



## Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 12:37 pm BST

PDB ID : 6ZJ3 / pdb\_00006zj3  
EMDB ID : EMD-11232  
Title : Cryo-EM structure of the highly atypical cytoplasmic ribosome of *Euglena gracilis*  
Authors : Matzov, D.; Halfon, H.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Gray, M.W.; Yonath, A.E.; Shalev-Benami, M.  
Deposited on : 2020-06-27  
Resolution : 3.15 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

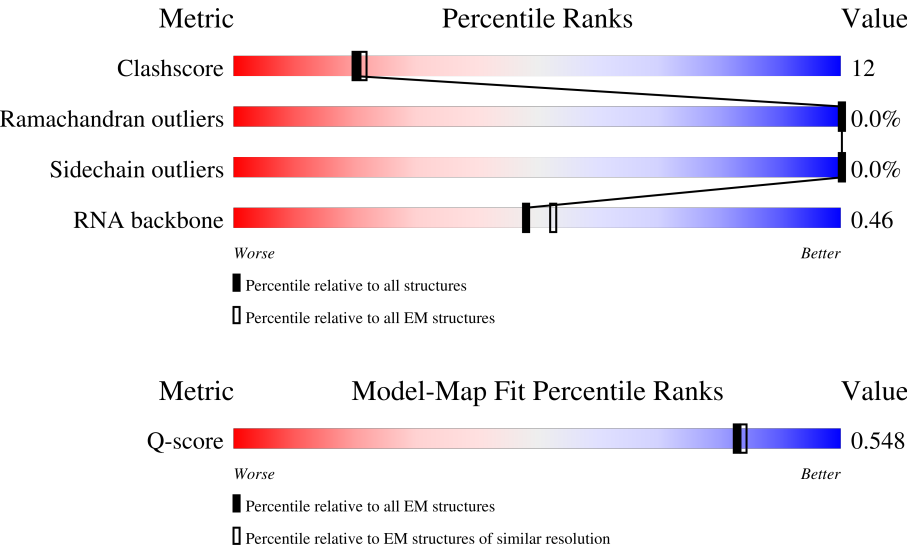
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.15 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14486 ( 2.65 - 3.65 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | S1    | 2315   |                  |
| 2   | S2    | 76     |                  |
| 3   | S3    | 76     |                  |

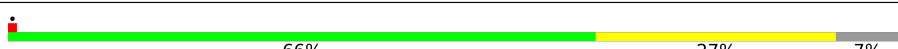
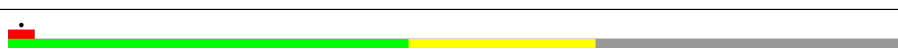
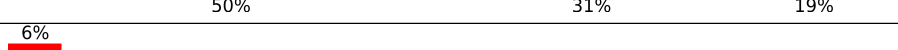
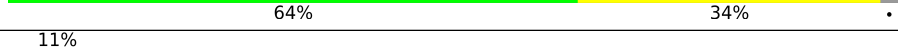
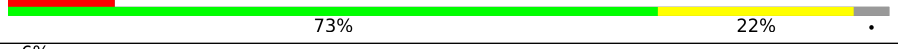
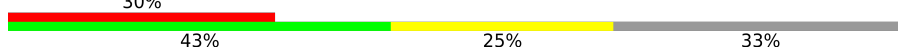
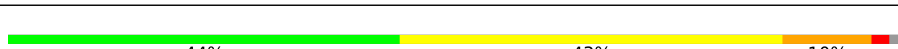
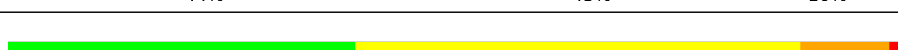
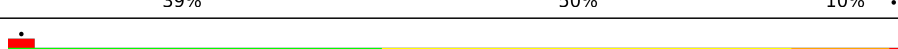
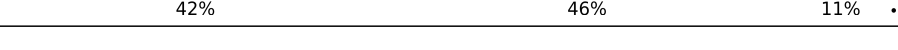
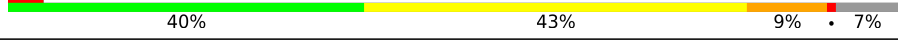
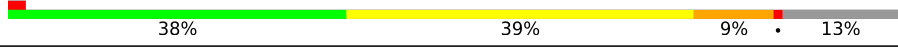
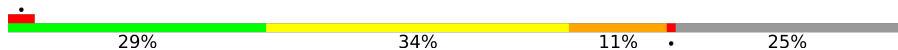
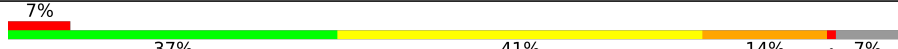
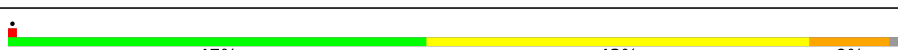
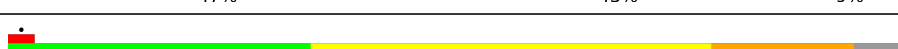
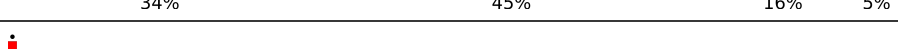
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | S4    | 76     |                  |
| 5   | S5    | 12     |                  |
| 6   | SA    | 249    |                  |
| 7   | SB    | 261    |                  |
| 8   | SC    | 220    |                  |
| 9   | SD    | 196    |                  |
| 10  | SE    | 271    |                  |
| 11  | SF    | 257    |                  |
| 12  | SG    | 283    |                  |
| 13  | SH    | 190    |                  |
| 14  | SI    | 200    |                  |
| 15  | SJ    | 130    |                  |
| 16  | SK    | 304    |                  |
| 17  | SL    | 151    |                  |
| 18  | SM    | 121    |                  |
| 19  | SN    | 152    |                  |
| 20  | SO    | 152    |                  |
| 21  | SP    | 143    |                  |
| 22  | SQ    | 139    |                  |
| 23  | SR    | 153    |                  |
| 24  | SS    | 55     |                  |
| 25  | ST    | 151    |                  |
| 26  | SU    | 164    |                  |
| 27  | SV    | 145    |                  |
| 28  | SW    | 150    |                  |

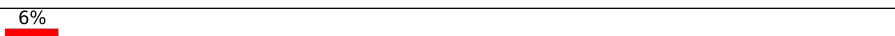
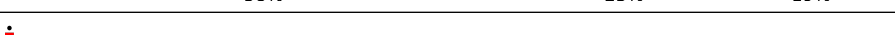
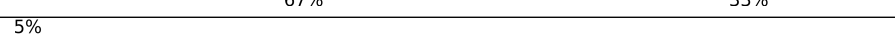
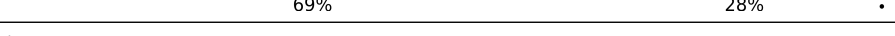
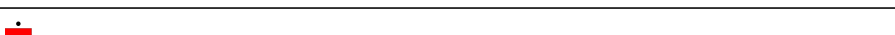
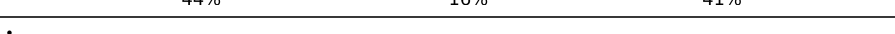
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | SX    | 148    |    |
| 30  | SY    | 96     |    |
| 31  | SZ    | 137    |    |
| 32  | Sa    | 119    |    |
| 33  | Sb    | 120    |    |
| 34  | Sc    | 86     |    |
| 35  | Sd    | 76     |    |
| 36  | Se    | 67     |    |
| 37  | Sf    | 157    |    |
| 38  | Sg    | 295    |    |
| 39  | Sh    | 317    |    |
| 40  | LA    | 163    |    |
| 41  | LB    | 133    |   |
| 42  | LC    | 350    |  |
| 43  | LD    | 116    |  |
| 44  | LE    | 698    |  |
| 45  | LF    | 527    |  |
| 46  | LG    | 234    |  |
| 47  | LH    | 744    |  |
| 48  | LI    | 617    |  |
| 49  | LJ    | 164    |  |
| 50  | LK    | 64     |  |
| 51  | LL    | 95     |  |
| 52  | LM    | 58     |  |
| 53  | LN    | 86     |  |

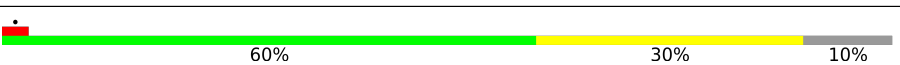
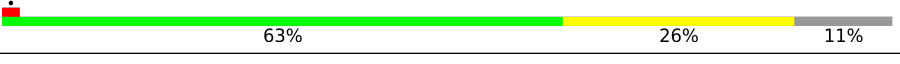
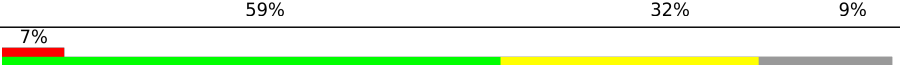
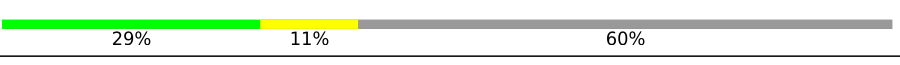
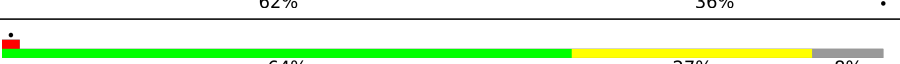
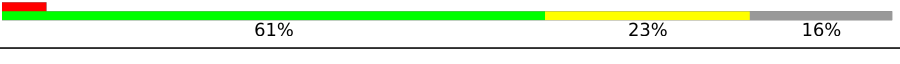
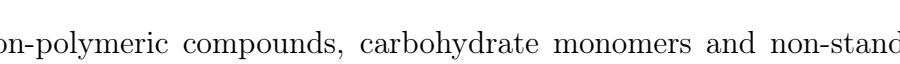
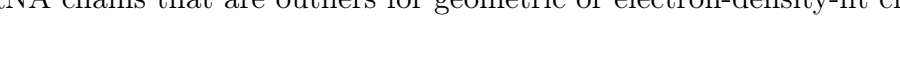
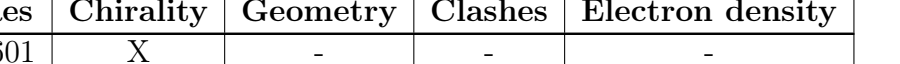
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | LO    | 120    |    |
| 55  | LP    | 264    |    |
| 56  | LQ    | 410    |    |
| 57  | LR    | 375    |    |
| 58  | LS    | 191    |    |
| 59  | LT    | 193    |    |
| 60  | LU    | 195    |    |
| 61  | LV    | 295    |    |
| 62  | LW    | 209    |    |
| 63  | LX    | 226    |    |
| 64  | LY    | 140    |    |
| 65  | LZ    | 219    |    |
| 66  | La    | 152    |   |
| 67  | Lb    | 204    |  |
| 68  | Lc    | 215    |  |
| 69  | Ld    | 260    |  |
| 70  | Le    | 193    |  |
| 71  | Lf    | 250    |  |
| 72  | Lg    | 182    |  |
| 73  | Lh    | 159    |  |
| 74  | Li    | 164    |  |
| 75  | Lj    | 170    |  |
| 76  | Lk    | 163    |  |
| 77  | Ll    | 146    |  |
| 78  | Lm    | 157    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 79  | Ln    | 134    |    |
| 80  | Lo    | 72     |    |
| 81  | Lp    | 123    |    |
| 82  | Lq    | 117    |    |
| 83  | Lr    | 242    |    |
| 84  | Ls    | 109    |    |
| 85  | Lt    | 151    |    |
| 86  | Lu    | 139    |    |
| 87  | Lv    | 115    |    |
| 88  | Lw    | 128    |   |
| 89  | Lx    | 106    |  |
| 90  | Ly    | 117    |  |
| 91  | Lz    | 82     |  |
| 92  | L1    | 51     |  |
| 93  | L2    | 126    |  |
| 94  | L3    | 34     |  |
| 95  | L5    | 92     |  |
| 96  | L4    | 106    |  |
| 97  | L6    | 69     |  |
| 98  | L7    | 64     |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1   | B8N  | S1    | 1601 | X         | -        | -       | -                |

## 2 Entry composition

There are 100 unique types of molecules in this entry. The entry contains 223607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | S1    | 2024     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 43278 | 19338 | 7765 | 14151 | 2024 |         |       |

- Molecule 2 is a RNA chain called A-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 2   | S2    | 76       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1626  | 729 | 290 | 531 | 75 | 1 |         |       |

- Molecule 3 is a RNA chain called P-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | S3    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1614  | 721 | 285 | 533 | 75 |         |       |

- Molecule 4 is a RNA chain called E-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4   | S4    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1621  | 724 | 292 | 530 | 75 |         |       |

- Molecule 5 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 5   | S5    | 12       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 251   | 113 | 43 | 83 | 12 |         |       |

- Molecule 6 is a protein called Ribosomal protein eS1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | SA    | 221      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1797  | 1133 | 331 | 323 | 10 |         |       |

- Molecule 7 is a protein called Ribosomal protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | SB    | 207      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1657  | 1058 | 295 | 293 | 11 |         |       |

- Molecule 8 is a protein called Ribosomal protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | SC    | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1675  | 1061 | 310 | 296 | 8 |         |       |

- Molecule 9 is a protein called Ribosomal protein uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | SD    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1436  | 913 | 277 | 240 | 6 |         |       |

- Molecule 10 is a protein called Ribosomal protein eS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | SE    | 265      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2125  | 1366 | 394 | 357 | 8 |         |       |

- Molecule 11 is a protein called Ribosomal protein uS5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | SF    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1713  | 1105 | 301 | 300 | 7 |         |       |

- Molecule 12 is a protein called Ribosomal protein eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | SG    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2016  | 1263 | 402 | 345 | 6 |         |       |

- Molecule 13 is a protein called Ribosomal protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | SH    | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1450  | 908 | 271 | 266 | 5 |         |       |

- Molecule 14 is a protein called Ribosomal protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | SI    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1514  | 967 | 284 | 262 | 1 |         |       |

- Molecule 15 is a protein called Ribosomal protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | SJ    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1037  | 658 | 194 | 178 | 7 |         |       |

- Molecule 16 is a protein called Ribosomal protein eS8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | SK    | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1644  | 1038 | 338 | 264 | 4 |         |       |

- Molecule 17 is a protein called Ribosomal protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | SL    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1144  | 725 | 220 | 194 | 5 |         |       |

- Molecule 18 is a protein called Ribosomal protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | SM    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 796   | 501 | 150 | 142 | 3 |         |       |

- Molecule 19 is a protein called Ribosomal protein eS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | SN    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 775   | 509 | 130 | 133 | 3 |         |       |

- Molecule 20 is a protein called Ribosomal protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | SO    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1010  | 616 | 198 | 189 | 7 |         |       |

- Molecule 21 is a protein called Ribosomal protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | SP    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1101  | 692 | 216 | 188 | 5 |         |       |

- Molecule 22 is a protein called Ribosomal protein eS12.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | SQ    | 122      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 919   | 574 | 164 | 171 | 10 |         |       |

- Molecule 23 is a protein called Ribosomal protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | SR    | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 737 | 234 | 204 | 6 |         |       |

- Molecule 24 is a protein called Ribosomal protein uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 24  | SS    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 433   | 267 | 95 | 68 | 3 |         |       |

- Molecule 25 is a protein called Ribosomal protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | ST    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1180  | 746 | 228 | 202 | 4 |         |       |

- Molecule 26 is a protein called Ribosomal protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | SU    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1225  | 793 | 230 | 199 | 3 |         |       |

- Molecule 27 is a protein called Ribosomal protein eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | SV    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 998   | 625 | 183 | 183 | 7 |         |       |

- Molecule 28 is a protein called Ribosomal protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | SW    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 990   | 632 | 186 | 167 | 5 |         |       |

- Molecule 29 is a protein called Ribosomal protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | SX    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1125  | 720 | 205 | 195 | 5 |         |       |

- Molecule 30 is a protein called Ribosomal protein eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | SY    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 624   | 391 | 111 | 119 | 3 |         |       |

- Molecule 31 is a protein called Ribosomal protein eS24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | SZ    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 668 | 205 | 174 | 5 |         |       |

- Molecule 32 is a protein called Ribosomal protein eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Sa    | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 405 | 118 | 108 | 2 |         |       |

- Molecule 33 is a protein called Ribosomal protein eS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Sb    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 780   | 481 | 162 | 129 | 8 |         |       |

- Molecule 34 is a protein called Ribosomal protein eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Sc    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 414 | 115 | 114 | 6 |         |       |

- Molecule 35 is a protein called Ribosomal protein eS28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 35  | Sd    | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 499   | 304 | 103 | 90 | 2 |         |       |

- Molecule 36 is a protein called Ribosomal protein eS30.

| Mol | Chain | Residues | Atoms |     |     |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|-------|
| 36  | Se    | 64       | Total | C   | N   | O  |  | 0       | 0     |
|     |       |          | 484   | 305 | 101 | 78 |  |         |       |

- Molecule 37 is a protein called Ribosomal protein eS31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37  | Sf    | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 508   | 322 | 95 | 85 | 6 |         |       |

- Molecule 38 is a protein called Ribosomal protein eSEug1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | Sg    | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1597  | 1022 | 301 | 267 | 7 |         |       |

- Molecule 39 is a protein called RACK1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39  | Sh    | 311      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2393  | 1516 | 407 | 454 | 16 |         |       |

- Molecule 40 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 40  | LA    | 160      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3423  | 1528 | 613 | 1122 | 160 |         |       |

- Molecule 41 is a RNA chain called LSU rRNA chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 41  | LB    | 133      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2847  | 1275 | 523 | 916 | 133 |         |       |

- Molecule 42 is a RNA chain called LSU rRNA chain 2.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 42  | LC    | 350      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 7516  | 3355 | 1368 | 2443 | 350 |         |       |

- Molecule 43 is a RNA chain called LSU rRNA chain 3.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 43  | LD    | 110      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2342  | 1043 | 418 | 771 | 110 |         |       |

- Molecule 44 is a RNA chain called LSU rRNA chain 4.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 44  | LE    | 652      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 13955 | 6233 | 2494 | 4576 | 652 |         |       |

- Molecule 45 is a RNA chain called LSU rRNA chain 5.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 45  | LF    | 456      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 9702  | 4340 | 1740 | 3166 | 456 |         |       |

- Molecule 46 is a RNA chain called LSU rRNA chain 6.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 46  | LG    | 207      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 4422  | 1975 | 789 | 1451 | 207 |         |       |

- Molecule 47 is a RNA chain called LSU rRNA chain 7.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 47  | LH    | 559      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 11980 | 5366 | 2143 | 3912 | 559 |         |       |

- Molecule 48 is a RNA chain called LSU rRNA chain 8.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 48  | LI    | 573      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 12233 | 5480 | 2170 | 4010 | 573 |         |       |

- Molecule 49 is a RNA chain called LSU rRNA chain 9.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 49  | LJ    | 163      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3486  | 1558 | 630 | 1135 | 163 |         |       |

- Molecule 50 is a RNA chain called LSU rRNA chain 10.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 50  | LK    | 61       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1301  | 581 | 237 | 422 | 61 |         |       |

- Molecule 51 is a RNA chain called LSU rRNA chain 11.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 51  | LL    | 92       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1983  | 882 | 366 | 643 | 92 |         |       |

- Molecule 52 is a RNA chain called LSU rRNA chain 12.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 52  | LM    | 54       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1158  | 517 | 214 | 373 | 54 |         |       |

- Molecule 53 is a RNA chain called LSU rRNA chain 13.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 53  | LN    | 79       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1696  | 753 | 307 | 557 | 79 |         |       |

- Molecule 54 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 54  | LO    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2559  | 1142 | 457 | 840 | 120 |         |       |

- Molecule 55 is a protein called Ribosomal protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | LP    | 249      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1901  | 1193 | 380 | 317 | 11 |         |       |

- Molecule 56 is a protein called Ribosomal protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | LQ    | 392      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3118  | 1987 | 592 | 521 | 18 |         |       |

- Molecule 57 is a protein called Ribosomal protein uL4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | LR    | 365      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2868  | 1807 | 572 | 482 | 7 |         |       |

- Molecule 58 is a protein called Ribosomal protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | LS    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1437  | 912 | 273 | 248 | 4 |         |       |

- Molecule 59 is a protein called Ribosomal protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 59  | LT    | 190      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1521  | 959 | 283 | 269 | 10 |         |       |

- Molecule 60 is a protein called Ribosomal protein eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | LU    | 194      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 1010 | 297 | 269 | 4 |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 61  | LV    | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1926  | 1236 | 365 | 321 | 4 |         |       |

- Molecule 62 is a protein called Ribosomal protein uL13.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 62  | LW    | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1713  | 1086 | 346 | 270 | 11 |         |       |

- Molecule 63 is a protein called Ribosomal protein eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 63  | LX    | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1115 | 357 | 292 | 5 |         |       |

- Molecule 64 is a protein called Ribosomal protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | LY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1001  | 634 | 187 | 173 | 7 |         |       |

- Molecule 65 is a protein called Ribosomal protein eL14.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65  | LZ    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1780  | 1126 | 357 | 293 | 4 |         |       |

- Molecule 66 is a protein called Ribosomal protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | La    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1210  | 759 | 254 | 193 | 4 |         |       |

- Molecule 67 is a protein called Ribosomal protein eL15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 67  | Lb    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1711  | 1080 | 363 | 259 | 9 |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 68  | Lc    | 203      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1643  | 1036 | 328 | 267 | 12 |         |       |

- Molecule 69 is a protein called Ribosomal protein uL18.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 69  | Ld    | 260      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2074  | 1313 | 384 | 367 | 10 |         |       |

- Molecule 70 is a protein called Ribosomal protein eL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | Le    | 192      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1526  | 963 | 313 | 241 | 9 |         |       |

- Molecule 71 is a protein called Ribosomal protein eL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | Lf    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1392  | 874 | 291 | 219 | 8 |         |       |

- Molecule 72 is a protein called Ribosomal protein eL20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | Lg    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1494  | 961 | 278 | 246 | 9 |         |       |

- Molecule 73 is a protein called Ribosomal protein eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | Lh    | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1279  | 814 | 254 | 209 | 2 |         |       |

- Molecule 74 is a protein called Ribosomal protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | Li    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1255  | 785 | 250 | 213 | 7 |         |       |

- Molecule 75 is a protein called Ribosomal protein eL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | Lj    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 540 | 140 | 146 | 1 |         |       |

- Molecule 76 is a protein called Ribosomal protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | Lk    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1073  | 684 | 204 | 182 | 3 |         |       |

- Molecule 77 is a protein called Ribosomal protein uL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | Ll    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1008  | 629 | 206 | 171 | 2 |         |       |

- Molecule 78 is a protein called Ribosomal protein eL24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 78  | Lm    | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 549   | 355 | 108 | 84 | 2 |         |       |

- Molecule 79 is a protein called Ribosomal protein eL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | Ln    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1084  | 695 | 213 | 172 | 4 |         |       |

- Molecule 80 is a protein called Ribosomal protein eLEgr1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | Lo    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 291 | 86 | 80 | 2 |         |       |

- Molecule 81 is a protein called Ribosomal protein uL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | Lp    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1010  | 645 | 198 | 164 | 3 |         |       |

- Molecule 82 is a protein called Ribosomal protein eL29.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 82  | Lq    | 91       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 767   | 478 | 164 | 125 |         |       |

- Molecule 83 is a protein called Ribosomal protein uL30.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 83  | Lr    | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1825  | 1184 | 346 | 285 | 10 |         |       |

- Molecule 84 is a protein called Ribosomal protein eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | Ls    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 747   | 466 | 132 | 143 | 6 |         |       |

- Molecule 85 is a protein called Ribosomal protein eL31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 85  | Lt    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 923   | 589 | 182 | 150 | 2 |         |       |

- Molecule 86 is a protein called Ribosomal protein eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 86  | Lu    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1068  | 680 | 219 | 167 | 2 |         |       |

- Molecule 87 is a protein called Ribosomal protein eL33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 87  | Lv    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 915   | 589 | 182 | 140 | 4 |         |       |

- Molecule 88 is a protein called Ribosomal protein eL34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 88  | Lw    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 922   | 577 | 197 | 147 | 1 |         |       |

- Molecule 89 is a protein called Ribosomal protein eL36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 89  | Lx    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 835   | 527 | 177 | 127 | 4 |         |       |

- Molecule 90 is a protein called Ribosomal protein eL37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 90  | Ly    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 859   | 525 | 189 | 137 | 8 |         |       |

- Molecule 91 is a protein called Ribosomal protein eL38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 91  | Lz    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 570   | 367 | 103 | 98 | 2 |         |       |

- Molecule 92 is a protein called Ribosomal protein eL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 92  | L1    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 447   | 287 | 93 | 65 | 2 |         |       |

- Molecule 93 is a protein called Ribosomal protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 93  | L2    | 51       | Total | C   | N  | O  | S  | 0       | 0     |
|     |       |          | 415   | 255 | 83 | 67 | 10 |         |       |

- Molecule 94 is a protein called Ribosomal protein eL41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 94  | L3    | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 180 | 81 | 38 | 3 |         |       |

- Molecule 95 is a protein called Ribosomal protein eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 95  | L5    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 719   | 449 | 147 | 117 | 6 |         |       |

- Molecule 96 is a protein called Ribosomal protein eL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 96  | L4    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 785   | 501 | 152 | 126 | 6 |         |       |

- Molecule 97 is a protein called Ribosomal protein eLEgr2.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 97  | L6    | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 493   | 308 | 99 | 85 | 1 |         |       |

- Molecule 98 is a protein called Ribosomal protein eLEgr3.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 98  | L7    | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 288 | 85 | 81 | 1 |         |       |

- Molecule 99 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 99  | Sb    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 99  | Ly    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 99  | L2    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 99  | L5    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 99  | L4    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 100 is water.

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 100 | S1    | 393      | Total | O   | 0       |
|     |       |          | 393   | 393 |         |
| 100 | S2    | 3        | Total | O   | 0       |
|     |       |          | 3     | 3   |         |
| 100 | S3    | 17       | Total | O   | 0       |
|     |       |          | 17    | 17  |         |
| 100 | S4    | 2        | Total | O   | 0       |
|     |       |          | 2     | 2   |         |
| 100 | S5    | 11       | Total | O   | 0       |
|     |       |          | 11    | 11  |         |
| 100 | SB    | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |
| 100 | SC    | 3        | Total | O   | 0       |
|     |       |          | 3     | 3   |         |
| 100 | SF    | 4        | Total | O   | 0       |
|     |       |          | 4     | 4   |         |
| 100 | SG    | 3        | Total | O   | 0       |
|     |       |          | 3     | 3   |         |
| 100 | SH    | 2        | Total | O   | 0       |
|     |       |          | 2     | 2   |         |
| 100 | SK    | 5        | Total | O   | 0       |
|     |       |          | 5     | 5   |         |
| 100 | SL    | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |

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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 100 | SM    | 1        | Total<br>1   | O<br>1   | 0       |
| 100 | SO    | 1        | Total<br>1   | O<br>1   | 0       |
| 100 | SP    | 4        | Total<br>4   | O<br>4   | 0       |
| 100 | SR    | 1        | Total<br>1   | O<br>1   | 0       |
| 100 | SS    | 2        | Total<br>2   | O<br>2   | 0       |
| 100 | SU    | 1        | Total<br>1   | O<br>1   | 0       |
| 100 | SX    | 2        | Total<br>2   | O<br>2   | 0       |
| 100 | SZ    | 2        | Total<br>2   | O<br>2   | 0       |
| 100 | Sb    | 1        | Total<br>1   | O<br>1   | 0       |
| 100 | Sh    | 1        | Total<br>1   | O<br>1   | 0       |
| 100 | LA    | 29       | Total<br>29  | O<br>29  | 0       |
| 100 | LB    | 15       | Total<br>15  | O<br>15  | 0       |
| 100 | LC    | 32       | Total<br>32  | O<br>32  | 0       |
| 100 | LD    | 9        | Total<br>9   | O<br>9   | 0       |
| 100 | LE    | 97       | Total<br>97  | O<br>97  | 0       |
| 100 | LF    | 93       | Total<br>93  | O<br>93  | 0       |
| 100 | LG    | 33       | Total<br>33  | O<br>33  | 0       |
| 100 | LH    | 174      | Total<br>174 | O<br>174 | 0       |
| 100 | LI    | 82       | Total<br>82  | O<br>82  | 0       |
| 100 | LJ    | 46       | Total<br>46  | O<br>46  | 0       |
| 100 | LK    | 3        | Total<br>3   | O<br>3   | 0       |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 100 | LL    | 5        | Total<br>5  | O<br>5  | 0       |
| 100 | LM    | 11       | Total<br>11 | O<br>11 | 0       |
| 100 | LN    | 12       | Total<br>12 | O<br>12 | 0       |
| 100 | LO    | 15       | Total<br>15 | O<br>15 | 0       |
| 100 | LP    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | LQ    | 8        | Total<br>8  | O<br>8  | 0       |
| 100 | LR    | 8        | Total<br>8  | O<br>8  | 0       |
| 100 | LU    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | LW    | 7        | Total<br>7  | O<br>7  | 0       |
| 100 | LY    | 3        | Total<br>3  | O<br>3  | 0       |
| 100 | La    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | Lb    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | Lc    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | Ld    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Lf    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Li    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | Lk    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Ll    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Lm    | 3        | Total<br>3  | O<br>3  | 0       |
| 100 | Lp    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Lq    | 3        | Total<br>3  | O<br>3  | 0       |

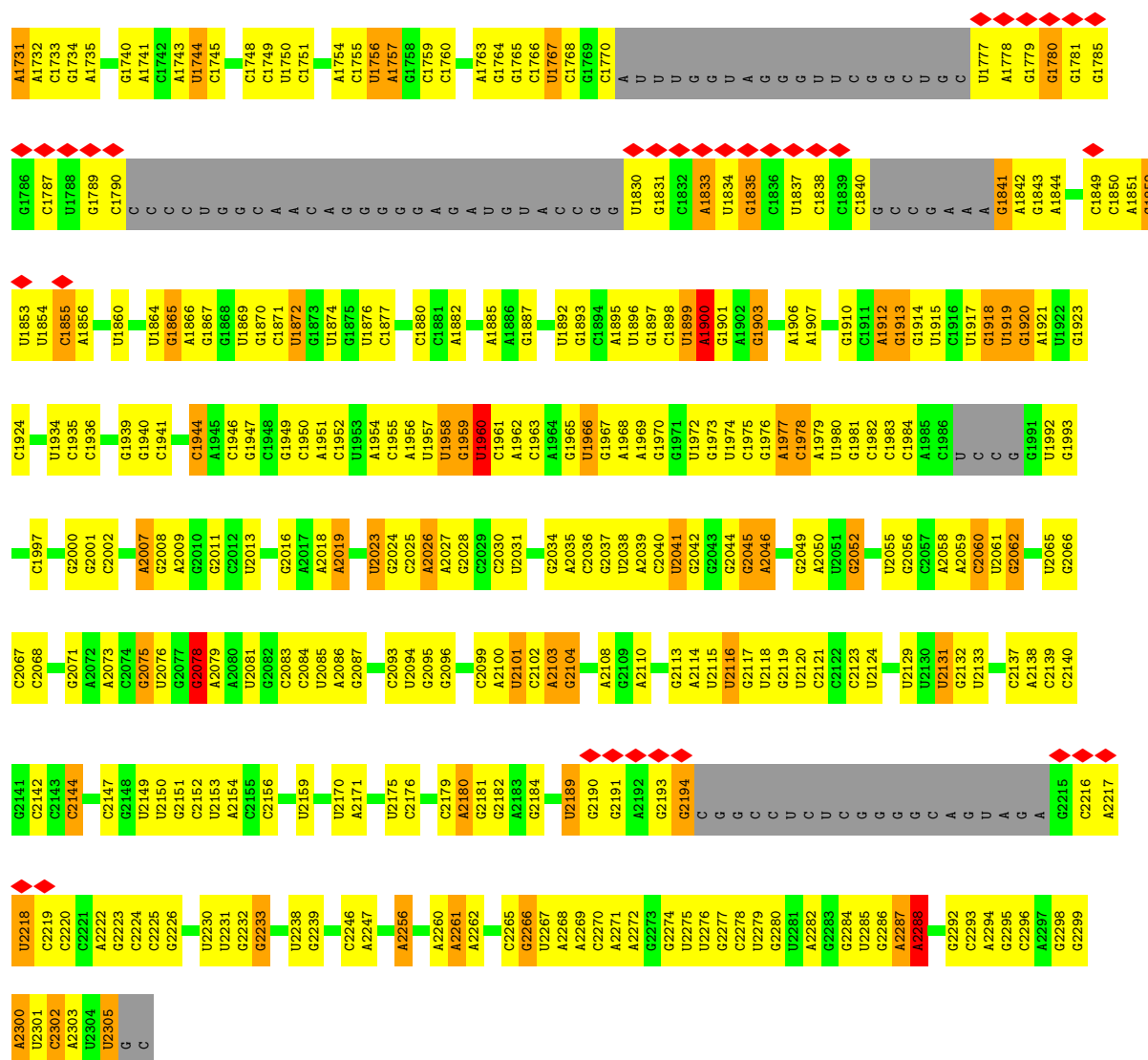
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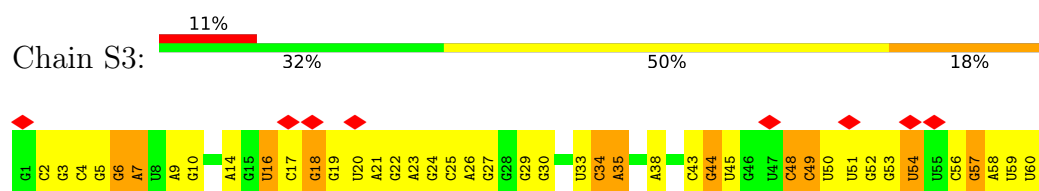
| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 100 | Lr    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Ls    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Lt    | 4        | Total<br>4  | O<br>4  | 0       |
| 100 | Lu    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | Lw    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | Ly    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | L2    | 3        | Total<br>3  | O<br>3  | 0       |
| 100 | L3    | 10       | Total<br>10 | O<br>10 | 0       |
| 100 | L5    | 2        | Total<br>2  | O<br>2  | 0       |
| 100 | L4    | 1        | Total<br>1  | O<br>1  | 0       |
| 100 | L7    | 1        | Total<br>1  | O<br>1  | 0       |



|       |         |       |       |       |       |       |       |      |      |   |      |
|-------|---------|-------|-------|-------|-------|-------|-------|------|------|---|------|
| G1853 | A1581   | C1417 | A1495 | U1342 | A1256 | G1136 | G1062 | A922 | U858 | C | U736 |
| A1654 | G1582   | C1418 | A1496 | U1343 | G1257 | C1137 | A1063 | A923 | G859 | C | C    |
| C1655 | U1583   | G1422 | A1497 | C1344 | U1258 | C1138 | C1064 | G924 | C960 | U | C740 |
| U1659 | U1584   | G1423 | C1498 | U1345 | G1259 | U     | G1065 | C925 | G861 | G | C741 |
| U1660 | C1585   | A1424 | C1499 | U1346 | U1260 | C1140 | U1068 | G926 | C962 | G | A743 |
| U1661 | C1586   | A1425 | A1501 | C1347 | U1261 | U1141 | G1069 | G927 | C963 | U | C744 |
| C1662 | C1587   | A1426 | C1502 | A1348 | C1266 | U1142 | A1070 | U928 | C964 | U | C745 |
| U1663 | U1588   | G1427 | A1503 | A1426 | U1267 | U1143 | A1071 | U929 | A865 | G | G746 |
| U1664 | C1589   | G1428 | C1504 | G1350 | U1270 | U1144 | U1072 | U930 | C966 | A | G747 |
| G1665 | C1590   | G1429 | C1505 | U1351 | C1271 | G1145 | G1073 | U931 | C967 | C | C748 |
| U1671 | C1591   | G1430 | C1506 | G1352 | U1272 | C1147 | U1074 | A931 | U    | C | U749 |
| U1672 | U1592   | G1431 | U1507 | C1353 | G1273 | U1148 | C1075 | U932 | C    | C | G750 |
| U1673 | U1593   | C1432 | G1508 | A1354 | U1274 | A1149 | U1076 | U933 | U    | U | G751 |
| C1676 | U1594   | G1433 | C1509 | C1355 | G1277 | U1150 | A1077 | C934 | C    | G | A752 |
| G1677 | U1595   | G1434 | G1510 | G1356 | U1281 | C1151 | U1078 | C935 | U    | C | G753 |
| G1678 | U1596   | G1435 | U1513 | U1357 | U1282 | U1152 | C1079 | G940 | C    | C | G754 |
| G1679 | U1597   | C1436 | U1514 | C1358 | U1283 | G1153 | G1084 | A941 | U    | U | G755 |
| U1682 | B8M1601 | G1439 | U1517 | C1359 | A1284 | G1154 | A1085 | A942 | G    | G | C756 |
| G1683 | C1602   | G1445 | G1518 | G1360 | U1289 | U1155 | C1090 | C943 | U    | U | U757 |
| U1686 | A1603   | G1446 | G1524 | G1363 | G1290 | G1156 | G1093 | U944 | G882 | G | G758 |
| U1691 | C1604   | A1448 | G1533 | A1364 | C1293 | U1157 | G1094 | U945 | A883 | G | U759 |
| U1692 | G1605   | A1453 | A1534 | U1365 | U1296 | U1158 | C1095 | G946 | G884 | U | U760 |
| U1693 | C1606   | A1454 | A1535 | C1366 | G1299 | G1159 | A1096 | C947 | A    | C | G761 |
| C1694 | G1607   | A1456 | G1536 | A1367 | U1300 | U1160 | U1097 | C950 | U    | U | G762 |
| U1695 | C1608   | A1457 | A1537 | U1370 | G1301 | U     | G1098 | G951 | U    | U | U763 |
| U1696 | G1609   | U1458 | A1538 | G1371 | U1302 | U     | G1099 | G952 | C    | C | U764 |
| U1697 | A1547   | C1459 | U1548 | G1372 | A1303 | U     | C1100 | A953 | U    | U | G765 |
| A1698 | U1617   | U1460 | A1549 | U1373 | A1304 | U     | C1101 | C954 | G889 | G | G766 |
| G1704 | A1618   | A1461 | G1550 | C1380 | U1305 | U     | A1104 | C955 | U891 | A | U767 |
| G1705 | U1624   | A1463 | U1551 | A1385 | U1309 | A     | U1105 | C956 | G890 | U | C768 |
| A1706 | C1625   | A1464 | U1552 | G1386 | A1310 | A     | U1106 | A958 | G895 | U | C769 |
| G1707 | U1554   | C1471 | U1555 | C1387 | G1311 | A     | G1107 | C959 | G899 | U | G770 |
| U1708 | A1626   | G1475 | G1556 | A1388 | A1312 | G     | U1108 | A961 | C960 | U | U772 |
| G1709 | G1627   | U1476 | C1557 | A1389 | U1313 | G     | G1109 | G962 | C961 | U | U773 |
| U1710 | G1628   | C1476 | C1558 | U1392 | G1314 | U     | G1110 | A966 | U901 | C | G774 |
| U1711 | U1629   | C1477 | G1559 | A1393 | G1315 | A     | A1111 | C967 | G902 | U | U775 |
| U1712 | C1635   | A     | G1560 | G1394 | C1316 | A     | U1112 | C968 | U903 | C | U776 |
| U1713 | U1636   | C     | U1563 | A1395 | U1317 | A     | U1113 | C969 | C904 | A | G777 |
| U1714 | G1637   | U     | U1564 | U1396 | G1318 | C     | G1114 | A970 | G905 | U | U778 |
| U1715 | G1638   | C     | C1568 | A1400 | C1319 | G     | G1115 | G971 | G    | C | U779 |
| C1716 | G1639   | U     | C1569 | C1401 | A1321 | A     | A1116 | C972 | C    | C | U780 |
| U1717 | A1640   | C     | U1570 | A1402 | G1322 | U     | A1117 | C    | U    | U | C781 |
| U1718 | U1641   | C     | C1571 | G1405 | U1323 | U     | U1120 | U905 | U    | U | U782 |
| U1719 | G1642   | A     | U1572 | U1409 | G1330 | U     | G1121 | G    | C    | C | U783 |
| G1722 | A1643   | C     | A1573 | A1410 | U1331 | C     | U1122 | G978 | C    | A | G784 |
| U1723 | C1645   | U     | G1574 | A1411 | C1332 | U     | G1126 | C979 | U    | U | U785 |
| U1724 | A1646   | A1489 | G1575 | C1414 | U1333 | C     | C1129 | U980 | G    | C | G786 |
| C1725 | G1647   | A1490 | C1576 | G1415 | G1334 | U     | U1130 | G981 | C    | A | C787 |
| U1726 | U1651   | G1492 | U1579 | G1416 | G1335 | C     | G1133 | G982 | G    | G | U850 |
|       | A1652   | G1494 | G1580 |       |       | U     | G1135 | G983 | G918 | U | A851 |
|       |         |       |       |       |       |       |       | U984 | C919 | U | G852 |
|       |         |       |       |       |       |       |       | A    | C920 | U | G853 |
|       |         |       |       |       |       |       |       |      | A921 | U | C788 |
|       |         |       |       |       |       |       |       |      |      | U | U854 |
|       |         |       |       |       |       |       |       |      |      | U | G855 |
|       |         |       |       |       |       |       |       |      |      | U | C856 |
|       |         |       |       |       |       |       |       |      |      | U | C857 |

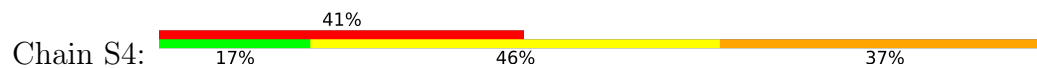


• Molecule 3: P-tRNA





• Molecule 4: E-tRNA



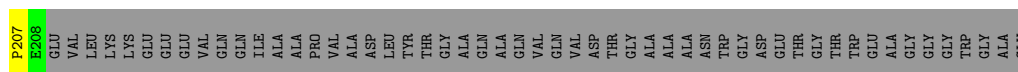
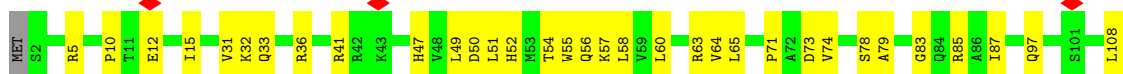
• Molecule 5: A-site tRNA



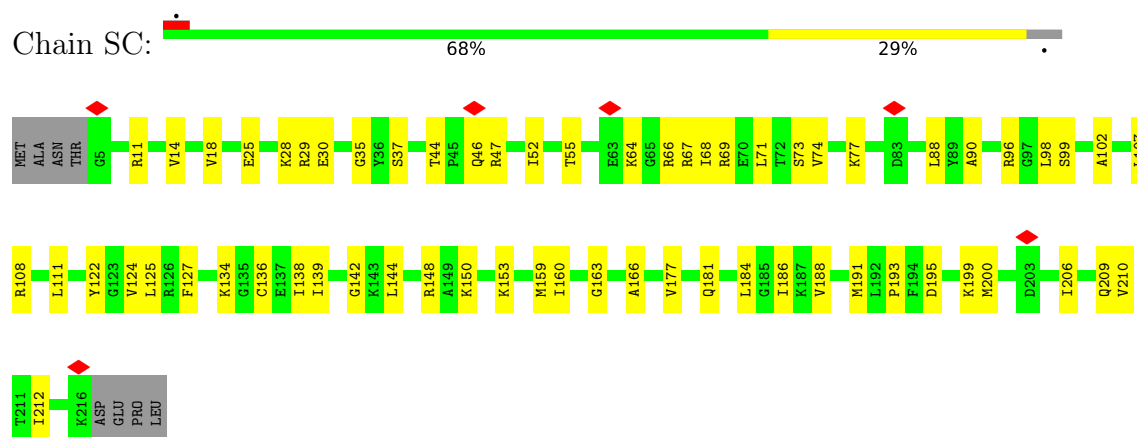
• Molecule 6: Ribosomal protein eS1



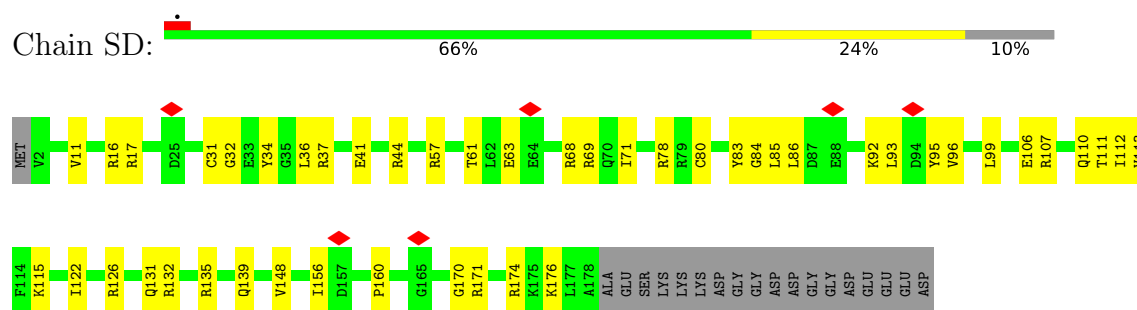
• Molecule 7: Ribosomal protein uS2



• Molecule 8: Ribosomal protein uS3



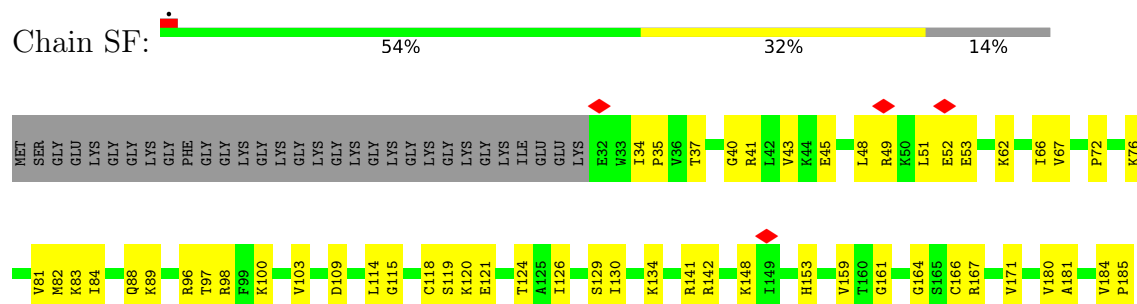
• Molecule 9: Ribosomal protein uS4

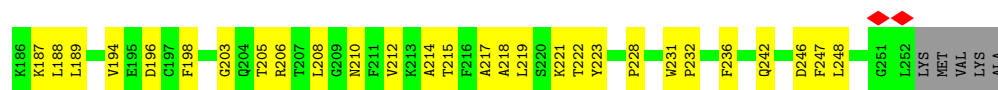


• Molecule 10: Ribosomal protein eS4

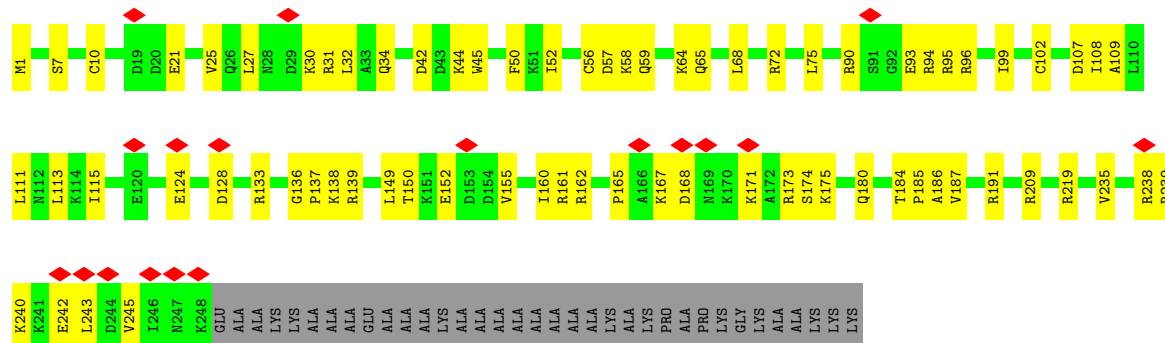


• Molecule 11: Ribosomal protein uS5

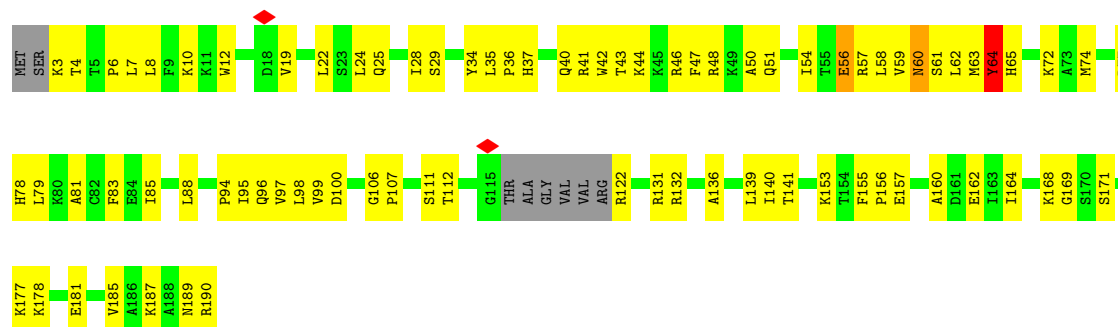




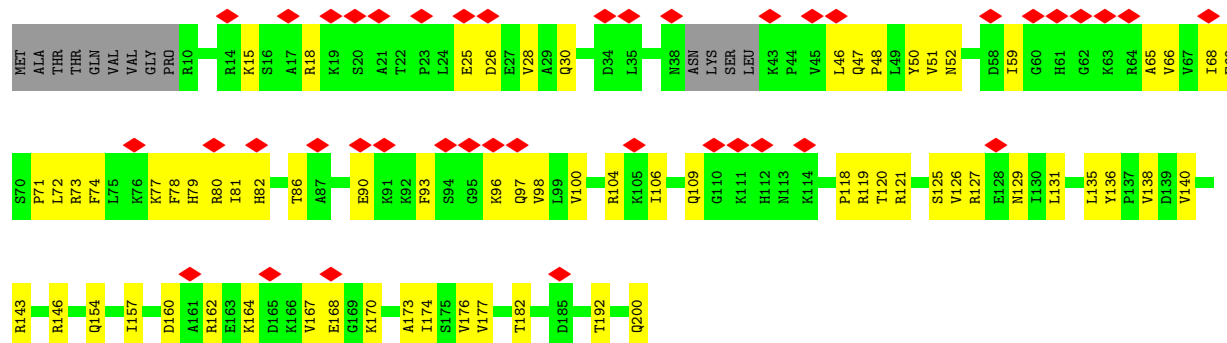
• Molecule 12: Ribosomal protein eS6



• Molecule 13: Ribosomal protein uS7



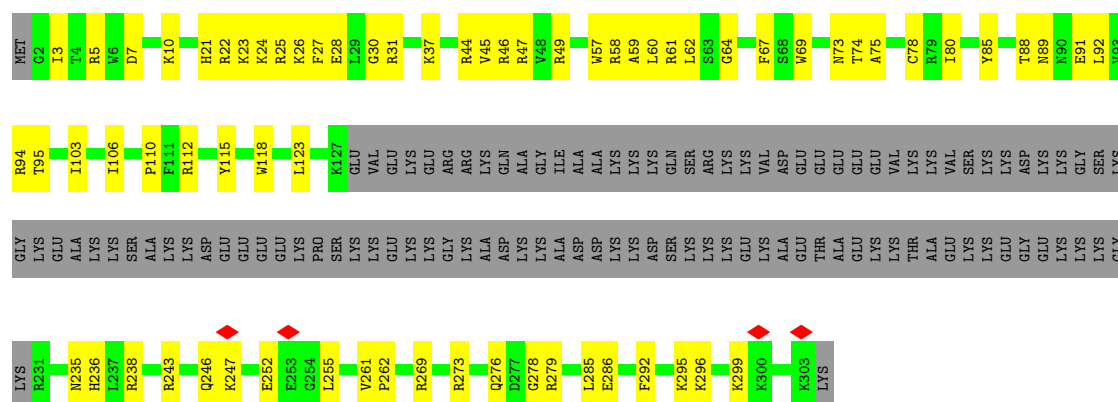
• Molecule 14: Ribosomal protein eS7



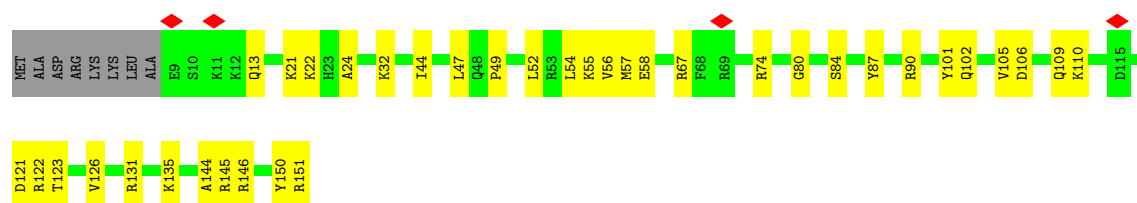
• Molecule 15: Ribosomal protein uS8

| Category | Number of Genes |
|----------|-----------------|
| MET      | 1               |
| V2       | 1               |
| R3       | 1               |
| K12      | 1               |
| K19      | 1               |
| R20      | 1               |
| L26      | 1               |
| C30      | 1               |
| S31      | 1               |
| K32      | 1               |
| R36      | 1               |
| F37      | 1               |
| L38      | 1               |
| M41      | 1               |
| D54      | 1               |
| N55      | 1               |
| H56      | 1               |
| R57      | 1               |
| S58      | 1               |
| N59      | 1               |
| K60      | 1               |
| N70      | 1               |
| K71      | 1               |
| L75      | 1               |
| S76      | 1               |
| P77      | 1               |
| D80      | 1               |
| I90      | 1               |
| T91      | 1               |
| S92      | 1               |
| L93      | 1               |
| L94      | 1               |
| R97      | 1               |
| I102     | 1               |
| H103     | 1               |
| L104     | 1               |
| S107     | 1               |
| M111     | 1               |
| D112     | 1               |
| H113     | 1               |
| K119     | 1               |
| K124     | 1               |
| L125     | 1               |

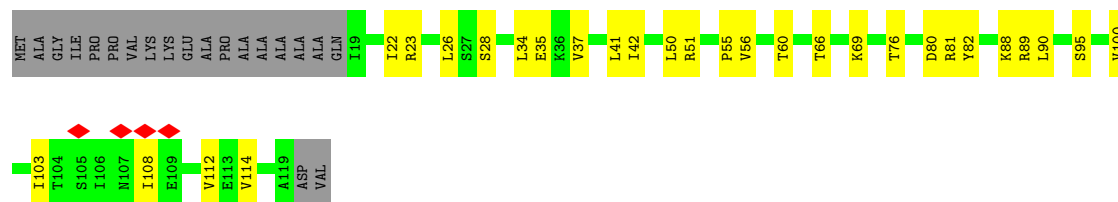
Chain SK: 



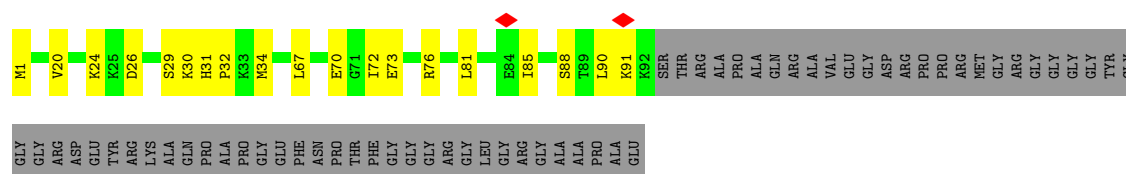
Chain SL: 



Chain SM: 



Chain SN: 



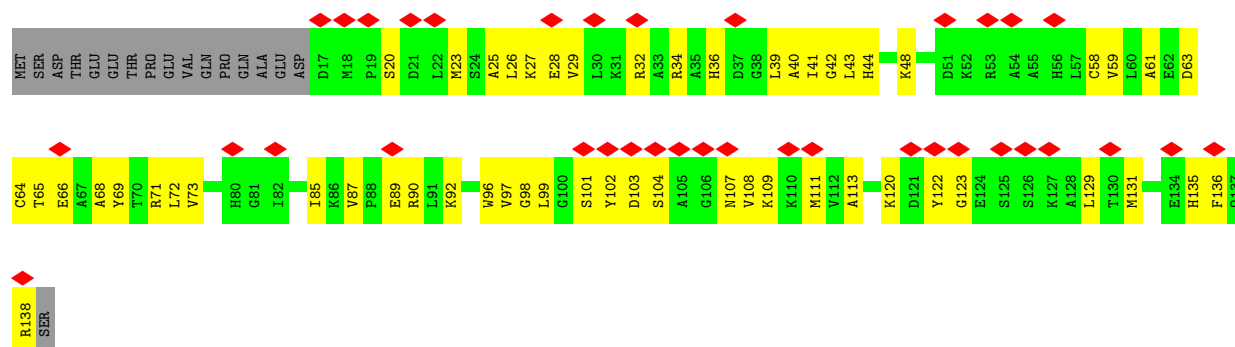
• Molecule 20: Ribosomal protein uS11



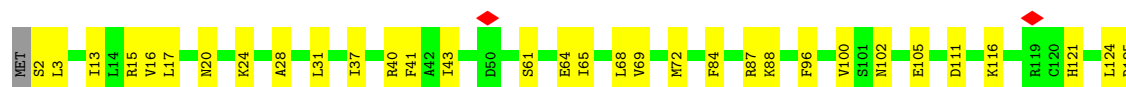
• Molecule 21: Ribosomal protein uS12



• Molecule 22: Ribosomal protein eS12

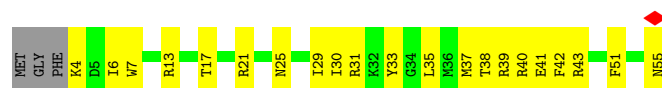


• Molecule 23: Ribosomal protein uS13





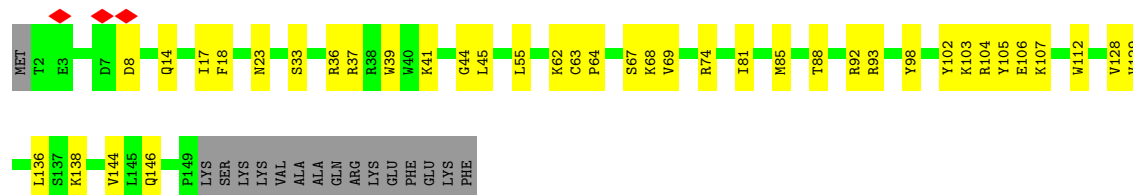
- Molecule 24: Ribosomal protein uS14



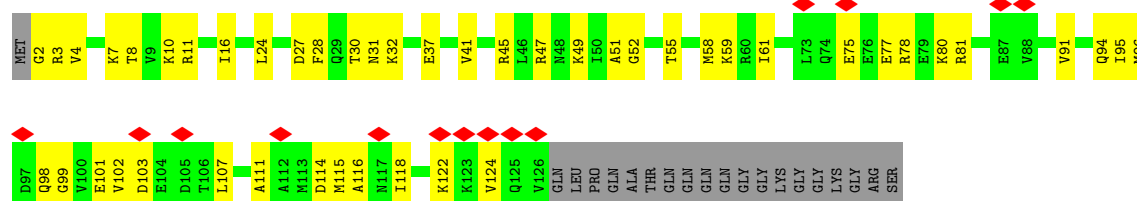
- Molecule 25: Ribosomal protein uS15



- Molecule 26: Ribosomal protein uS17

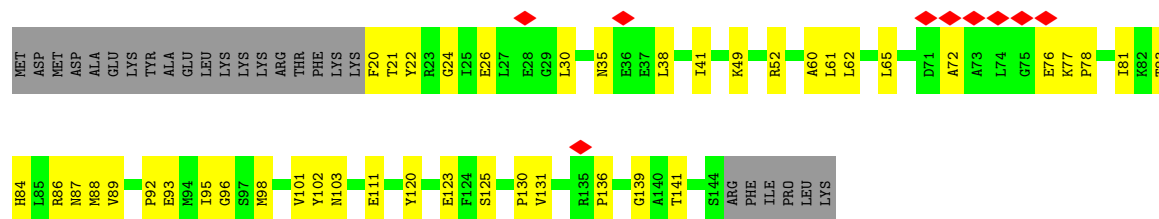


- Molecule 27: Ribosomal protein eS17

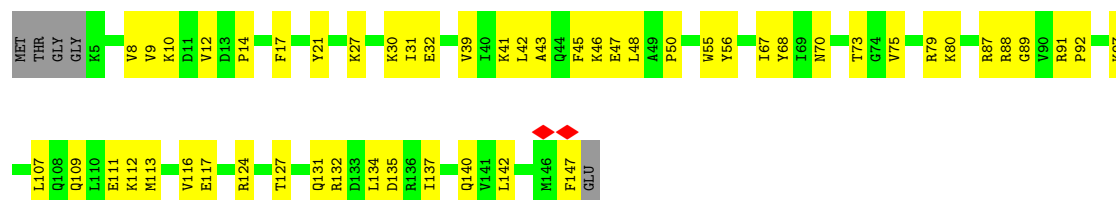


- Molecule 28: Ribosomal protein uS19





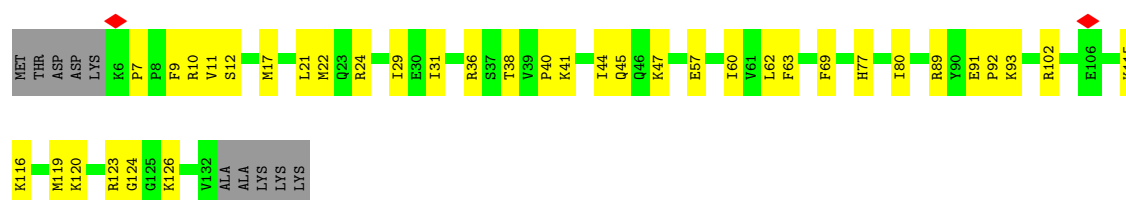
• Molecule 29: Ribosomal protein eS19



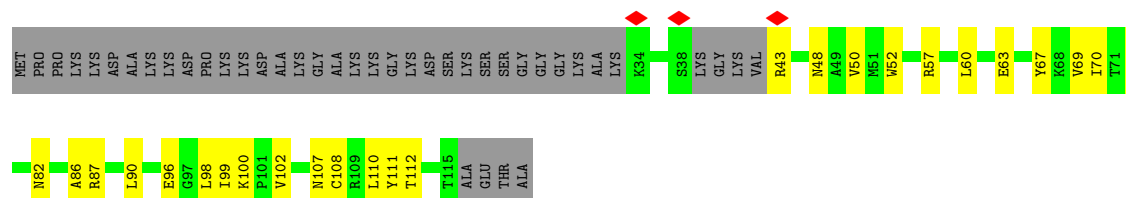
• Molecule 30: Ribosomal protein eS21



• Molecule 31: Ribosomal protein eS24



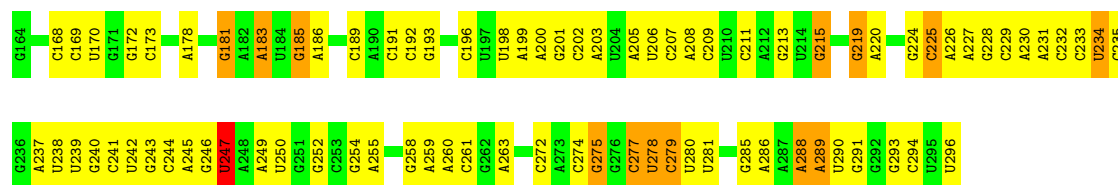
• Molecule 32: Ribosomal protein eS25



• Molecule 33: Ribosomal protein eS26

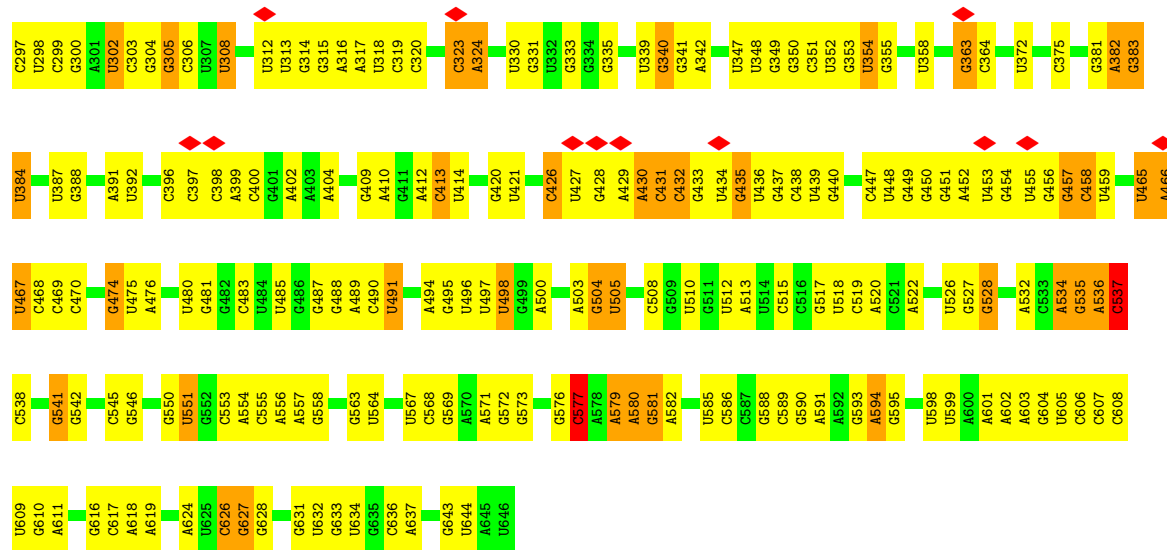






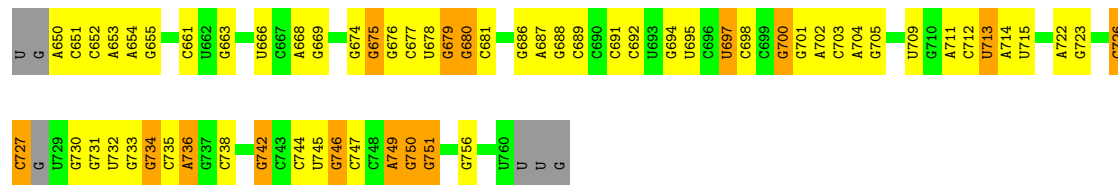
• Molecule 42: LSU rRNA chain 2

Chain LC: 42% 46% 11%



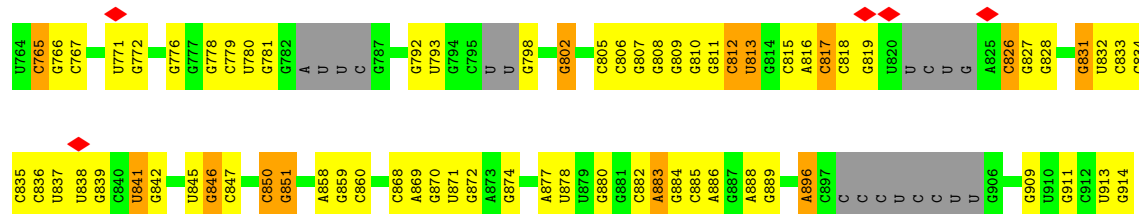
• Molecule 43: LSU rRNA chain 3

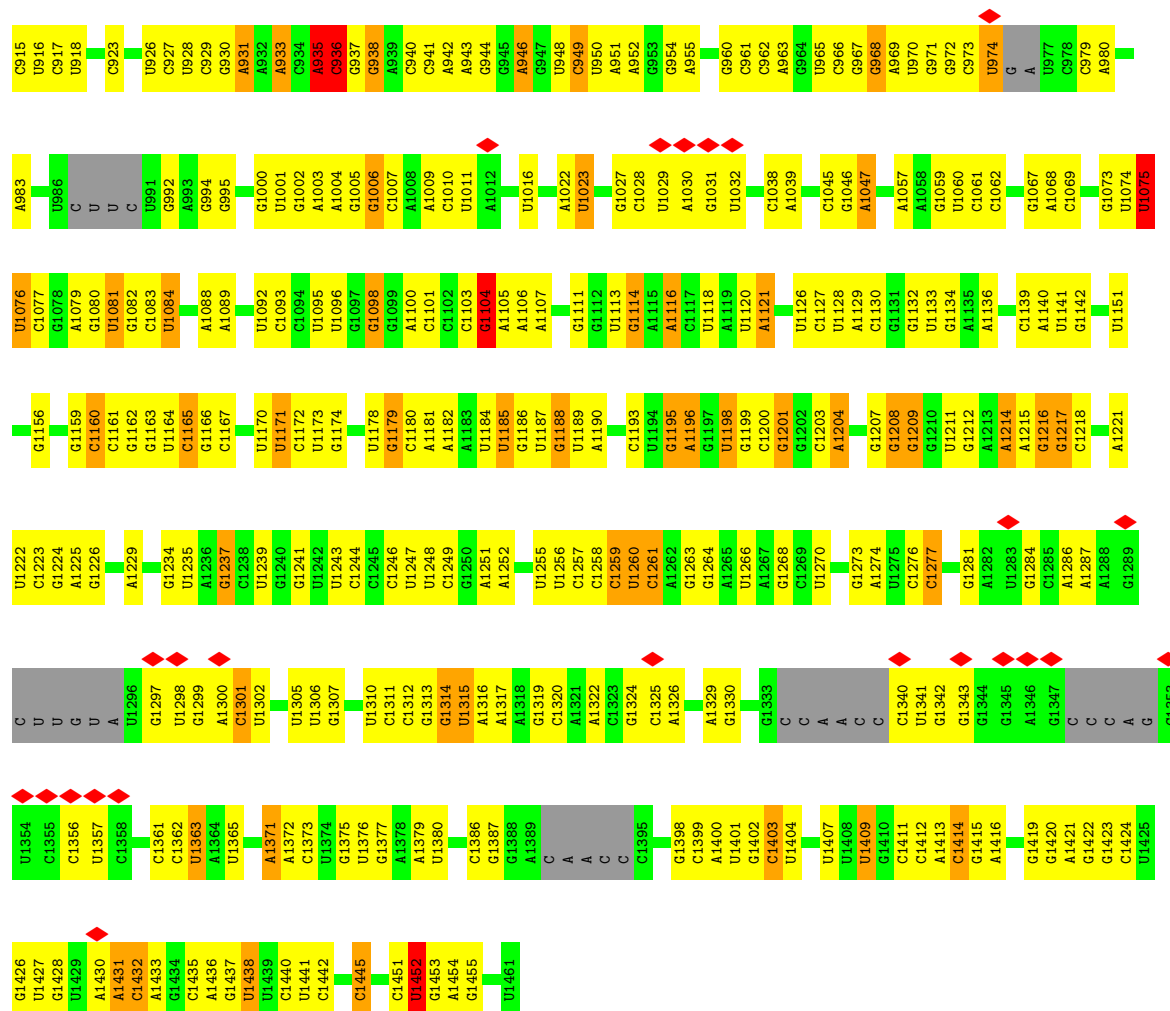
Chain LD: 41% 41% 13% 5%



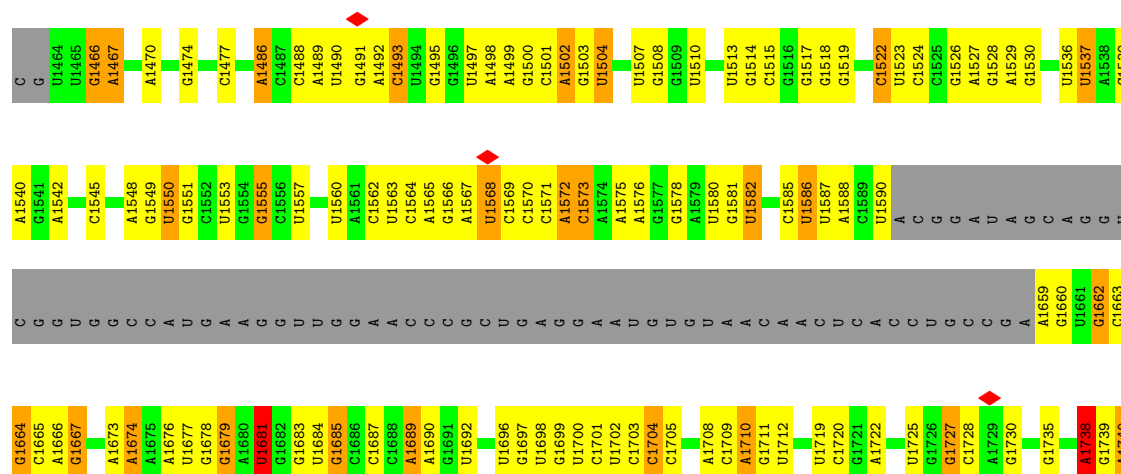
• Molecule 44: LSU rRNA chain 4

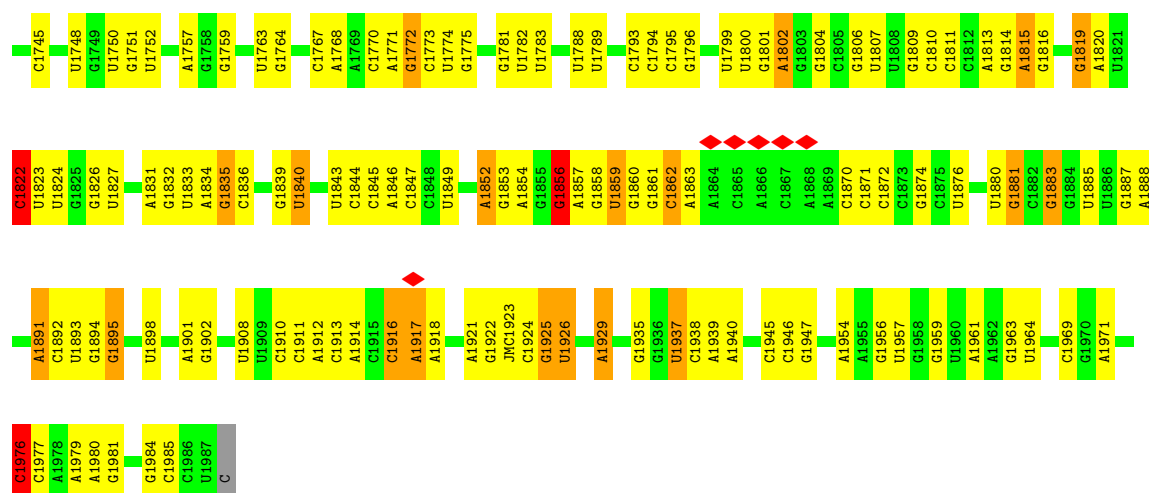
Chain LE: 40% 43% 9% 7%



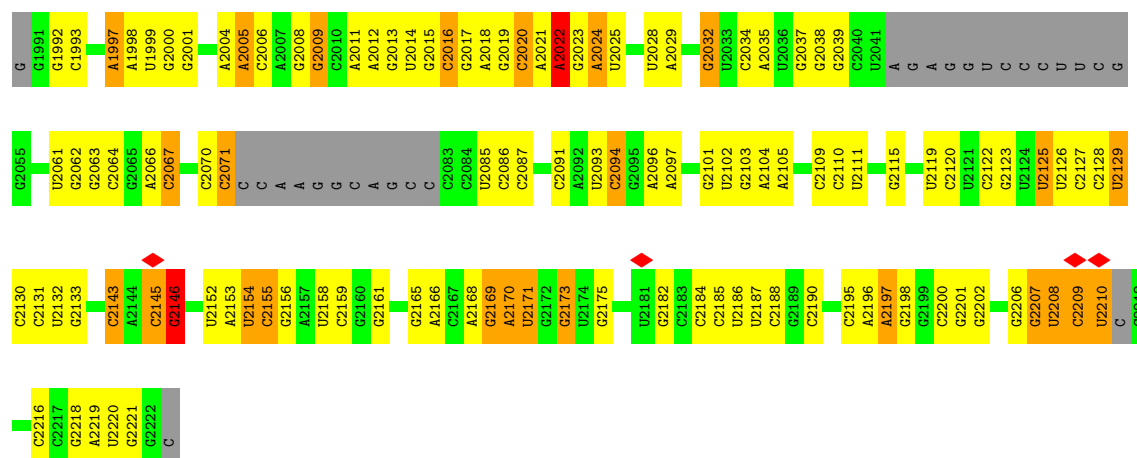


• Molecule 45: LSU rRNA chain 5

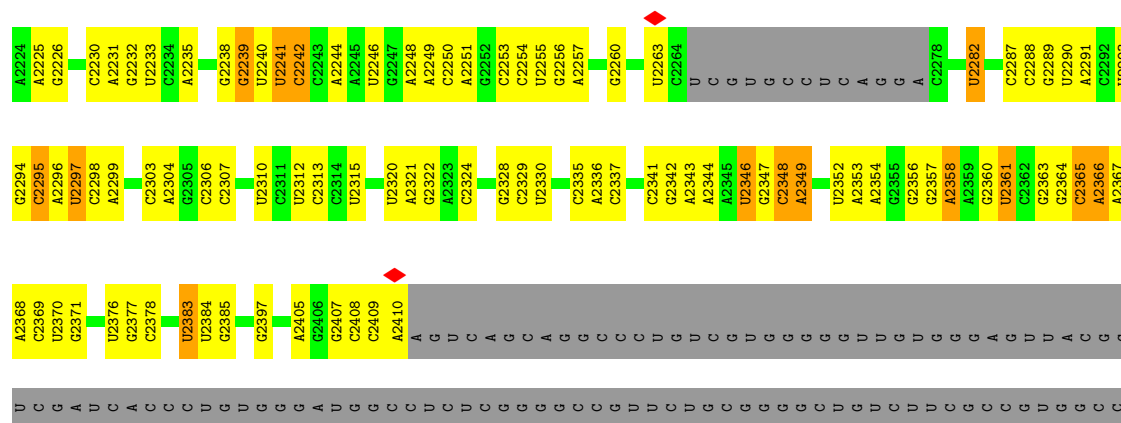


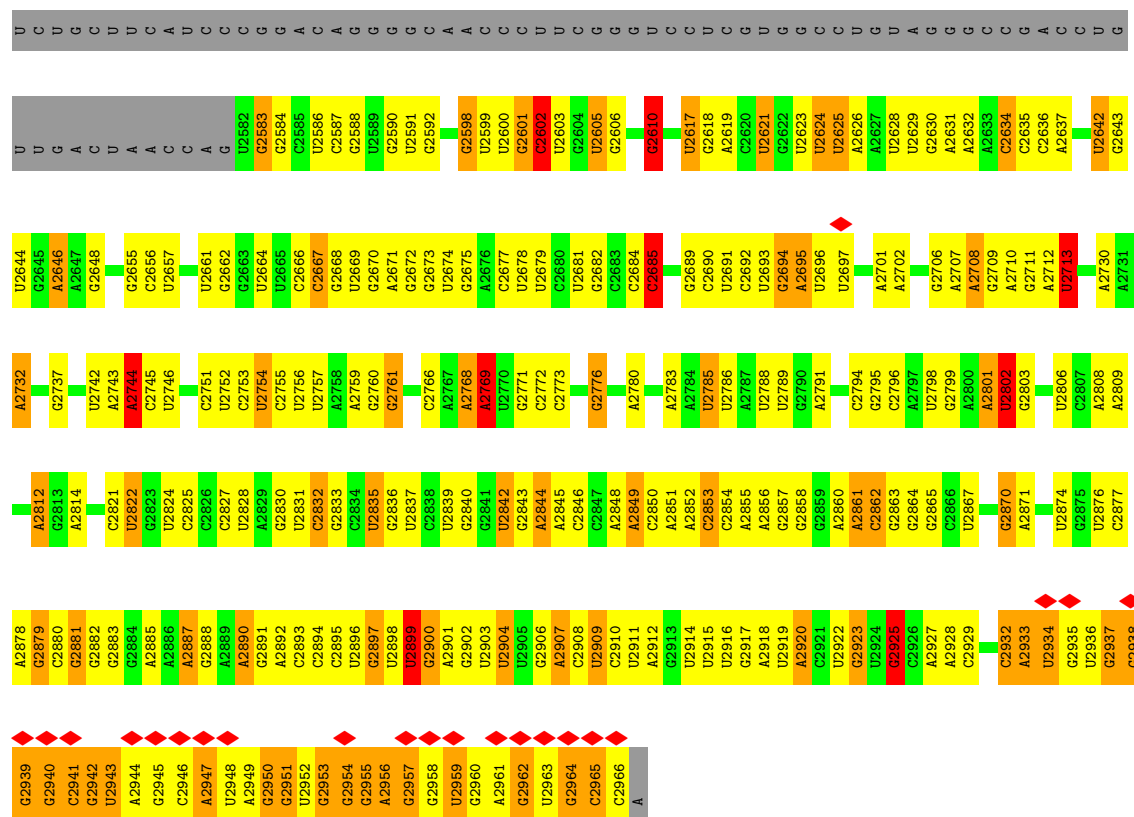


• Molecule 46: LSU rRNA chain 6

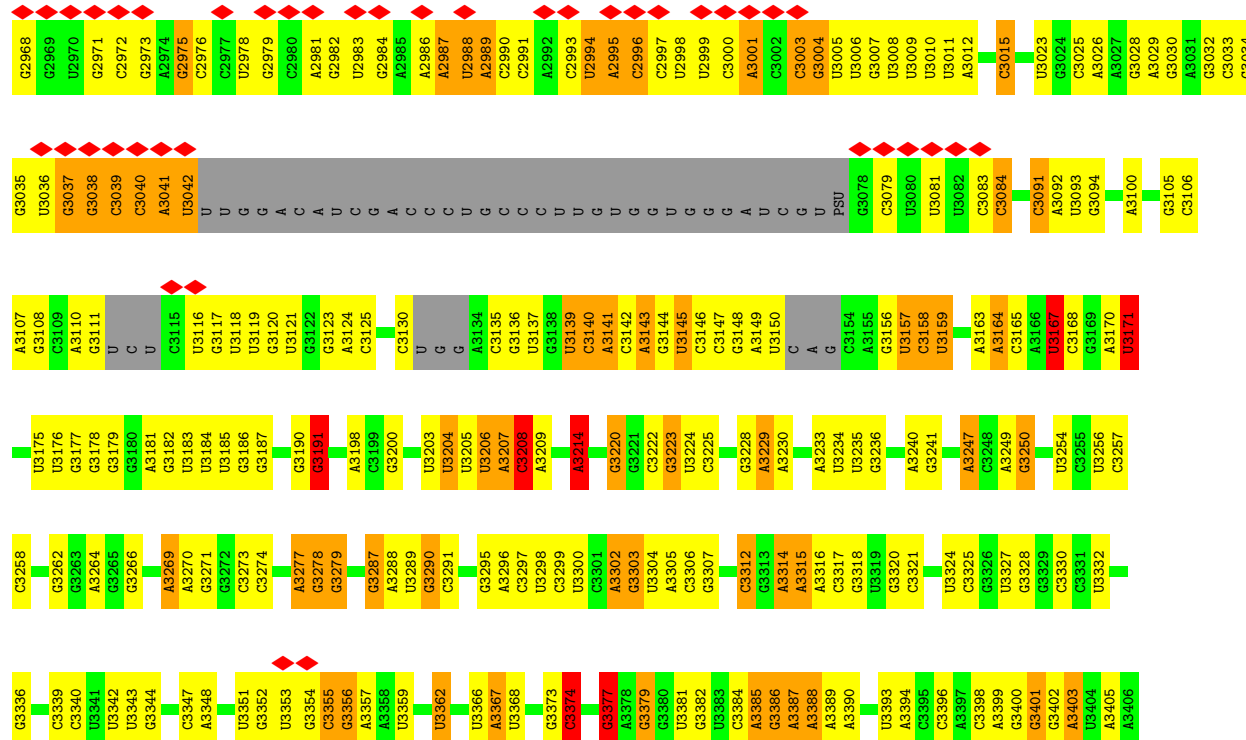


• Molecule 47: LSU rRNA chain 7



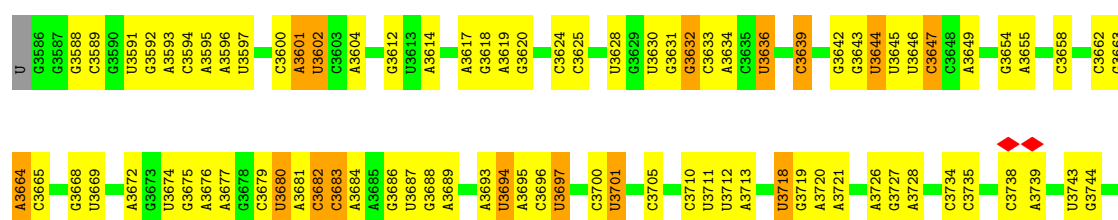


# Molecule 48: LSU rRNA chain 8

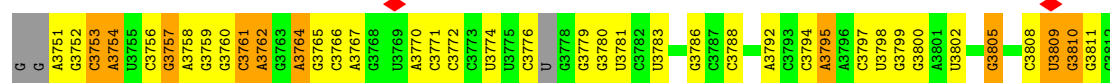




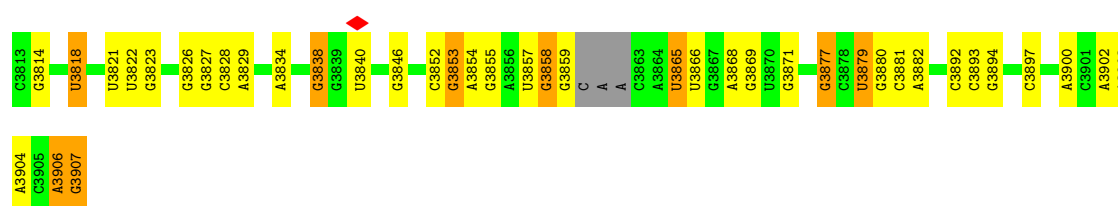
• Molecule 49: LSU rRNA chain 9



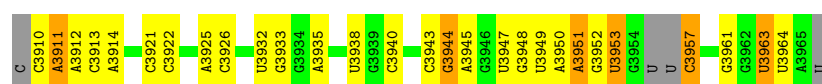
• Molecule 50: LSU rRNA chain 10



• Molecule 51: LSU rRNA chain 11

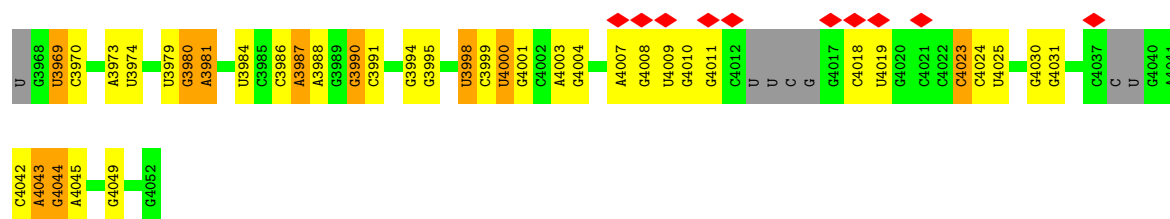


• Molecule 52: LSU rRNA chain 12



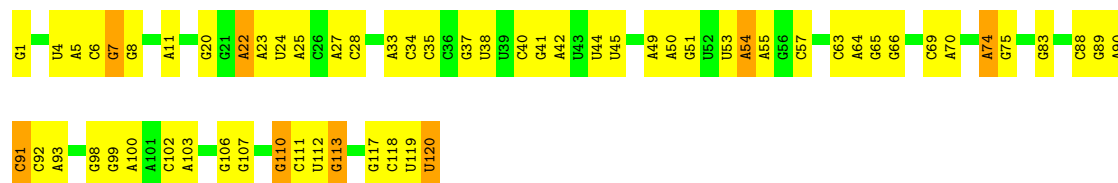
• Molecule 53: LSU rRNA chain 13





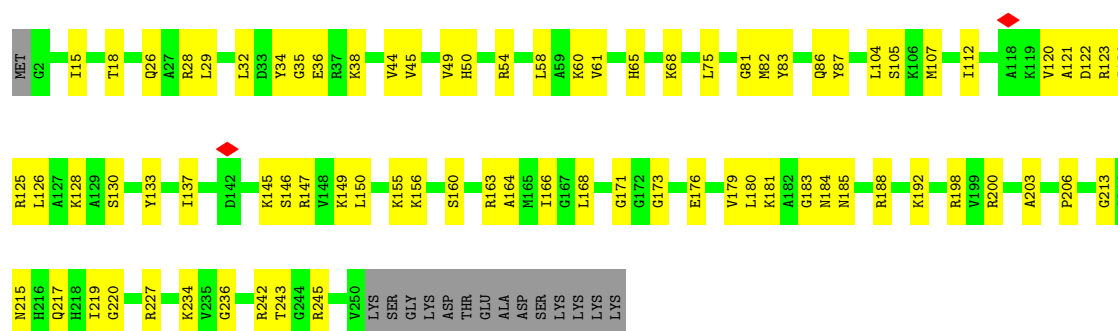
• Molecule 54: 5S rRNA

Chain LO: 49% 44% 7%



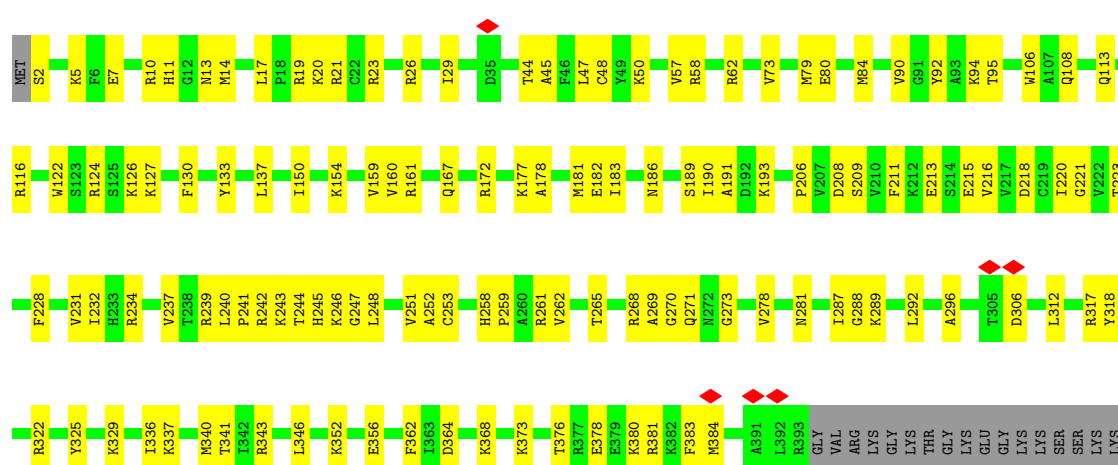
• Molecule 55: Ribosomal protein uL2

Chain LP: 64% 30% 6%

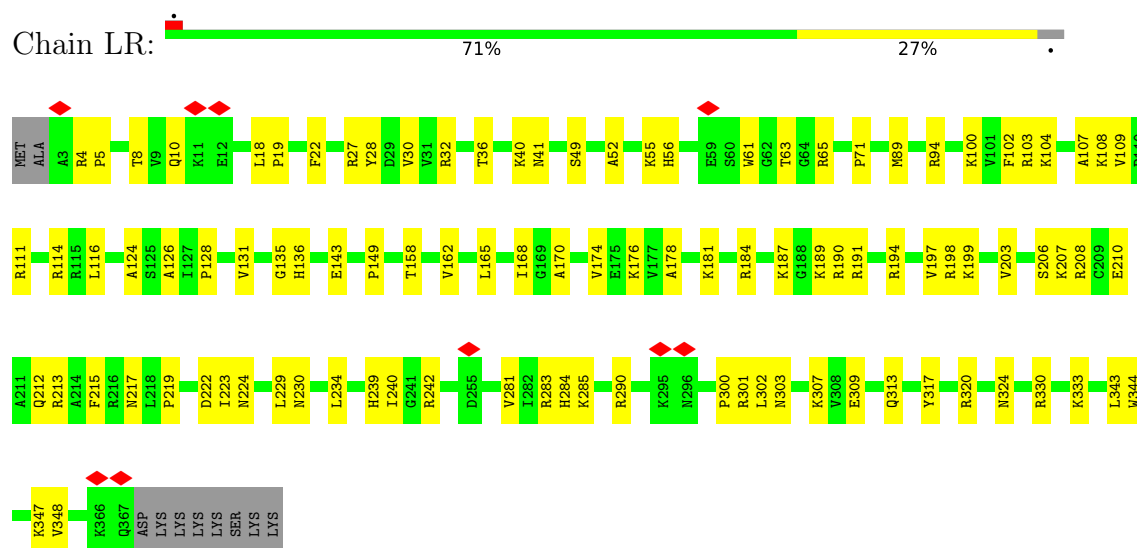


• Molecule 56: Ribosomal protein uL3

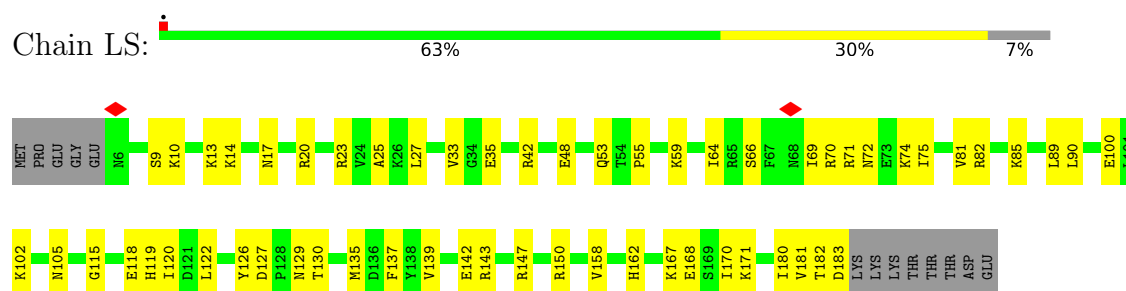
Chain LQ: 64% 32%



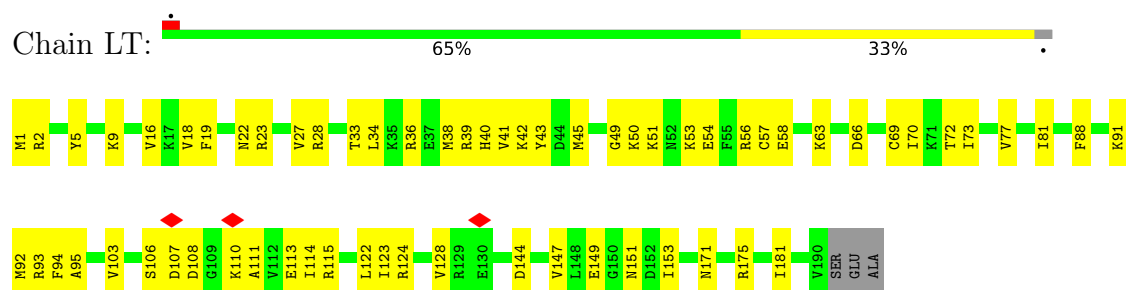
• Molecule 57: Ribosomal protein uL4



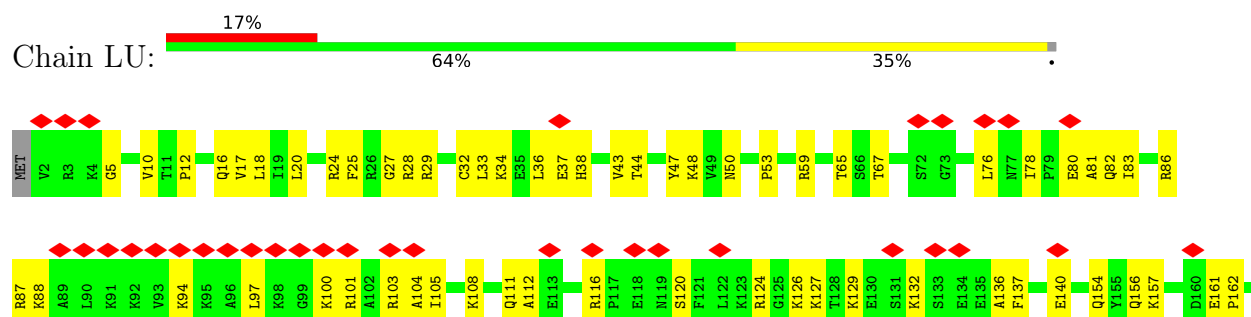
• Molecule 58: Ribosomal protein uL5

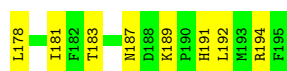


• Molecule 59: Ribosomal protein uL6

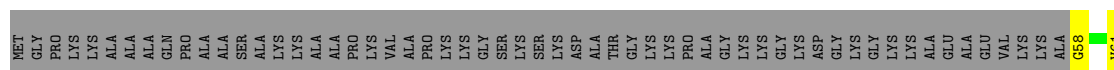


• Molecule 60: Ribosomal protein eL6





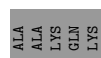
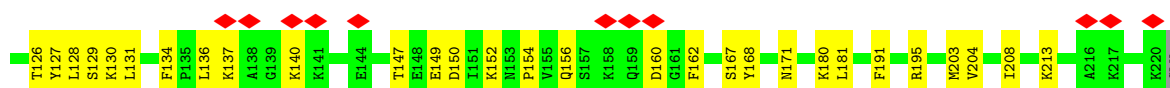
- Molecule 61: 60S ribosomal protein L7a



- Molecule 62: Ribosomal protein uL13

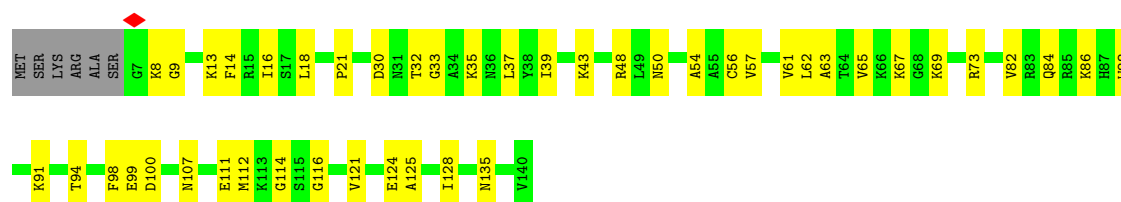


- Molecule 63: Ribosomal protein eL13

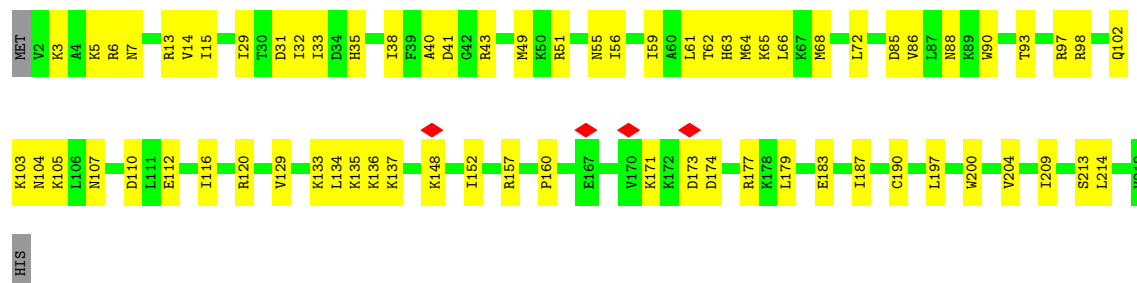


- Molecule 64: Ribosomal protein uL14

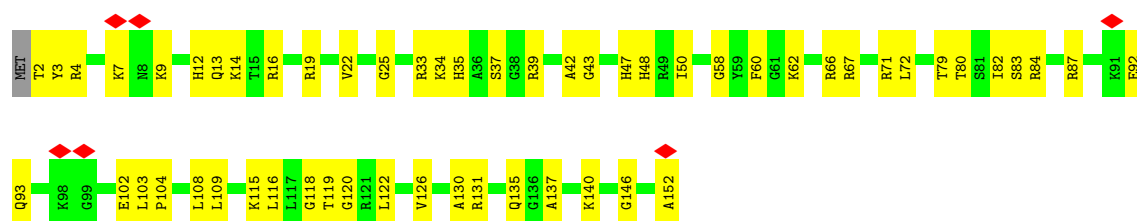




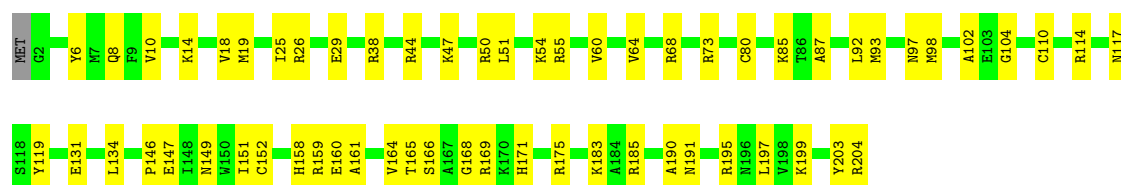
• Molecule 65: Ribosomal protein eL14



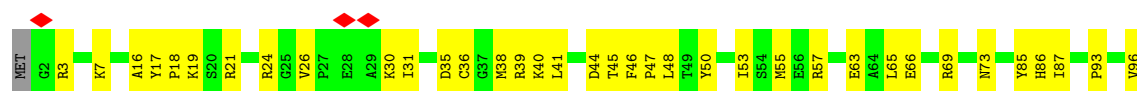
• Molecule 66: Ribosomal protein uL15

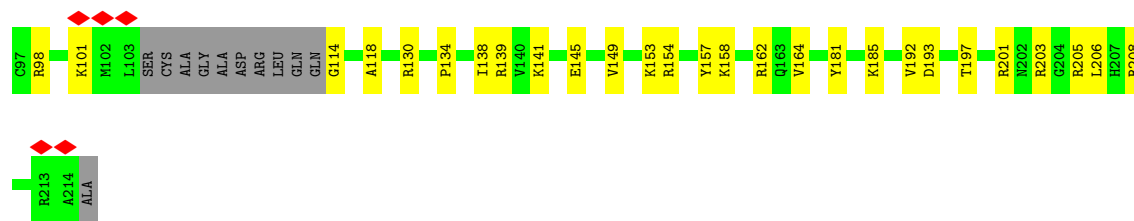


• Molecule 67: Ribosomal protein eL15

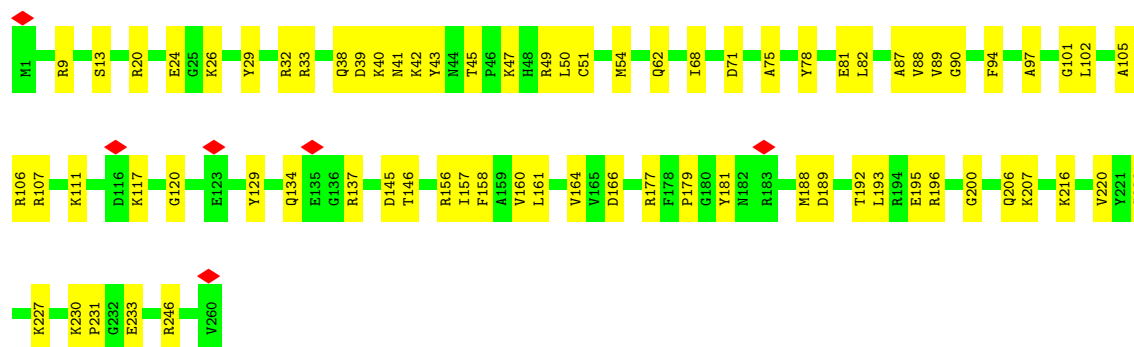
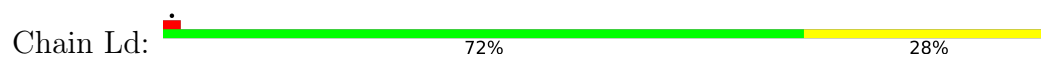


• Molecule 68: 60S ribosomal protein L10

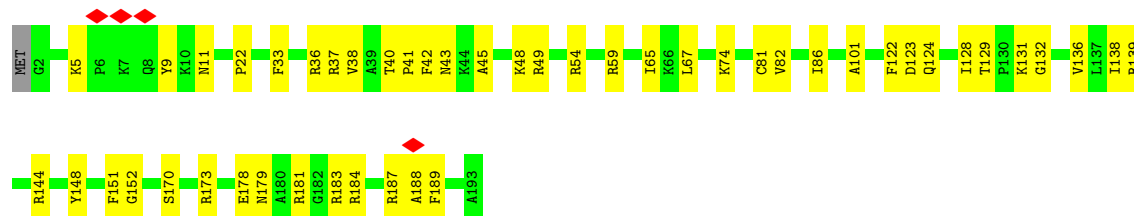
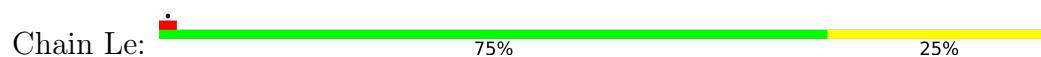




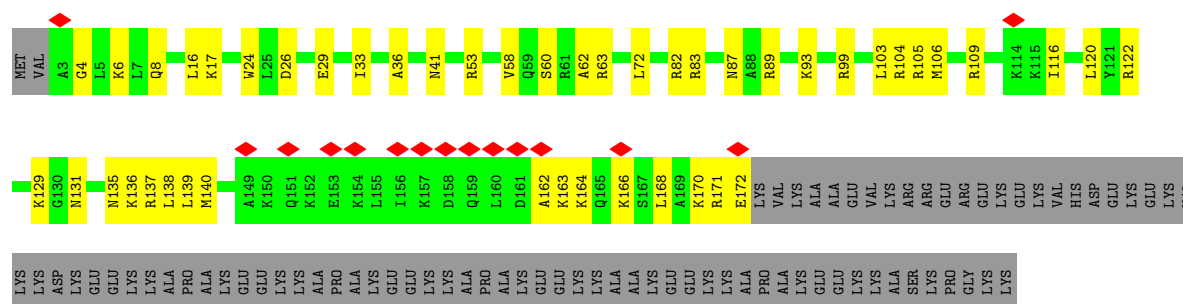
• Molecule 69: Ribosomal protein uL18



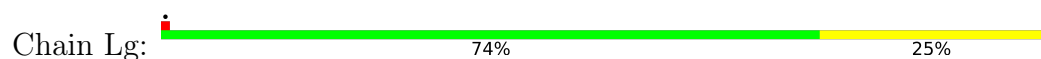
• Molecule 70: Ribosomal protein eL18



• Molecule 71: Ribosomal protein eL19



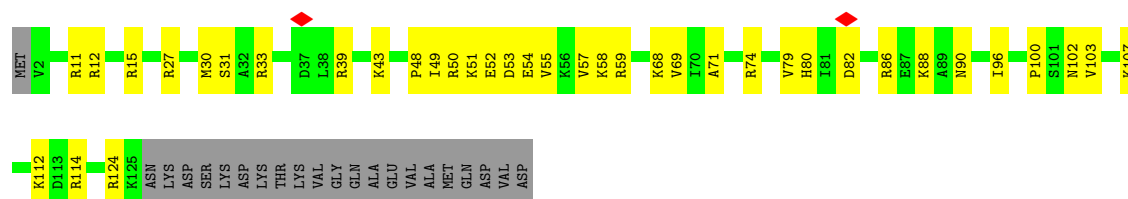
• Molecule 72: Ribosomal protein eL20



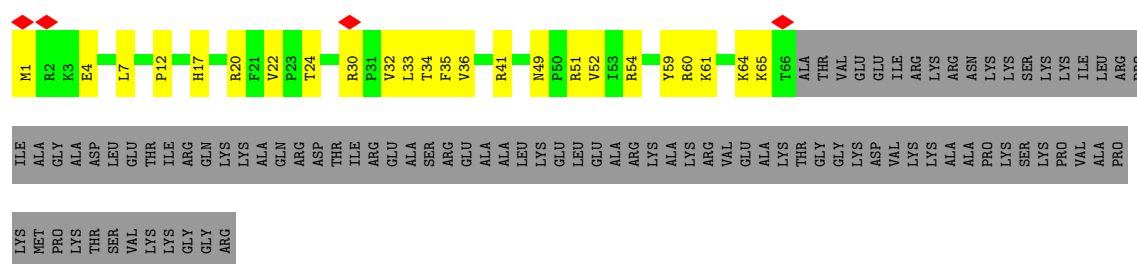




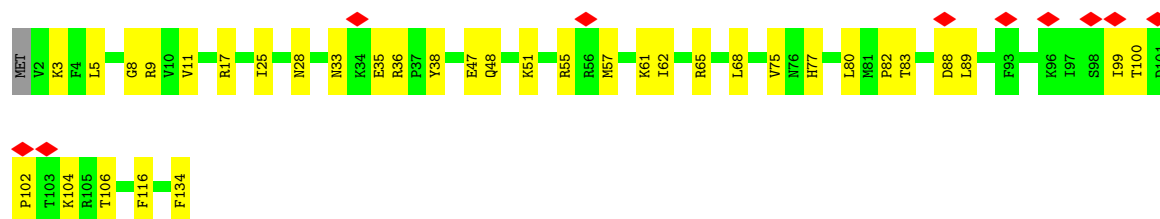
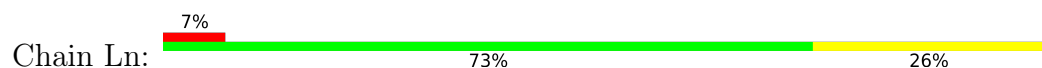
• Molecule 77: Ribosomal protein uL24



• Molecule 78: Ribosomal protein eL24



• Molecule 79: Ribosomal protein eL27

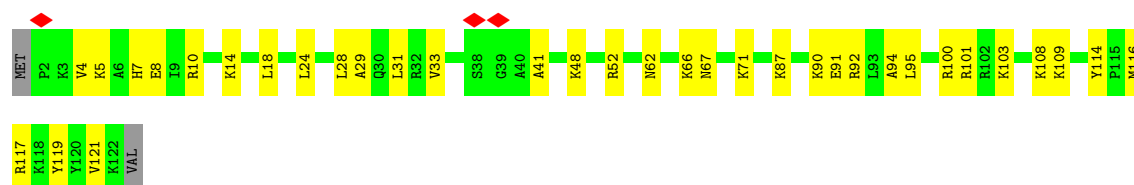


• Molecule 80: Ribosomal protein eLEgr1

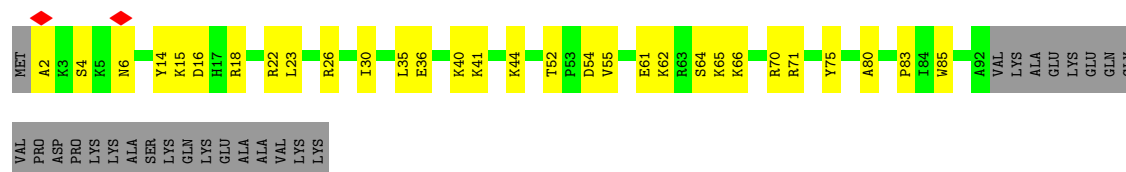


• Molecule 81: Ribosomal protein uL29

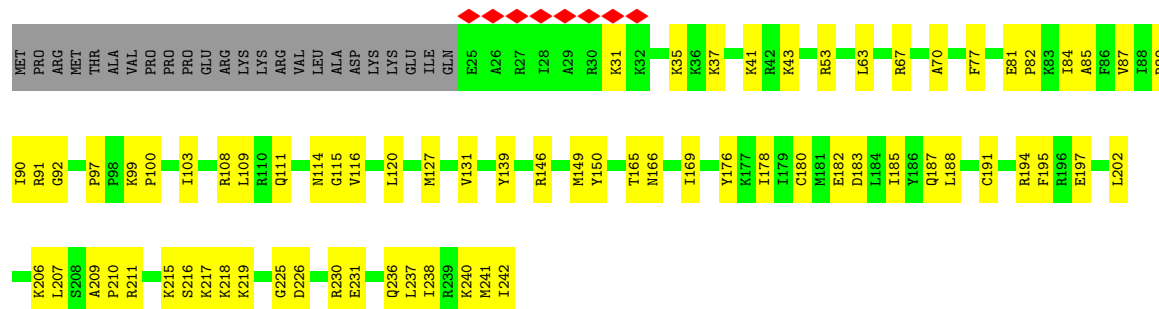




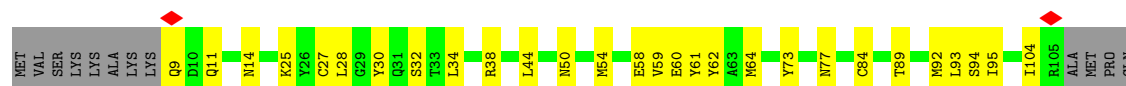
- Molecule 82: Ribosomal protein eL29



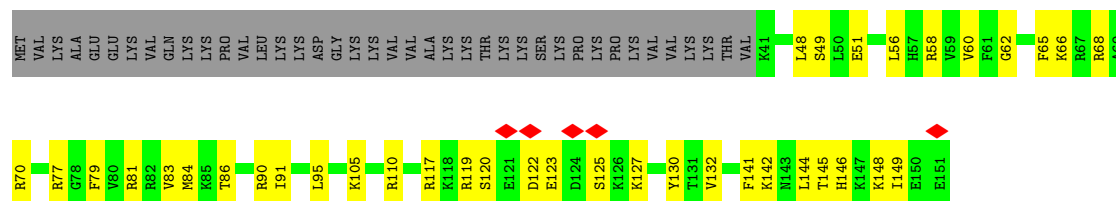
- Molecule 83: Ribosomal protein uL30



- Molecule 84: Ribosomal protein eL30



- Molecule 85: Ribosomal protein eL31



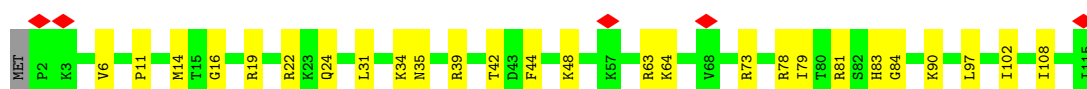
- Molecule 86: Ribosomal protein eL32

Chain Lu:  71% 21% 8%



- Molecule 87: Ribosomal protein eL33

Chain Lv:  77% 23%



- Molecule 88: Ribosomal protein eL34

Chain Lw:  60% 29% 11%



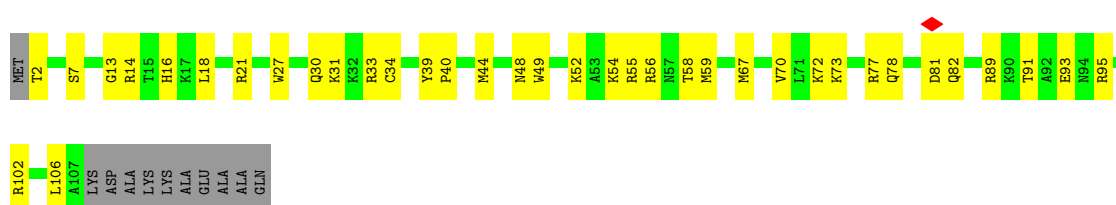
- Molecule 89: Ribosomal protein eL36

Chain Lx:  77% 19%



- Molecule 90: Ribosomal protein eL37

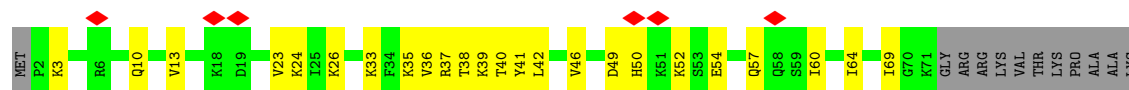
Chain Ly:  59% 32% 9%



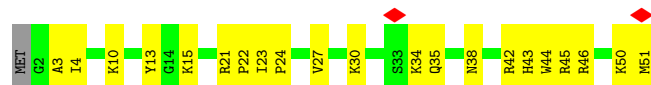
- Molecule 91: Ribosomal protein eL38

Chain Lz:  7% 56% 29% 15%

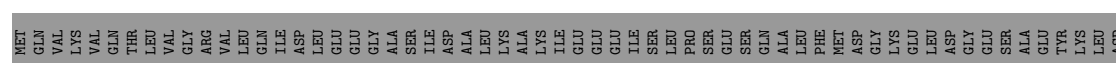




- Molecule 92: Ribosomal protein eL39



- Molecule 93: Ribosomal protein eL40



- Molecule 94: Ribosomal protein eL41



- Molecule 95: Ribosomal protein eL42



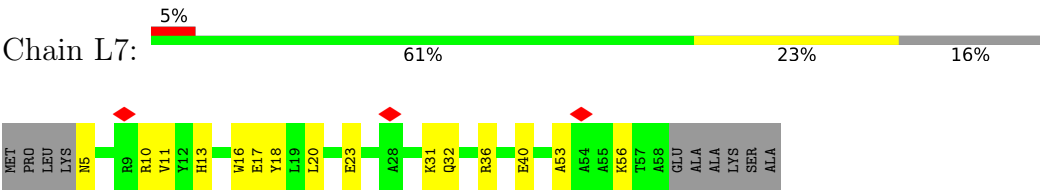
- Molecule 96: Ribosomal protein eL43



- Molecule 97: Ribosomal protein eLEgr2



● Molecule 98: Ribosomal protein eLEgr3



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 176308                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.52                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.408                                   | Depositor |
| Minimum map value                    | -0.214                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.011                                   | Depositor |
| Recommended contour level            | 0.035                                   | Depositor |
| Map size (Å)                         | 419.99997, 419.99997, 419.99997         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.05, 1.05, 1.05                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, ZN, JMH, MA6, A2M, JMC, OMG, 7MG, B8H, OMC, MIA, B8N, UR3, 5MC, OMU, 6MZ, 1MA

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   | S1    | 0.31         | 2/46353 (0.0%) | 0.36        | 3/72230 (0.0%) |
| 2   | S2    | 0.18         | 0/1783         | 0.34        | 0/2776         |
| 3   | S3    | 0.26         | 0/1802         | 0.38        | 0/2807         |
| 4   | S4    | 0.18         | 0/1812         | 0.37        | 0/2824         |
| 5   | S5    | 0.43         | 0/279          | 0.37        | 0/431          |
| 6   | SA    | 0.27         | 0/1828         | 0.50        | 0/2458         |
| 7   | SB    | 0.24         | 0/1694         | 0.46        | 0/2301         |
| 8   | SC    | 0.26         | 0/1701         | 0.45        | 0/2281         |
| 9   | SD    | 0.25         | 0/1461         | 0.45        | 0/1955         |
| 10  | SE    | 0.29         | 0/2169         | 0.51        | 0/2909         |
| 11  | SF    | 0.28         | 0/1752         | 0.44        | 0/2371         |
| 12  | SG    | 0.27         | 0/2036         | 0.53        | 0/2709         |
| 13  | SH    | 0.71         | 4/1472 (0.3%)  | 0.90        | 7/1982 (0.4%)  |
| 14  | SI    | 0.25         | 0/1538         | 0.49        | 0/2060         |
| 15  | SJ    | 0.29         | 0/1056         | 0.47        | 0/1415         |
| 16  | SK    | 0.30         | 0/1678         | 0.55        | 0/2240         |
| 17  | SL    | 0.27         | 0/1162         | 0.46        | 0/1554         |
| 18  | SM    | 0.26         | 0/808          | 0.47        | 0/1089         |
| 19  | SN    | 0.25         | 0/796          | 0.43        | 0/1072         |
| 20  | SO    | 0.34         | 0/1024         | 0.63        | 1/1375 (0.1%)  |
| 21  | SP    | 0.36         | 0/1119         | 0.59        | 0/1493         |
| 22  | SQ    | 0.22         | 0/931          | 0.58        | 0/1252         |
| 23  | SR    | 0.33         | 0/1198         | 0.58        | 0/1603         |
| 24  | SS    | 0.32         | 0/441          | 0.57        | 0/583          |
| 25  | ST    | 0.26         | 0/1201         | 0.50        | 0/1608         |
| 26  | SU    | 0.30         | 0/1259         | 0.44        | 0/1695         |
| 27  | SV    | 0.32         | 0/1006         | 0.52        | 0/1344         |
| 28  | SW    | 0.27         | 0/1008         | 0.48        | 0/1346         |
| 29  | SX    | 0.28         | 0/1148         | 0.47        | 0/1543         |
| 30  | SY    | 0.23         | 0/631          | 0.42        | 0/849          |
| 31  | SZ    | 0.30         | 0/1070         | 0.51        | 0/1412         |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 32  | Sa    | 0.32         | 0/642          | 0.52        | 0/862          |
| 33  | Sb    | 0.34         | 0/791          | 0.57        | 1/1057 (0.1%)  |
| 34  | Sc    | 0.24         | 0/663          | 0.43        | 0/891          |
| 35  | Sd    | 0.27         | 0/500          | 0.59        | 0/669          |
| 36  | Se    | 0.32         | 0/490          | 0.61        | 0/646          |
| 37  | Sf    | 0.33         | 0/519          | 0.67        | 2/691 (0.3%)   |
| 38  | Sg    | 0.45         | 0/1623         | 0.75        | 0/2158         |
| 39  | Sh    | 0.34         | 0/2454         | 0.60        | 1/3339 (0.0%)  |
| 40  | LA    | 0.30         | 0/3674         | 0.32        | 0/5722         |
| 41  | LB    | 0.32         | 0/3021         | 0.31        | 0/4708         |
| 42  | LC    | 0.28         | 0/8081         | 0.36        | 0/12607        |
| 43  | LD    | 0.23         | 0/2613         | 0.31        | 0/4069         |
| 44  | LE    | 0.30         | 0/14709        | 0.34        | 0/22917        |
| 45  | LF    | 0.33         | 0/10013        | 0.32        | 0/15601        |
| 46  | LG    | 0.30         | 1/4698 (0.0%)  | 0.30        | 0/7316         |
| 47  | LH    | 0.35         | 1/12014 (0.0%) | 0.34        | 0/18729        |
| 48  | LI    | 0.30         | 0/12455        | 0.33        | 2/19402 (0.0%) |
| 49  | LJ    | 0.33         | 0/3692         | 0.34        | 0/5756         |
| 50  | LK    | 0.23         | 0/1453         | 0.30        | 0/2260         |
| 51  | LL    | 0.21         | 0/2170         | 0.26        | 0/3384         |
| 52  | LM    | 0.29         | 0/1228         | 0.33        | 0/1914         |
| 53  | LN    | 0.21         | 0/1871         | 0.30        | 0/2914         |
| 54  | LO    | 0.24         | 0/2860         | 0.28        | 0/4456         |
| 55  | LP    | 0.30         | 0/1941         | 0.48        | 0/2604         |
| 56  | LQ    | 0.30         | 0/3177         | 0.47        | 0/4254         |
| 57  | LR    | 0.27         | 0/2918         | 0.44        | 0/3918         |
| 58  | LS    | 0.23         | 0/1456         | 0.48        | 0/1937         |
| 59  | LT    | 0.24         | 0/1545         | 0.43        | 0/2068         |
| 60  | LU    | 0.22         | 0/1606         | 0.47        | 0/2142         |
| 61  | LV    | 0.23         | 0/1963         | 0.42        | 0/2627         |
| 62  | LW    | 0.30         | 0/1745         | 0.49        | 0/2327         |
| 63  | LX    | 0.26         | 0/1803         | 0.48        | 0/2404         |
| 64  | LY    | 0.30         | 0/1017         | 0.49        | 0/1368         |
| 65  | LZ    | 0.25         | 0/1809         | 0.43        | 0/2409         |
| 66  | La    | 0.28         | 0/1238         | 0.47        | 0/1650         |
| 67  | Lb    | 0.30         | 0/1757         | 0.49        | 0/2355         |
| 68  | Lc    | 0.23         | 0/1675         | 0.43        | 0/2237         |
| 69  | Ld    | 0.24         | 0/2112         | 0.42        | 0/2838         |
| 70  | Le    | 0.28         | 0/1554         | 0.50        | 0/2073         |
| 71  | Lf    | 0.30         | 0/1410         | 0.53        | 0/1870         |
| 72  | Lg    | 0.27         | 0/1532         | 0.43        | 0/2056         |
| 73  | Lh    | 0.26         | 0/1306         | 0.47        | 0/1748         |
| 74  | Li    | 0.36         | 0/1281         | 0.54        | 0/1721         |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 75  | Lj    | 0.19         | 0/841           | 0.43        | 0/1125           |
| 76  | Lk    | 0.32         | 0/1088          | 0.52        | 0/1455           |
| 77  | Ll    | 0.24         | 0/1019          | 0.45        | 0/1350           |
| 78  | Lm    | 0.26         | 0/562           | 0.44        | 0/756            |
| 79  | Ln    | 0.23         | 0/1103          | 0.44        | 0/1470           |
| 80  | Lo    | 0.26         | 0/470           | 0.43        | 0/631            |
| 81  | Lp    | 0.23         | 0/1020          | 0.40        | 0/1352           |
| 82  | Lq    | 0.22         | 0/780           | 0.39        | 0/1027           |
| 83  | Lr    | 0.29         | 0/1867          | 0.46        | 0/2500           |
| 84  | Ls    | 0.27         | 0/756           | 0.46        | 0/1014           |
| 85  | Lt    | 0.30         | 0/941           | 0.51        | 0/1257           |
| 86  | Lu    | 0.27         | 0/1093          | 0.44        | 0/1462           |
| 87  | Lv    | 0.31         | 0/935           | 0.44        | 0/1247           |
| 88  | Lw    | 0.30         | 0/937           | 0.49        | 0/1254           |
| 89  | Lx    | 0.23         | 0/847           | 0.43        | 0/1122           |
| 90  | Ly    | 0.30         | 0/872           | 0.50        | 0/1151           |
| 91  | Lz    | 0.22         | 0/577           | 0.47        | 0/767            |
| 92  | L1    | 0.26         | 0/457           | 0.42        | 0/603            |
| 93  | L2    | 0.25         | 0/420           | 0.45        | 0/554            |
| 94  | L3    | 0.51         | 0/304           | 0.80        | 0/390            |
| 95  | L5    | 0.30         | 0/732           | 0.52        | 0/975            |
| 96  | L4    | 0.30         | 0/798           | 0.48        | 0/1054           |
| 97  | L6    | 0.21         | 0/500           | 0.47        | 0/665            |
| 98  | L7    | 0.21         | 0/463           | 0.38        | 0/616            |
| All | All   | 0.30         | 8/231677 (0.0%) | 0.41        | 17/340038 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | S1    | 1                   | 0                   |
| 45  | LF    | 1                   | 0                   |
| All | All   | 2                   | 0                   |

All (8) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 13  | SH    | 60   | ASN  | C-O   | 14.41 | 1.41        | 1.24     |
| 13  | SH    | 57   | ARG  | C-O   | 10.43 | 1.36        | 1.24     |
| 1   | S1    | 2180 | A2M  | O3'-P | 8.05  | 1.64        | 1.56     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 13  | SH    | 64   | TYR  | N-CA  | 7.02 | 1.55        | 1.46     |
| 47  | LH    | 2744 | A2M  | O3'-P | 5.56 | 1.61        | 1.56     |
| 1   | S1    | 649  | A2M  | O3'-P | 5.24 | 1.61        | 1.56     |
| 13  | SH    | 64   | TYR  | CA-C  | 5.17 | 1.59        | 1.52     |
| 46  | LG    | 2005 | A2M  | O3'-P | 5.08 | 1.61        | 1.56     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | SH    | 64   | TYR  | CA-C-N      | 12.84 | 146.07      | 121.54   |
| 13  | SH    | 64   | TYR  | C-N-CA      | 12.84 | 146.07      | 121.54   |
| 48  | LI    | 3566 | U    | OP2-P-O3'   | -9.30 | 80.11       | 108.00   |
| 1   | S1    | 1959 | G    | C4'-C3'-O3' | 8.05  | 125.07      | 113.00   |
| 48  | LI    | 3566 | U    | OP1-P-O3'   | -7.21 | 86.36       | 108.00   |
| 13  | SH    | 64   | TYR  | N-CA-C      | 6.97  | 125.64      | 110.80   |
| 1   | S1    | 282  | C    | C4'-C3'-O3' | 6.59  | 119.29      | 109.40   |
| 13  | SH    | 60   | ASN  | CA-C-N      | -6.56 | 111.49      | 120.28   |
| 13  | SH    | 60   | ASN  | C-N-CA      | -6.56 | 111.49      | 120.28   |
| 1   | S1    | 1959 | G    | C1'-C2'-O2' | -6.54 | 98.59       | 108.40   |
| 37  | Sf    | 87   | THR  | CA-C-N      | 6.44  | 132.91      | 122.48   |
| 37  | Sf    | 87   | THR  | C-N-CA      | 6.44  | 132.91      | 122.48   |
| 13  | SH    | 64   | TYR  | CA-CB-CG    | -6.41 | 102.37      | 113.90   |
| 20  | SO    | 139  | ASP  | CB-CA-C     | 5.98  | 121.75      | 110.62   |
| 13  | SH    | 56   | GLU  | O-C-N       | -5.77 | 115.17      | 122.27   |
| 33  | Sb    | 84   | ILE  | N-CA-C      | -5.42 | 105.24      | 110.72   |
| 39  | Sh    | 306  | TYR  | N-CA-C      | 5.29  | 115.53      | 108.23   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | S1    | 1601 | B8N  | C33  |
| 45  | LF    | 1923 | JMC  | C4   |

There are no planarity outliers.

## 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   | S1    | 43278 | 0        | 21953    | 921     | 0            |
| 2   | S2    | 1626  | 0        | 834      | 33      | 0            |
| 3   | S3    | 1614  | 0        | 821      | 43      | 0            |
| 4   | S4    | 1621  | 0        | 822      | 59      | 0            |
| 5   | S5    | 251   | 0        | 130      | 5       | 0            |
| 6   | SA    | 1797  | 0        | 1849     | 56      | 0            |
| 7   | SB    | 1657  | 0        | 1688     | 55      | 0            |
| 8   | SC    | 1675  | 0        | 1748     | 41      | 0            |
| 9   | SD    | 1436  | 0        | 1532     | 46      | 0            |
| 10  | SE    | 2125  | 0        | 2262     | 77      | 0            |
| 11  | SF    | 1713  | 0        | 1780     | 63      | 0            |
| 12  | SG    | 2016  | 0        | 2197     | 62      | 0            |
| 13  | SH    | 1450  | 0        | 1498     | 78      | 0            |
| 14  | SI    | 1514  | 0        | 1611     | 48      | 0            |
| 15  | SJ    | 1037  | 0        | 1076     | 32      | 0            |
| 16  | SK    | 1644  | 0        | 1725     | 63      | 0            |
| 17  | SL    | 1144  | 0        | 1219     | 30      | 0            |
| 18  | SM    | 796   | 0        | 853      | 25      | 0            |
| 19  | SN    | 775   | 0        | 791      | 14      | 0            |
| 20  | SO    | 1010  | 0        | 1024     | 34      | 0            |
| 21  | SP    | 1101  | 0        | 1161     | 37      | 0            |
| 22  | SQ    | 919   | 0        | 939      | 48      | 0            |
| 23  | SR    | 1181  | 0        | 1238     | 38      | 0            |
| 24  | SS    | 433   | 0        | 442      | 21      | 0            |
| 25  | ST    | 1180  | 0        | 1257     | 30      | 0            |
| 26  | SU    | 1225  | 0        | 1263     | 30      | 0            |
| 27  | SV    | 998   | 0        | 1060     | 42      | 0            |
| 28  | SW    | 990   | 0        | 1052     | 34      | 0            |
| 29  | SX    | 1125  | 0        | 1158     | 41      | 0            |
| 30  | SY    | 624   | 0        | 629      | 29      | 0            |
| 31  | SZ    | 1052  | 0        | 1124     | 30      | 0            |
| 32  | Sa    | 633   | 0        | 680      | 19      | 0            |
| 33  | Sb    | 780   | 0        | 818      | 26      | 0            |
| 34  | Sc    | 649   | 0        | 673      | 22      | 0            |
| 35  | Sd    | 499   | 0        | 538      | 18      | 0            |
| 36  | Se    | 484   | 0        | 540      | 18      | 0            |
| 37  | Sf    | 508   | 0        | 532      | 15      | 0            |
| 38  | Sg    | 1597  | 0        | 1720     | 75      | 0            |
| 39  | Sh    | 2393  | 0        | 2327     | 71      | 0            |
| 40  | LA    | 3423  | 0        | 1736     | 75      | 0            |
| 41  | LB    | 2847  | 0        | 1448     | 73      | 0            |
| 42  | LC    | 7516  | 0        | 3791     | 146     | 0            |
| 43  | LD    | 2342  | 0        | 1194     | 39      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | LE    | 13955 | 0        | 7088     | 297     | 0            |
| 45  | LF    | 9702  | 0        | 4907     | 188     | 0            |
| 46  | LG    | 4422  | 0        | 2249     | 84      | 0            |
| 47  | LH    | 11980 | 0        | 6071     | 255     | 0            |
| 48  | LI    | 12233 | 0        | 6237     | 253     | 0            |
| 49  | LJ    | 3486  | 0        | 1769     | 59      | 0            |
| 50  | LK    | 1301  | 0        | 663      | 33      | 0            |
| 51  | LL    | 1983  | 0        | 1000     | 33      | 0            |
| 52  | LM    | 1158  | 0        | 590      | 23      | 0            |
| 53  | LN    | 1696  | 0        | 858      | 28      | 0            |
| 54  | LO    | 2559  | 0        | 1294     | 52      | 0            |
| 55  | LP    | 1901  | 0        | 1984     | 65      | 0            |
| 56  | LQ    | 3118  | 0        | 3260     | 111     | 0            |
| 57  | LR    | 2868  | 0        | 3081     | 84      | 0            |
| 58  | LS    | 1437  | 0        | 1533     | 46      | 0            |
| 59  | LT    | 1521  | 0        | 1580     | 44      | 0            |
| 60  | LU    | 1580  | 0        | 1703     | 46      | 0            |
| 61  | LV    | 1926  | 0        | 2075     | 51      | 0            |
| 62  | LW    | 1713  | 0        | 1850     | 57      | 0            |
| 63  | LX    | 1769  | 0        | 1895     | 55      | 0            |
| 64  | LY    | 1001  | 0        | 1063     | 33      | 0            |
| 65  | LZ    | 1780  | 0        | 1923     | 62      | 0            |
| 66  | La    | 1210  | 0        | 1251     | 52      | 0            |
| 67  | Lb    | 1711  | 0        | 1776     | 54      | 0            |
| 68  | Lc    | 1643  | 0        | 1714     | 48      | 0            |
| 69  | Ld    | 2074  | 0        | 2122     | 58      | 0            |
| 70  | Le    | 1526  | 0        | 1662     | 38      | 0            |
| 71  | Lf    | 1392  | 0        | 1530     | 40      | 0            |
| 72  | Lg    | 1494  | 0        | 1558     | 38      | 0            |
| 73  | Lh    | 1279  | 0        | 1363     | 45      | 0            |
| 74  | Li    | 1255  | 0        | 1290     | 38      | 0            |
| 75  | Lj    | 827   | 0        | 876      | 23      | 0            |
| 76  | Lk    | 1073  | 0        | 1161     | 31      | 0            |
| 77  | Ll    | 1008  | 0        | 1105     | 32      | 0            |
| 78  | Lm    | 549   | 0        | 604      | 21      | 0            |
| 79  | Ln    | 1084  | 0        | 1183     | 32      | 0            |
| 80  | Lo    | 459   | 0        | 457      | 14      | 0            |
| 81  | Lp    | 1010  | 0        | 1153     | 31      | 0            |
| 82  | Lq    | 767   | 0        | 828      | 24      | 0            |
| 83  | Lr    | 1825  | 0        | 1947     | 63      | 0            |
| 84  | Ls    | 747   | 0        | 760      | 22      | 0            |
| 85  | Lt    | 923   | 0        | 986      | 26      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86  | Lu    | 1068  | 0        | 1130     | 22      | 0            |
| 87  | Lv    | 915   | 0        | 1001     | 21      | 0            |
| 88  | Lw    | 922   | 0        | 1017     | 34      | 0            |
| 89  | Lx    | 835   | 0        | 931      | 15      | 0            |
| 90  | Ly    | 859   | 0        | 915      | 38      | 0            |
| 91  | Lz    | 570   | 0        | 636      | 16      | 0            |
| 92  | L1    | 447   | 0        | 490      | 23      | 0            |
| 93  | L2    | 415   | 0        | 440      | 13      | 0            |
| 94  | L3    | 302   | 0        | 348      | 17      | 0            |
| 95  | L5    | 719   | 0        | 750      | 25      | 0            |
| 96  | L4    | 785   | 0        | 860      | 22      | 0            |
| 97  | L6    | 493   | 0        | 539      | 11      | 0            |
| 98  | L7    | 455   | 0        | 462      | 14      | 0            |
| 99  | L2    | 1     | 0        | 0        | 0       | 0            |
| 99  | L4    | 1     | 0        | 0        | 0       | 0            |
| 99  | L5    | 1     | 0        | 0        | 0       | 0            |
| 99  | Ly    | 1     | 0        | 0        | 0       | 0            |
| 99  | Sb    | 1     | 0        | 0        | 0       | 0            |
| 100 | L2    | 3     | 0        | 0        | 0       | 0            |
| 100 | L3    | 10    | 0        | 0        | 2       | 0            |
| 100 | L4    | 1     | 0        | 0        | 0       | 0            |
| 100 | L5    | 2     | 0        | 0        | 0       | 0            |
| 100 | L7    | 1     | 0        | 0        | 0       | 0            |
| 100 | LA    | 29    | 0        | 0        | 1       | 0            |
| 100 | LB    | 15    | 0        | 0        | 2       | 0            |
| 100 | LC    | 32    | 0        | 0        | 2       | 0            |
| 100 | LD    | 9     | 0        | 0        | 0       | 0            |
| 100 | LE    | 97    | 0        | 0        | 21      | 0            |
| 100 | LF    | 93    | 0        | 0        | 13      | 0            |
| 100 | LG    | 33    | 0        | 0        | 2       | 0            |
| 100 | LH    | 174   | 0        | 0        | 23      | 0            |
| 100 | LI    | 82    | 0        | 0        | 13      | 0            |
| 100 | LJ    | 46    | 0        | 0        | 2       | 0            |
| 100 | LK    | 3     | 0        | 0        | 0       | 0            |
| 100 | LL    | 5     | 0        | 0        | 1       | 0            |
| 100 | LM    | 11    | 0        | 0        | 0       | 0            |
| 100 | LN    | 12    | 0        | 0        | 1       | 0            |
| 100 | LO    | 15    | 0        | 0        | 2       | 0            |
| 100 | LP    | 2     | 0        | 0        | 0       | 0            |
| 100 | LQ    | 8     | 0        | 0        | 1       | 0            |
| 100 | LR    | 8     | 0        | 0        | 0       | 0            |
| 100 | LU    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 100 | LW    | 7      | 0        | 0        | 2       | 0            |
| 100 | LY    | 3      | 0        | 0        | 1       | 0            |
| 100 | La    | 2      | 0        | 0        | 1       | 0            |
| 100 | Lb    | 2      | 0        | 0        | 0       | 0            |
| 100 | Lc    | 2      | 0        | 0        | 0       | 0            |
| 100 | Ld    | 1      | 0        | 0        | 0       | 0            |
| 100 | Lf    | 1      | 0        | 0        | 0       | 0            |
| 100 | Li    | 2      | 0        | 0        | 0       | 0            |
| 100 | Lk    | 1      | 0        | 0        | 0       | 0            |
| 100 | Ll    | 1      | 0        | 0        | 0       | 0            |
| 100 | Lm    | 3      | 0        | 0        | 0       | 0            |
| 100 | Lp    | 1      | 0        | 0        | 0       | 0            |
| 100 | Lq    | 3      | 0        | 0        | 0       | 0            |
| 100 | Lr    | 1      | 0        | 0        | 0       | 0            |
| 100 | Ls    | 1      | 0        | 0        | 0       | 0            |
| 100 | Lt    | 4      | 0        | 0        | 1       | 0            |
| 100 | Lu    | 1      | 0        | 0        | 0       | 0            |
| 100 | Lw    | 2      | 0        | 0        | 1       | 0            |
| 100 | Ly    | 2      | 0        | 0        | 2       | 0            |
| 100 | S1    | 393    | 0        | 0        | 33      | 0            |
| 100 | S2    | 3      | 0        | 0        | 0       | 0            |
| 100 | S3    | 17     | 0        | 0        | 1       | 0            |
| 100 | S4    | 2      | 0        | 0        | 1       | 0            |
| 100 | S5    | 11     | 0        | 0        | 0       | 0            |
| 100 | SB    | 1      | 0        | 0        | 0       | 0            |
| 100 | SC    | 3      | 0        | 0        | 0       | 0            |
| 100 | SF    | 4      | 0        | 0        | 1       | 0            |
| 100 | SG    | 3      | 0        | 0        | 3       | 0            |
| 100 | SH    | 2      | 0        | 0        | 0       | 0            |
| 100 | SK    | 5      | 0        | 0        | 0       | 0            |
| 100 | SL    | 1      | 0        | 0        | 0       | 0            |
| 100 | SM    | 1      | 0        | 0        | 0       | 0            |
| 100 | SO    | 1      | 0        | 0        | 1       | 0            |
| 100 | SP    | 4      | 0        | 0        | 1       | 0            |
| 100 | SR    | 1      | 0        | 0        | 0       | 0            |
| 100 | SS    | 2      | 0        | 0        | 0       | 0            |
| 100 | SU    | 1      | 0        | 0        | 0       | 0            |
| 100 | SX    | 2      | 0        | 0        | 0       | 0            |
| 100 | SZ    | 2      | 0        | 0        | 0       | 0            |
| 100 | Sb    | 1      | 0        | 0        | 0       | 0            |
| 100 | Sh    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 223607 | 0        | 164251   | 4643    | 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 12.

All (4643) 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:S1:1456:A:OP1    | 6:SA:193:LYS:NZ    | 1.65                     | 1.27              |
| 10:SE:151:ASP:OD1  | 10:SE:152:PRO:HD2  | 1.50                     | 1.08              |
| 20:SO:100:ALA:H    | 20:SO:134:THR:HG22 | 1.36                     | 0.91              |
| 22:SQ:85:ILE:HG12  | 22:SQ:136:PHE:HE2  | 1.34                     | 0.91              |
| 56:LQ:352:LYS:O    | 56:LQ:356:GLU:HB2  | 1.70                     | 0.90              |
| 38:Sg:69:LYS:HD3   | 38:Sg:73:LYS:HE3   | 1.53                     | 0.89              |
| 4:S4:22:G:N7       | 4:S4:46:G:N2       | 2.21                     | 0.89              |
| 1:S1:128:G:C6      | 1:S1:193:U:C4      | 2.61                     | 0.88              |
| 10:SE:151:ASP:OD1  | 10:SE:152:PRO:CD   | 2.22                     | 0.88              |
| 4:S4:8:U:H3        | 4:S4:14:A:H62      | 1.21                     | 0.87              |
| 9:SD:71:ILE:CD1    | 10:SE:249:ILE:HD12 | 2.03                     | 0.87              |
| 74:Li:6:TYR:HE2    | 74:Li:18:LYS:HB3   | 1.37                     | 0.87              |
| 47:LH:2667:C:H5    | 55:LP:173:GLY:H    | 1.22                     | 0.87              |
| 47:LH:2932:C:N3    | 48:LI:3004:G:N1    | 2.21                     | 0.87              |
| 1:S1:1161:G:N2     | 1:S1:1241:C:C2     | 2.42                     | 0.87              |
| 45:LF:1673:A:H4'   | 45:LF:1674:A:H5''  | 1.56                     | 0.86              |
| 4:S4:76:A:H8       | 48:LI:3339:C:H42   | 1.23                     | 0.86              |
| 39:Sh:278:LEU:HD22 | 39:Sh:288:PRO:HD2  | 1.57                     | 0.86              |
| 4:S4:54:U:O2'      | 4:S4:58:A:N7       | 2.09                     | 0.86              |
| 1:S1:369:U:O4      | 1:S1:370:G:O6      | 1.94                     | 0.85              |
| 1:S1:154:C:N4      | 1:S1:193:U:O4      | 2.08                     | 0.85              |
| 1:S1:1108:U:H5''   | 1:S1:1109:G:H5'    | 1.57                     | 0.85              |
| 1:S1:128:G:N1      | 1:S1:193:U:C4      | 2.44                     | 0.85              |
| 1:S1:1310:A:N3     | 47:LH:2694:G:N1    | 2.23                     | 0.84              |
| 1:S1:984:U:H1'     | 38:Sg:63:MET:HG2   | 1.59                     | 0.84              |
| 38:Sg:70:LYS:HG3   | 38:Sg:71:VAL:HG23  | 1.60                     | 0.84              |
| 47:LH:2354:A:H61   | 47:LH:2827:C:H42   | 1.25                     | 0.84              |
| 1:S1:579:G:H22     | 1:S1:614:G:H1      | 1.27                     | 0.83              |
| 3:S3:2:C:N3        | 3:S3:71:G:N1       | 2.26                     | 0.83              |
| 47:LH:2932:C:O2    | 48:LI:3004:G:N2    | 2.11                     | 0.83              |
| 42:LC:372:U:H3     | 42:LC:437:G:H1     | 1.25                     | 0.83              |
| 40:LA:65:C:O2'     | 40:LA:95:A:N6      | 2.11                     | 0.82              |
| 1:S1:133:C:O2      | 1:S1:145:G:N2      | 2.10                     | 0.82              |
| 45:LF:1571:C:H4'   | 45:LF:1572:A:H5'   | 1.61                     | 0.82              |
| 45:LF:1895:G:N3    | 47:LH:2315:U:O2'   | 2.11                     | 0.82              |
| 13:SH:61:SER:HB2   | 13:SH:141:THR:HG21 | 1.60                     | 0.82              |
| 63:LX:29:ARG:HE    | 67:Lb:197:LEU:HD21 | 1.44                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:618:G:N7      | 9:SD:171:ARG:NH1   | 2.27                     | 0.81              |
| 94:L3:10:MET:HE1   | 94:L3:18:ARG:HD3   | 1.61                     | 0.81              |
| 62:LW:7:ARG:NH1    | 100:LW:301:HOH:O   | 2.13                     | 0.81              |
| 9:SD:71:ILE:HD11   | 10:SE:249:ILE:HG13 | 1.64                     | 0.80              |
| 38:Sg:74:SER:HB2   | 38:Sg:83:LEU:HD22  | 1.62                     | 0.80              |
| 79:Ln:5:LEU:O      | 79:Ln:28:ASN:ND2   | 2.14                     | 0.80              |
| 45:LF:1843:U:OP1   | 85:Lt:70:ARG:NH2   | 2.15                     | 0.80              |
| 7:SB:165:ASN:HA    | 7:SB:171:ILE:HD11  | 1.64                     | 0.80              |
| 42:LC:354:U:O2     | 42:LC:454:G:O6     | 2.00                     | 0.79              |
| 1:S1:1161:G:N2     | 1:S1:1241:C:O2     | 2.16                     | 0.79              |
| 27:SV:41:VAL:HG21  | 27:SV:47:ARG:HB2   | 1.63                     | 0.79              |
| 35:Sd:36:ARG:HH22  | 35:Sd:74:ARG:HH21  | 1.30                     | 0.79              |
| 4:S4:12:U:O2       | 4:S4:23:A:N6       | 2.15                     | 0.79              |
| 10:SE:45:ILE:HB    | 10:SE:80:ILE:HG12  | 1.65                     | 0.79              |
| 10:SE:229:GLY:HA2  | 10:SE:236:LEU:HD23 | 1.64                     | 0.79              |
| 27:SV:28:PHE:HA    | 27:SV:55:THR:HG21  | 1.64                     | 0.78              |
| 42:LC:409:G:OP1    | 77:Ll:15:ARG:NH2   | 2.16                     | 0.78              |
| 87:Lv:11:PRO:HG2   | 87:Lv:34:LYS:HG3   | 1.66                     | 0.78              |
| 1:S1:2159:U:HO2'   | 47:LH:2780:A:HO2'  | 1.28                     | 0.78              |
| 41:LB:286:A:N6     | 61:LV:165:GLY:O    | 2.16                     | 0.78              |
| 45:LF:1519:G:N2    | 47:LH:2867:U:O2    | 2.16                     | 0.78              |
| 38:Sg:134:ARG:NH1  | 38:Sg:177:LYS:O    | 2.17                     | 0.78              |
| 47:LH:2231:A:H2'   | 47:LH:2232:G:C8    | 2.18                     | 0.78              |
| 4:S4:33:U:OP1      | 13:SH:122:ARG:NH2  | 2.16                     | 0.78              |
| 1:S1:1756:U:OP2    | 18:SM:23:ARG:NH1   | 2.16                     | 0.78              |
| 42:LC:426:C:H4'    | 42:LC:431:C:H42    | 1.48                     | 0.78              |
| 6:SA:137:VAL:HG12  | 6:SA:210:VAL:HG12  | 1.66                     | 0.78              |
| 1:S1:1935:C:O2'    | 24:SS:7:TRP:O      | 2.02                     | 0.77              |
| 54:LO:28:C:OP1     | 58:LS:147:ARG:NH1  | 2.18                     | 0.77              |
| 42:LC:489:A:OP2    | 96:L4:41:ARG:NH1   | 2.18                     | 0.77              |
| 1:S1:941:C:H41     | 38:Sg:169:LYS:HD2  | 1.48                     | 0.77              |
| 44:LE:971:G:OP1    | 63:LX:45:ARG:NH2   | 2.17                     | 0.77              |
| 69:Ld:88:VAL:HG11  | 97:L6:14:CYS:HB3   | 1.67                     | 0.77              |
| 1:S1:1282:A:OP1    | 6:SA:214:LYS:NZ    | 2.17                     | 0.77              |
| 57:LR:224:ASN:HD21 | 57:LR:230:ASN:H    | 1.32                     | 0.77              |
| 44:LE:886:A:N7     | 60:LU:103:ARG:NH2  | 2.31                     | 0.77              |
| 44:LE:1239:U:OP2   | 66:La:33:ARG:NH1   | 2.14                     | 0.77              |
| 3:S3:26:A:H61      | 3:S3:44:G:H1       | 1.32                     | 0.76              |
| 4:S4:9:A:H2'       | 4:S4:11:C:H41      | 1.48                     | 0.76              |
| 1:S1:641:OMG:C4    | 9:SD:171:ARG:HD3   | 2.20                     | 0.76              |
| 51:LL:3826:G:H21   | 65:LZ:160:PRO:HG3  | 1.50                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:LH:2354:A:H61   | 47:LH:2827:C:N4    | 1.82                     | 0.76              |
| 90:Ly:21:ARG:NH2   | 90:Ly:44:MET:SD    | 2.59                     | 0.76              |
| 1:S1:1007:G:OP1    | 12:SG:238:ARG:NH2  | 2.19                     | 0.76              |
| 12:SG:242:GLU:HA   | 12:SG:245:VAL:HG22 | 1.67                     | 0.76              |
| 1:S1:128:G:O6      | 1:S1:193:U:O4      | 2.04                     | 0.76              |
| 1:S1:293:G:H5'     | 38:Sg:167:PRO:HG2  | 1.67                     | 0.76              |
| 44:LE:1258:C:OP1   | 100:LE:1502:HOH:O  | 2.03                     | 0.76              |
| 47:LH:2605:OMU:H3' | 47:LH:2606:G:H21   | 1.51                     | 0.75              |
| 56:LQ:80:GLU:OE1   | 56:LQ:318:TYR:OH   | 2.04                     | 0.75              |
| 4:S4:36:A:N6       | 100:S4:101:HOH:O   | 2.20                     | 0.75              |
| 9:SD:71:ILE:HD11   | 10:SE:249:ILE:CG1  | 2.17                     | 0.75              |
| 44:LE:930:G:O6     | 100:LE:1501:HOH:O  | 2.03                     | 0.75              |
| 74:Li:6:TYR:CE2    | 74:Li:18:LYS:HB3   | 2.22                     | 0.75              |
| 44:LE:1120:U:H2'   | 44:LE:1121:A2M:H8  | 1.69                     | 0.75              |
| 48:LI:3578:C:O2    | 74:Li:71:ARG:NH2   | 2.17                     | 0.75              |
| 20:SO:133:VAL:O    | 20:SO:133:VAL:HG12 | 1.87                     | 0.75              |
| 60:LU:50:ASN:ND2   | 60:LU:178:LEU:O    | 2.20                     | 0.75              |
| 1:S1:1158:U:O4     | 1:S1:1244:C:N3     | 2.20                     | 0.75              |
| 48:LI:3091:C:N4    | 84:Ls:60:GLU:OE2   | 2.20                     | 0.75              |
| 48:LI:3482:C:O2'   | 93:L2:98:TYR:O     | 2.03                     | 0.75              |
| 1:S1:1241:C:O2     | 1:S1:1242:A:N6     | 2.16                     | 0.75              |
| 3:S3:2:C:O2        | 3:S3:71:G:N2       | 2.14                     | 0.75              |
| 44:LE:885:C:OP2    | 60:LU:103:ARG:NH1  | 2.20                     | 0.75              |
| 48:LI:3303:G:N7    | 73:Lh:87:LYS:NZ    | 2.32                     | 0.75              |
| 100:LE:1501:HOH:O  | 48:LI:3403:A:OP1   | 2.05                     | 0.74              |
| 91:Lz:49:ASP:HB3   | 91:Lz:52:LYS:HB2   | 1.69                     | 0.74              |
| 8:SC:108:ARG:HG3   | 8:SC:177:VAL:HG22  | 1.70                     | 0.74              |
| 2:S2:75:C:H42      | 48:LI:3509:OMG:HN1 | 1.34                     | 0.74              |
| 26:SU:129:VAL:HG12 | 26:SU:146:GLN:HB2  | 1.69                     | 0.74              |
| 41:LB:207:C:H5''   | 63:LX:16:LYS:HB3   | 1.70                     | 0.74              |
| 83:Lr:108:ARG:NH2  | 83:Lr:202:LEU:O    | 2.21                     | 0.74              |
| 1:S1:1357:U:OP2    | 25:ST:55:ARG:NH1   | 2.21                     | 0.74              |
| 4:S4:5:G:H2'       | 4:S4:6:G:C8        | 2.23                     | 0.74              |
| 44:LE:1251:A:OP1   | 82:Lq:18:ARG:NH2   | 2.19                     | 0.74              |
| 68:Lc:73:ASN:OD1   | 68:Lc:85:TYR:OH    | 2.06                     | 0.74              |
| 1:S1:1100:A:H4'    | 1:S1:1150:C:H42    | 1.52                     | 0.74              |
| 6:SA:101:MET:HG3   | 6:SA:213:VAL:HB    | 1.70                     | 0.74              |
| 61:LV:217:LYS:O    | 61:LV:221:ASN:ND2  | 2.20                     | 0.74              |
| 91:Lz:37:ARG:NH1   | 91:Lz:38:THR:O     | 2.20                     | 0.74              |
| 47:LH:2673:G:O2'   | 47:LH:2802:PSU:OP2 | 2.06                     | 0.73              |
| 38:Sg:60:PHE:CE1   | 38:Sg:109:VAL:HG11 | 2.23                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:LE:1171:PSU:N3  | 44:LE:1188:G:O6    | 2.16                     | 0.73              |
| 61:LV:140:PHE:HA   | 61:LV:143:ARG:HE   | 1.53                     | 0.73              |
| 1:S1:269:U:O2      | 1:S1:349:G:N2      | 2.21                     | 0.73              |
| 1:S1:2295:G:OP2    | 20:SO:147:ARG:NH2  | 2.20                     | 0.73              |
| 41:LB:285:G:O2'    | 41:LB:288:A:N1     | 2.22                     | 0.73              |
| 15:SJ:26:LEU:HD11  | 15:SJ:60:LYS:HD3   | 1.71                     | 0.73              |
| 31:SZ:7:PRO:O      | 31:SZ:36:ARG:NH2   | 2.21                     | 0.73              |
| 73:Lh:117:ARG:HH12 | 98:L7:36:ARG:HG2   | 1.53                     | 0.73              |
| 78:Lm:60:ARG:HD3   | 78:Lm:65:LYS:HB2   | 1.70                     | 0.73              |
| 87:Lv:79:ILE:HD11  | 87:Lv:108:ILE:HD13 | 1.69                     | 0.73              |
| 1:S1:2137:C:N4     | 100:S1:2427:HOH:O  | 2.21                     | 0.73              |
| 22:SQ:65:THR:HG22  | 22:SQ:66:GLU:H     | 1.53                     | 0.73              |
| 47:LH:2934:U:O2    | 48:LI:3001:A:N6    | 2.19                     | 0.73              |
| 85:Lt:84:MET:HE3   | 85:Lt:117:ARG:HB2  | 1.70                     | 0.73              |
| 92:L1:34:LYS:HG3   | 92:L1:35:GLN:H     | 1.54                     | 0.73              |
| 1:S1:623:C:O2'     | 1:S1:625:A:N7      | 2.21                     | 0.73              |
| 9:SD:71:ILE:HD11   | 10:SE:249:ILE:CD1  | 2.19                     | 0.72              |
| 49:LJ:3682:C:O2'   | 49:LJ:3684:A:OP2   | 2.07                     | 0.72              |
| 63:LX:86:GLU:OE2   | 63:LX:111:ASN:ND2  | 2.21                     | 0.72              |
| 34:Sc:42:CYS:SG    | 34:Sc:43:TRP:N     | 2.62                     | 0.72              |
| 44:LE:961:C:H41    | 70:Le:54:ARG:NH1   | 1.86                     | 0.72              |
| 44:LE:1162:G:OP2   | 100:LE:1503:HOH:O  | 2.07                     | 0.72              |
| 52:LM:3932:U:O2'   | 52:LM:3935:A:N3    | 2.22                     | 0.72              |
| 68:Lc:3:ARG:NH1    | 68:Lc:63:GLU:OE2   | 2.21                     | 0.72              |
| 13:SH:78:HIS:HD2   | 13:SH:155:PHE:HD2  | 1.34                     | 0.72              |
| 78:Lm:7:LEU:HD11   | 78:Lm:30:ARG:HH11  | 1.53                     | 0.72              |
| 1:S1:21:C:O2       | 9:SD:16:ARG:NH2    | 2.23                     | 0.72              |
| 9:SD:71:ILE:CD1    | 10:SE:249:ILE:CD1  | 2.66                     | 0.72              |
| 20:SO:99:ARG:NH2   | 20:SO:133:VAL:HG12 | 2.03                     | 0.72              |
| 1:S1:1874:U:OP1    | 27:SV:59:LYS:NZ    | 2.22                     | 0.72              |
| 35:Sd:34:GLN:NE2   | 35:Sd:52:ASN:OD1   | 2.22                     | 0.72              |
| 47:LH:2407:G:OP1   | 71:Lf:105:ARG:NH1  | 2.23                     | 0.72              |
| 47:LH:2644:U:H3    | 47:LH:2668:G:H1    | 1.37                     | 0.72              |
| 7:SB:108:LEU:HB2   | 7:SB:136:GLU:HB3   | 1.70                     | 0.72              |
| 42:LC:331:G:H5''   | 67:Lb:55:ARG:HG3   | 1.72                     | 0.72              |
| 44:LE:1237:G:N2    | 44:LE:1261:C:OP1   | 2.23                     | 0.72              |
| 64:LY:82:VAL:HB    | 64:LY:121:VAL:HG23 | 1.71                     | 0.72              |
| 1:S1:74:G:OP2      | 1:S1:74:G:N2       | 2.23                     | 0.71              |
| 40:LA:64:U:O2'     | 81:Lp:10:ARG:NH2   | 2.23                     | 0.71              |
| 56:LQ:271:GLN:NE2  | 56:LQ:273:GLY:O    | 2.23                     | 0.71              |
| 1:S1:773:U:H3      | 1:S1:829:G:H21     | 1.38                     | 0.71              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:S3:75:C:OP1       | 100:S3:101:HOH:O   | 2.09                     | 0.71              |
| 100:LE:1502:HOH:O   | 48:LI:3384:C:OP1   | 2.07                     | 0.71              |
| 56:LQ:160:VAL:HG11  | 56:LQ:193:LYS:HB3  | 1.70                     | 0.71              |
| 22:SQ:85:ILE:HG12   | 22:SQ:136:PHE:CE2  | 2.23                     | 0.71              |
| 23:SR:61:SER:OG     | 23:SR:64:GLU:OE1   | 2.06                     | 0.71              |
| 40:LA:57:G:OP1      | 40:LA:104:G:N2     | 2.23                     | 0.71              |
| 40:LA:86:G:OP2      | 81:Lp:5:LYS:NZ     | 2.23                     | 0.71              |
| 1:S1:1504:G:H21     | 15:SJ:20:ARG:HH22  | 1.38                     | 0.71              |
| 10:SE:54:TYR:OH     | 10:SE:97:ASP:OD2   | 2.06                     | 0.71              |
| 21:SP:87:LYS:HG2    | 21:SP:131:MET:HE1  | 1.72                     | 0.71              |
| 1:S1:458:C:OP2      | 100:S1:2401:HOH:O  | 2.09                     | 0.71              |
| 1:S1:533:A2M:O5'    | 1:S1:533:A2M:H8    | 1.91                     | 0.71              |
| 41:LB:224:G:OP1     | 67:Lb:185:ARG:NH1  | 2.23                     | 0.71              |
| 45:LF:1557:U:OP1    | 45:LF:1582:PSU:O2' | 2.07                     | 0.71              |
| 56:LQ:10:ARG:NH2    | 56:LQ:265:THR:O    | 2.23                     | 0.71              |
| 23:SR:16:VAL:HG12   | 23:SR:17:LEU:HD23  | 1.71                     | 0.71              |
| 84:Ls:27:CYS:HB3    | 84:Ls:32:SER:HB3   | 1.73                     | 0.71              |
| 16:SK:59:ALA:HB2    | 16:SK:278:GLY:HA2  | 1.72                     | 0.71              |
| 26:SU:63:CYS:O      | 26:SU:67:SER:OG    | 2.07                     | 0.71              |
| 57:LR:222:ASP:OD2   | 57:LR:242:ARG:NH2  | 2.18                     | 0.71              |
| 1:S1:109:C:O2       | 26:SU:74:ARG:NH2   | 2.24                     | 0.71              |
| 13:SH:78:HIS:CD2    | 13:SH:155:PHE:HD2  | 2.08                     | 0.70              |
| 15:SJ:54:ASP:OD1    | 15:SJ:59:ASN:ND2   | 2.23                     | 0.70              |
| 39:Sh:199:LEU:HA    | 39:Sh:215:GLY:HA3  | 1.73                     | 0.70              |
| 47:LH:2919:U:H2'    | 47:LH:2920:A2M:H8  | 1.72                     | 0.70              |
| 66:La:79:THR:HG22   | 66:La:115:LYS:HB3  | 1.72                     | 0.70              |
| 1:S1:154:C:C4       | 1:S1:193:U:O4      | 2.44                     | 0.70              |
| 45:LF:1856:OMG:HM22 | 74:Li:98:LYS:HG2   | 1.71                     | 0.70              |
| 68:Lc:38:MET:HB3    | 68:Lc:41:LEU:HD13  | 1.73                     | 0.70              |
| 20:SO:132:ASP:HB2   | 33:Sb:44:MET:HE1   | 1.72                     | 0.70              |
| 83:Lr:150:TYR:OH    | 83:Lr:182:GLU:OE2  | 2.09                     | 0.70              |
| 90:Ly:21:ARG:HD2    | 90:Ly:39:TYR:HD1   | 1.56                     | 0.70              |
| 48:LI:3413:U:O2'    | 48:LI:3415:U:O4    | 2.08                     | 0.70              |
| 57:LR:210:GLU:OE1   | 57:LR:213:ARG:NH1  | 2.24                     | 0.70              |
| 72:Lg:94:SER:O      | 72:Lg:139:ARG:NH2  | 2.25                     | 0.70              |
| 96:L4:9:LYS:HA      | 96:L4:21:GLN:O     | 1.92                     | 0.70              |
| 43:LD:735:C:O2'     | 72:Lg:69:GLU:O     | 2.10                     | 0.70              |
| 48:LI:3040:C:N3     | 48:LI:3081:U:O4    | 2.24                     | 0.70              |
| 1:S1:2179:C:OP2     | 16:SK:46:ARG:NH2   | 2.24                     | 0.70              |
| 1:S1:2190:G:H2'     | 1:S1:2191:G:C8     | 2.27                     | 0.70              |
| 45:LF:1697:G:O2'    | 45:LF:1701:C:N3    | 2.22                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:LH:2678:U:OP1   | 95:L5:21:ASN:ND2   | 2.24                     | 0.70              |
| 23:SR:40:ARG:NH2   | 29:SX:39:VAL:O     | 2.24                     | 0.70              |
| 25:ST:129:TYR:HB3  | 25:ST:135:LEU:HD13 | 1.74                     | 0.70              |
| 45:LF:1815:A2M:OP1 | 100:LF:2001:HOH:O  | 2.09                     | 0.70              |
| 1:S1:429:U:P       | 16:SK:58:ARG:HH22  | 2.13                     | 0.70              |
| 47:LH:2244:A:H4'   | 95:L5:52:VAL:HG21  | 1.72                     | 0.70              |
| 48:LI:3460:G:O6    | 100:LI:3601:HOH:O  | 2.09                     | 0.70              |
| 90:Ly:27:TRP:HA    | 90:Ly:34:CYS:HA    | 1.73                     | 0.70              |
| 13:SH:140:ILE:HG23 | 13:SH:162:GLU:OE1  | 1.92                     | 0.70              |
| 23:SR:15:ARG:NH1   | 23:SR:20:ASN:OD1   | 2.25                     | 0.70              |
| 48:LI:3506:A:OP1   | 100:LI:3602:HOH:O  | 2.10                     | 0.70              |
| 22:SQ:34:ARG:HD3   | 22:SQ:98:GLY:H     | 1.56                     | 0.70              |
| 1:S1:1713:U:OP2    | 100:S1:2403:HOH:O  | 2.09                     | 0.69              |
| 1:S1:1962:A:OP2    | 29:SX:87:ARG:NH2   | 2.25                     | 0.69              |
| 47:LH:2328:G:OP2   | 100:LH:3001:HOH:O  | 2.08                     | 0.69              |
| 49:LJ:3735:C:H2'   | 62:LW:108:ARG:HH12 | 1.57                     | 0.69              |
| 65:LZ:174:ASP:O    | 65:LZ:177:ARG:NH2  | 2.25                     | 0.69              |
| 23:SR:116:LYS:HD3  | 23:SR:127:MET:HB3  | 1.74                     | 0.69              |
| 47:LH:2871:A:N7    | 62:LW:96:ARG:NH1   | 2.40                     | 0.69              |
| 48:LI:3137:U:H3    | 48:LI:3144:G:H1    | 1.40                     | 0.69              |
| 1:S1:958:A:H2'     | 1:S1:959:A:H8      | 1.57                     | 0.69              |
| 1:S1:617:U:H2'     | 1:S1:618:G:C8      | 2.27                     | 0.69              |
| 1:S1:2133:U:OP1    | 100:S1:2402:HOH:O  | 2.09                     | 0.69              |
| 17:SL:13:GLN:HE21  | 17:SL:32:LYS:HD2   | 1.58                     | 0.69              |
| 1:S1:745:G:H2'     | 1:S1:746:G:H8      | 1.57                     | 0.69              |
| 6:SA:185:LYS:O     | 6:SA:188:LEU:O     | 2.09                     | 0.69              |
| 29:SX:68:TYR:HE1   | 29:SX:131:GLN:HG3  | 1.57                     | 0.69              |
| 49:LJ:3728:A:H5'   | 56:LQ:346:LEU:HD23 | 1.74                     | 0.69              |
| 56:LQ:364:ASP:OD2  | 78:Lm:17:HIS:NE2   | 2.25                     | 0.69              |
| 1:S1:2038:U:OP2    | 32:Sa:48:ASN:ND2   | 2.25                     | 0.69              |
| 6:SA:224:ASN:ND2   | 61:LV:293:ALA:O    | 2.25                     | 0.69              |
| 44:LE:1203:C:H2'   | 44:LE:1204:A2M:H8  | 1.74                     | 0.69              |
| 12:SG:93:GLU:OE2   | 12:SG:95:ARG:NH2   | 2.26                     | 0.69              |
| 42:LC:598:U:O3'    | 77:Ll:86:ARG:NH2   | 2.24                     | 0.69              |
| 68:Lc:192:VAL:HA   | 68:Lc:197:THR:HG22 | 1.75                     | 0.69              |
| 1:S1:501:G:O2'     | 12:SG:93:GLU:OE1   | 2.11                     | 0.69              |
| 14:SI:160:ASP:OD2  | 14:SI:162:ARG:NH1  | 2.25                     | 0.69              |
| 42:LC:563:G:O6     | 92:L1:50:LYS:NZ    | 2.25                     | 0.69              |
| 44:LE:1174:G:OP1   | 100:LE:1504:HOH:O  | 2.09                     | 0.69              |
| 44:LE:1193:C:OP2   | 100:LE:1503:HOH:O  | 2.11                     | 0.69              |
| 47:LH:2357:G:O2'   | 47:LH:2822:U:O4    | 2.08                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:LW:82:ARG:HB3   | 62:LW:111:GLU:HG3  | 1.75                     | 0.69              |
| 1:S1:55:A:OP1      | 31:SZ:116:LYS:NZ   | 2.25                     | 0.69              |
| 1:S1:2049:G:H2'    | 1:S1:2050:A:H8     | 1.58                     | 0.69              |
| 41:LB:224:G:OP1    | 67:Lb:169:ARG:NH2  | 2.26                     | 0.69              |
| 47:LH:2629:U:OP2   | 100:LH:3003:HOH:O  | 2.10                     | 0.69              |
| 94:L3:10:MET:HE3   | 94:L3:15:ARG:HB3   | 1.75                     | 0.69              |
| 1:S1:1044:U:OP1    | 9:SD:78:ARG:NH1    | 2.26                     | 0.69              |
| 1:S1:1426:A:OP1    | 1:S1:2295:G:O2'    | 2.11                     | 0.69              |
| 6:SA:43:LYS:NZ     | 20:SO:21:GLN:O     | 2.26                     | 0.69              |
| 1:S1:1113:U:O2     | 1:S1:1134:G:O6     | 2.10                     | 0.68              |
| 1:S1:1656:C:O2     | 37:Sf:91:LYS:NZ    | 2.25                     | 0.68              |
| 29:SX:32:GLU:O     | 29:SX:109:GLN:NE2  | 2.26                     | 0.68              |
| 39:Sh:42:LEU:HD21  | 39:Sh:70:VAL:HG11  | 1.75                     | 0.68              |
| 48:LI:3457:G:OP2   | 100:LI:3603:HOH:O  | 2.10                     | 0.68              |
| 54:LO:34:C:O2      | 69:Ld:196:ARG:NH2  | 2.26                     | 0.68              |
| 54:LO:91:C:OP1     | 68:Lc:57:ARG:NH1   | 2.21                     | 0.68              |
| 56:LQ:58:ARG:NH1   | 56:LQ:356:GLU:OE2  | 2.26                     | 0.68              |
| 1:S1:128:G:C6      | 1:S1:193:U:O4      | 2.45                     | 0.68              |
| 45:LF:1809:G:H1'   | 80:Lo:31:SER:HB2   | 1.76                     | 0.68              |
| 63:LX:53:PHE:O     | 63:LX:156:GLN:NE2  | 2.26                     | 0.68              |
| 1:S1:85:U:H2'      | 1:S1:86:C:C6       | 2.29                     | 0.68              |
| 47:LH:2290:U:O4    | 100:LH:3002:HOH:O  | 2.10                     | 0.68              |
| 47:LH:2290:U:OP2   | 92:L1:10:LYS:NZ    | 2.25                     | 0.68              |
| 47:LH:2629:U:HO2'  | 48:LI:3563:G:HO2'  | 1.39                     | 0.68              |
| 56:LQ:7:GLU:OE2    | 100:LQ:501:HOH:O   | 2.12                     | 0.68              |
| 7:SB:141:ASN:ND2   | 30:SY:31:SER:O     | 2.24                     | 0.68              |
| 12:SG:59:GLN:OE1   | 12:SG:72:ARG:NH2   | 2.27                     | 0.68              |
| 45:LF:1720:C:O2'   | 70:Le:9:TYR:O      | 2.12                     | 0.68              |
| 57:LR:187:LYS:HG3  | 57:LR:190:ARG:HE   | 1.58                     | 0.68              |
| 63:LX:130:LYS:HB3  | 81:Lp:121:VAL:HG13 | 1.76                     | 0.68              |
| 1:S1:68:A:N6       | 12:SG:165:PRO:O    | 2.18                     | 0.68              |
| 1:S1:369:U:C4      | 1:S1:370:G:O6      | 2.46                     | 0.68              |
| 45:LF:1939:A:OP2   | 100:LH:3002:HOH:O  | 2.11                     | 0.68              |
| 63:LX:131:LEU:HD11 | 81:Lp:119:TYR:HB2  | 1.74                     | 0.68              |
| 4:S4:35:A:H2'      | 4:S4:36:A:H4'      | 1.75                     | 0.68              |
| 11:SF:82:MET:HG2   | 11:SF:187:LYS:HD2  | 1.76                     | 0.68              |
| 27:SV:99:GLY:HA3   | 27:SV:122:LYS:HE3  | 1.75                     | 0.68              |
| 40:LA:109:G:H4'    | 90:Ly:21:ARG:HG2   | 1.73                     | 0.68              |
| 45:LF:1893:U:OP2   | 100:LH:3001:HOH:O  | 2.11                     | 0.68              |
| 40:LA:31:U:H5''    | 40:LA:32:C:H5'     | 1.75                     | 0.68              |
| 45:LF:1712:U:H5''  | 83:Lr:206:LYS:HB3  | 1.75                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:LI:3434:OMG:OP1 | 93:L2:98:TYR:OH    | 2.12                     | 0.68              |
| 1:S1:964:G:H5'     | 38:Sg:129:ARG:HH22 | 1.58                     | 0.68              |
| 10:SE:69:TYR:CE1   | 31:SZ:21:LEU:HD22  | 2.28                     | 0.68              |
| 47:LH:2937:G:N1    | 48:LI:2997:C:O2    | 2.25                     | 0.68              |
| 1:S1:1453:A:O2'    | 1:S1:1464:A:N1     | 2.27                     | 0.68              |
| 17:SL:58:GLU:OE1   | 17:SL:90:ARG:NH2   | 2.26                     | 0.68              |
| 33:Sb:94:LYS:O     | 33:Sb:96:ARG:NH1   | 2.26                     | 0.68              |
| 50:LK:3757:G:OP2   | 62:LW:172:ARG:NH1  | 2.27                     | 0.68              |
| 44:LE:960:G:OP1    | 57:LR:27:ARG:NH1   | 2.27                     | 0.67              |
| 46:LG:2008:G:OP1   | 88:Lw:40:LYS:NZ    | 2.20                     | 0.67              |
| 47:LH:2354:A:N6    | 47:LH:2827:C:H42   | 1.92                     | 0.67              |
| 48:LI:3038:G:H3'   | 48:LI:3039:C:H3'   | 1.76                     | 0.67              |
| 1:S1:1743:A:H2'    | 1:S1:1744:OMU:H6   | 1.76                     | 0.67              |
| 3:S3:48:C:H5'      | 3:S3:49:C:H5'      | 1.75                     | 0.67              |
| 44:LE:1103:C:OP1   | 57:LR:94:ARG:NH2   | 2.19                     | 0.67              |
| 45:LF:1562:C:N4    | 48:LI:3497:A:OP1   | 2.27                     | 0.67              |
| 1:S1:1161:G:N1     | 1:S1:1241:C:N3     | 2.41                     | 0.67              |
| 56:LQ:57:VAL:HB    | 56:LQ:362:PHE:HB3  | 1.75                     | 0.67              |
| 81:Lp:87:LYS:HB3   | 81:Lp:91:GLU:HG3   | 1.75                     | 0.67              |
| 84:Ls:14:ASN:ND2   | 84:Ls:73:TYR:OH    | 2.28                     | 0.67              |
| 7:SB:109:THR:O     | 11:SF:62:LYS:NZ    | 2.27                     | 0.67              |
| 40:LA:49:A:OP2     | 92:L1:21:ARG:NH1   | 2.28                     | 0.67              |
| 42:LC:534:A:N6     | 63:LX:25:LYS:O     | 2.25                     | 0.67              |
| 45:LF:1495:G:OP1   | 68:Lc:98:ARG:NH2   | 2.26                     | 0.67              |
| 56:LQ:218:ASP:OD2  | 56:LQ:343:ARG:NH2  | 2.27                     | 0.67              |
| 57:LR:165:LEU:HD23 | 57:LR:168:ILE:HD11 | 1.75                     | 0.67              |
| 64:LY:116:GLY:HA2  | 64:LY:135:ASN:HB3  | 1.75                     | 0.67              |
| 29:SX:56:TYR:OH    | 29:SX:109:GLN:OE1  | 2.09                     | 0.67              |
| 48:LI:3041:A:N6    | 48:LI:3079:C:OP2   | 2.27                     | 0.67              |
| 60:LU:97:LEU:HD11  | 60:LU:100:LYS:HG2  | 1.75                     | 0.67              |
| 30:SY:16:LYS:HG2   | 30:SY:23:LEU:HD23  | 1.77                     | 0.67              |
| 66:La:84:ARG:HB3   | 66:La:87:ARG:HE    | 1.59                     | 0.67              |
| 84:Ls:9:GLN:O      | 84:Ls:11:GLN:NE2   | 2.27                     | 0.67              |
| 41:LB:245:A:H5'    | 41:LB:247:OMU:H1'  | 1.76                     | 0.67              |
| 48:LI:3229:A:OP2   | 100:LI:3604:HOH:O  | 2.11                     | 0.67              |
| 68:Lc:19:LYS:HG3   | 68:Lc:26:VAL:HG11  | 1.76                     | 0.67              |
| 79:Ln:9:ARG:NH1    | 79:Ln:83:THR:O     | 2.28                     | 0.67              |
| 1:S1:977:A:H62     | 38:Sg:220:ARG:HH12 | 1.43                     | 0.67              |
| 41:LB:199:A:N7     | 100:LB:301:HOH:O   | 2.28                     | 0.67              |
| 43:LD:700:G:O2'    | 72:Lg:151:LYS:NZ   | 2.22                     | 0.67              |
| 44:LE:1190:A:N3    | 47:LH:2812:A2M:H2  | 2.09                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:LE:1301:C:O2'   | 82:Lq:26:ARG:NH1   | 2.28                     | 0.67              |
| 65:LZ:13:ARG:NH2   | 65:LZ:62:THR:O     | 2.26                     | 0.67              |
| 83:Lr:216:SER:N    | 83:Lr:226:ASP:OD2  | 2.27                     | 0.67              |
| 27:SV:37:GLU:OE1   | 39:Sh:154:TRP:NE1  | 2.23                     | 0.67              |
| 64:LY:13:LYS:NZ    | 64:LY:56:CYS:SG    | 2.68                     | 0.67              |
| 10:SE:22:LYS:HG3   | 10:SE:23:LEU:HD12  | 1.76                     | 0.66              |
| 16:SK:296:LYS:NZ   | 26:SU:8:ASP:O      | 2.26                     | 0.66              |
| 45:LF:1767:C:OP2   | 57:LR:184:ARG:NH1  | 2.26                     | 0.66              |
| 52:LM:3944:G:H4'   | 56:LQ:312:LEU:HB3  | 1.75                     | 0.66              |
| 54:LO:83:G:OP1     | 100:LO:201:HOH:O   | 2.13                     | 0.66              |
| 74:Li:49:TYR:HD1   | 74:Li:58:ARG:HD2   | 1.59                     | 0.66              |
| 77:LI:57:VAL:HA    | 77:LI:103:VAL:HG12 | 1.77                     | 0.66              |
| 1:S1:625:A:O2'     | 31:SZ:38:THR:O     | 2.14                     | 0.66              |
| 7:SB:134:ILE:HG23  | 7:SB:156:TYR:HB2   | 1.78                     | 0.66              |
| 46:LG:2062:G:N7    | 79:Ln:17:ARG:NH1   | 2.44                     | 0.66              |
| 47:LH:2904:B8H:OP1 | 100:LH:3005:HOH:O  | 2.13                     | 0.66              |
| 77:LI:86:ARG:HB2   | 77:LI:96:ILE:HD11  | 1.76                     | 0.66              |
| 92:L1:21:ARG:NH2   | 92:L1:22:PRO:O     | 2.27                     | 0.66              |
| 1:S1:827:C:H2'     | 1:S1:828:G:H8      | 1.59                     | 0.66              |
| 1:S1:1574:G:O2'    | 1:S1:2115:U:O2     | 2.13                     | 0.66              |
| 55:LP:81:GLY:HA2   | 95:L5:64:MET:HE3   | 1.78                     | 0.66              |
| 1:S1:1136:C:H2'    | 1:S1:1137:C:H6     | 1.59                     | 0.66              |
| 16:SK:89:ASN:HD21  | 16:SK:92:LEU:HG    | 1.59                     | 0.66              |
| 44:LE:961:C:H41    | 70:Le:54:ARG:HH12  | 1.42                     | 0.66              |
| 1:S1:188:C:OP2     | 100:S1:2404:HOH:O  | 2.13                     | 0.66              |
| 4:S4:75:A:O2'      | 96:L4:56:PRO:O     | 2.14                     | 0.66              |
| 9:SD:86:LEU:HD11   | 9:SD:99:LEU:HD21   | 1.77                     | 0.66              |
| 26:SU:62:LYS:HA    | 26:SU:69:VAL:HG21  | 1.76                     | 0.66              |
| 44:LE:1454:A:H2'   | 44:LE:1455:G:C8    | 2.30                     | 0.66              |
| 47:LH:2932:C:C2    | 48:LI:3004:G:N2    | 2.63                     | 0.66              |
| 48:LI:2979:G:H5''  | 48:LI:2984:G:H22   | 1.61                     | 0.66              |
| 1:S1:1645:C:O2     | 37:Sf:139:ARG:NH1  | 2.28                     | 0.66              |
| 15:SJ:80:ASP:OD1   | 15:SJ:124:LYS:NZ   | 2.23                     | 0.66              |
| 100:LE:1502:HOH:O  | 48:LI:3385:A:OP1   | 2.13                     | 0.66              |
| 47:LH:2289:G:O2'   | 92:L1:3:ALA:O      | 2.13                     | 0.66              |
| 47:LH:2709:G:N7    | 89:Lx:68:LYS:NZ    | 2.38                     | 0.66              |
| 48:LI:3015:C:OP2   | 48:LI:3157:U:N3    | 2.27                     | 0.66              |
| 48:LI:3235:U:H2'   | 48:LI:3236:G:C8    | 2.31                     | 0.66              |
| 9:SD:84:GLY:H      | 9:SD:107:ARG:HD2   | 1.61                     | 0.66              |
| 39:Sh:66:HIS:NE2   | 39:Sh:84:SER:OG    | 2.24                     | 0.66              |
| 42:LC:494:A:H5''   | 67:Lb:97:ASN:HB3   | 1.78                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:Lc:201:ARG:HD2  | 68:Lc:203:ARG:HH11 | 1.61                     | 0.66              |
| 1:S1:586:C:H2'     | 1:S1:587:G:H8      | 1.60                     | 0.66              |
| 1:S1:2108:A:OP1    | 18:SM:81:ARG:NH2   | 2.28                     | 0.66              |
| 45:LF:1536:U:O2'   | 83:Lr:209:ALA:O    | 2.13                     | 0.66              |
| 47:LH:2880:C:O2'   | 56:LQ:268:ARG:NH2  | 2.29                     | 0.66              |
| 16:SK:3:ILE:O      | 16:SK:30:GLY:N     | 2.27                     | 0.66              |
| 26:SU:36:ARG:NH2   | 26:SU:55:LEU:O     | 2.28                     | 0.66              |
| 39:Sh:278:LEU:HD12 | 39:Sh:278:LEU:O    | 1.95                     | 0.66              |
| 44:LE:1105:A:OP2   | 100:LE:1505:HOH:O  | 2.13                     | 0.66              |
| 47:LH:2707:A:H2'   | 47:LH:2708:A2M:H8  | 1.79                     | 0.66              |
| 47:LH:2900:G:OP1   | 100:LH:3004:HOH:O  | 2.12                     | 0.66              |
| 59:LT:95:ALA:HB2   | 93:L2:80:LEU:HD22  | 1.79                     | 0.66              |
| 67:Lb:152:CYS:HB2  | 81:Lp:95:LEU:HD12  | 1.77                     | 0.66              |
| 81:Lp:4:VAL:HG21   | 81:Lp:24:LEU:HD11  | 1.78                     | 0.66              |
| 1:S1:2267:U:OP2    | 5:S5:5:A:O2'       | 2.13                     | 0.65              |
| 4:S4:19:G:N3       | 4:S4:57:G:N2       | 2.44                     | 0.65              |
| 42:LC:303:C:OP1    | 81:Lp:101:ARG:NH2  | 2.29                     | 0.65              |
| 43:LD:745:U:H4'    | 43:LD:746:G:H5'    | 1.78                     | 0.65              |
| 44:LE:1234:G:OP1   | 100:LE:1505:HOH:O  | 2.14                     | 0.65              |
| 57:LR:215:PHE:HB2  | 57:LR:223:ILE:HD11 | 1.76                     | 0.65              |
| 3:S3:2:C:H2'       | 3:S3:3:G:C8        | 2.31                     | 0.65              |
| 30:SY:40:ASP:HB3   | 30:SY:46:ILE:HD11  | 1.77                     | 0.65              |
| 44:LE:810:G:H5''   | 68:Lc:208:ARG:HH12 | 1.61                     | 0.65              |
| 45:LF:1685:G:O2'   | 45:LF:1690:A:N1    | 2.28                     | 0.65              |
| 55:LP:122:ASP:OD1  | 55:LP:123:ARG:N    | 2.29                     | 0.65              |
| 57:LR:109:VAL:O    | 57:LR:114:ARG:NH1  | 2.29                     | 0.65              |
| 68:Lc:21:ARG:O     | 68:Lc:24:ARG:NH1   | 2.28                     | 0.65              |
| 1:S1:179:OMU:H2'   | 1:S1:180:OMG:H8    | 1.62                     | 0.65              |
| 47:LH:2605:OMU:H3' | 47:LH:2606:G:N2    | 2.10                     | 0.65              |
| 48:LI:3457:G:H5''  | 48:LI:3458:A:H5''  | 1.77                     | 0.65              |
| 65:LZ:65:LYS:NZ    | 65:LZ:66:LEU:O     | 2.29                     | 0.65              |
| 1:S1:469:G:O2'     | 1:S1:715:C:N3      | 2.29                     | 0.65              |
| 1:S1:1094:G:N2     | 1:S1:1094:G:OP2    | 2.25                     | 0.65              |
| 1:S1:1966:OMU:H2'  | 1:S1:1967:G:O4'    | 1.96                     | 0.65              |
| 7:SB:181:GLU:HG3   | 7:SB:185:MET:HE3   | 1.78                     | 0.65              |
| 13:SH:56:GLU:O     | 13:SH:59:VAL:HG12  | 1.96                     | 0.65              |
| 29:SX:107:LEU:HD22 | 29:SX:124:ARG:HG3  | 1.76                     | 0.65              |
| 41:LB:207:C:OP2    | 41:LB:208:A:O2'    | 2.14                     | 0.65              |
| 61:LV:185:LYS:NZ   | 61:LV:237:VAL:O    | 2.28                     | 0.65              |
| 1:S1:768:C:N4      | 1:S1:831:U:O4      | 2.30                     | 0.65              |
| 1:S1:1158:U:N3     | 1:S1:1244:C:O2     | 2.29                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:2000:G:O6     | 1:S1:2013:U:O2     | 2.15                     | 0.65              |
| 1:S1:2277:G:O2'    | 94:L3:2:GLY:O      | 2.13                     | 0.65              |
| 41:LB:286:A:OP2    | 61:LV:174:ARG:NH2  | 2.27                     | 0.65              |
| 47:LH:2358:A2M:H2  | 47:LH:2365:C:H41   | 1.61                     | 0.65              |
| 10:SE:181:LEU:HD21 | 10:SE:225:VAL:HB   | 1.77                     | 0.65              |
| 14:SI:90:GLU:O     | 14:SI:93:PHE:N     | 2.29                     | 0.65              |
| 15:SJ:94:LEU:HD21  | 15:SJ:102:ILE:HG13 | 1.79                     | 0.65              |
| 39:Sh:130:ASP:O    | 39:Sh:132:LEU:N    | 2.29                     | 0.65              |
| 48:LI:3343:U:O2'   | 96:L4:82:GLN:NE2   | 2.30                     | 0.65              |
| 49:LJ:3642:G:OP1   | 78:Lm:41:ARG:NH1   | 2.27                     | 0.65              |
| 78:Lm:22:VAL:HG22  | 78:Lm:32:VAL:HG22  | 1.77                     | 0.65              |
| 1:S1:1136:C:H2'    | 1:S1:1137:C:C6     | 2.32                     | 0.65              |
| 1:S1:2002:C:OP1    | 29:SX:124:ARG:NH1  | 2.30                     | 0.65              |
| 4:S4:7:A:N1        | 4:S4:67:C:N4       | 2.45                     | 0.65              |
| 38:Sg:237:PRO:O    | 38:Sg:241:ILE:HG13 | 1.96                     | 0.65              |
| 40:LA:150:G:H2'    | 40:LA:151:U:C6     | 2.32                     | 0.65              |
| 78:Lm:54:ARG:NH1   | 78:Lm:59:TYR:OH    | 2.29                     | 0.65              |
| 96:L4:25:VAL:HG22  | 96:L4:72:LEU:HD22  | 1.79                     | 0.65              |
| 1:S1:977:A:N7      | 38:Sg:220:ARG:NH1  | 2.45                     | 0.65              |
| 4:S4:51:U:O2       | 4:S4:63:G:O6       | 2.14                     | 0.65              |
| 44:LE:1159:G:O2'   | 44:LE:1195:G:H4'   | 1.97                     | 0.65              |
| 57:LR:49:SER:HB3   | 57:LR:52:ALA:HB2   | 1.77                     | 0.65              |
| 63:LX:136:LEU:O    | 63:LX:140:LYS:NZ   | 2.29                     | 0.65              |
| 85:Lt:91:ILE:HG23  | 85:Lt:95:LEU:HD23  | 1.78                     | 0.65              |
| 9:SD:71:ILE:HD12   | 10:SE:249:ILE:HD12 | 1.78                     | 0.65              |
| 30:SY:20:THR:HG22  | 30:SY:21:ASN:H     | 1.61                     | 0.65              |
| 51:LL:3877:G:OP2   | 65:LZ:157:ARG:NH1  | 2.30                     | 0.65              |
| 1:S1:1947:G:O2'    | 3:S3:30:G:OP1      | 2.15                     | 0.65              |
| 10:SE:136:THR:OG1  | 12:SG:209:ARG:NH2  | 2.30                     | 0.65              |
| 18:SM:37:VAL:HG11  | 18:SM:112:VAL:HG11 | 1.78                     | 0.65              |
| 41:LB:232:C:O2'    | 63:LX:73:ASN:OD1   | 2.15                     | 0.65              |
| 45:LF:1493:C:O2'   | 48:LI:3207:A:OP1   | 2.14                     | 0.65              |
| 64:LY:18:LEU:HD13  | 64:LY:54:ALA:HB3   | 1.79                     | 0.65              |
| 74:Li:49:TYR:CD1   | 74:Li:58:ARG:HD2   | 2.32                     | 0.65              |
| 4:S4:58:A:O2'      | 4:S4:60:U:OP2      | 2.14                     | 0.64              |
| 24:SS:13:ARG:NH2   | 24:SS:17:THR:OG1   | 2.30                     | 0.64              |
| 45:LF:1563:U:OP1   | 100:LF:2003:HOH:O  | 2.14                     | 0.64              |
| 45:LF:1924:C:OP2   | 100:LF:2004:HOH:O  | 2.14                     | 0.64              |
| 48:LI:3094:G:O2'   | 79:Ln:134:PHE:O    | 2.14                     | 0.64              |
| 58:LS:42:ARG:HD2   | 58:LS:130:THR:HA   | 1.76                     | 0.64              |
| 66:La:109:LEU:HD11 | 66:La:131:ARG:HG3  | 1.78                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 73:Lh:136:LEU:HD11 | 83:Lr:70:ALA:HB2   | 1.77                     | 0.64              |
| 1:S1:5:U:OP2       | 11:SF:205:THR:OG1  | 2.15                     | 0.64              |
| 9:SD:80:CYS:HB3    | 9:SD:86:LEU:HD13   | 1.79                     | 0.64              |
| 22:SQ:44:HIS:HA    | 37:Sf:103:VAL:HG21 | 1.77                     | 0.64              |
| 46:LG:2104:A:H2'   | 46:LG:2105:A:C8    | 2.31                     | 0.64              |
| 60:LU:29:ARG:NH2   | 65:LZ:110:ASP:OD1  | 2.30                     | 0.64              |
| 74:Li:60:ILE:HD12  | 74:Li:86:PRO:HD2   | 1.78                     | 0.64              |
| 1:S1:502:C:O2'     | 12:SG:94:ARG:O     | 2.14                     | 0.64              |
| 9:SD:126:ARG:HD3   | 36:Se:33:ARG:HD3   | 1.79                     | 0.64              |
| 45:LF:1486:A:OP2   | 100:LF:2005:HOH:O  | 2.15                     | 0.64              |
| 48:LI:3003:C:H3'   | 48:LI:3004:G:H8    | 1.63                     | 0.64              |
| 48:LI:3480:C:O2    | 59:LT:171:ASN:ND2  | 2.31                     | 0.64              |
| 51:LL:3853:G:O2'   | 51:LL:3868:A:N6    | 2.31                     | 0.64              |
| 53:LN:4003:A:H2'   | 53:LN:4004:G:C8    | 2.32                     | 0.64              |
| 56:LQ:376:THR:HG22 | 56:LQ:378:GLU:H    | 1.62                     | 0.64              |
| 59:LT:54:GLU:OE2   | 59:LT:56:ARG:NH2   | 2.30                     | 0.64              |
| 65:LZ:43:ARG:HH12  | 65:LZ:51:ARG:HD3   | 1.63                     | 0.64              |
| 71:Lf:16:LEU:HD22  | 71:Lf:53:ARG:HB2   | 1.78                     | 0.64              |
| 10:SE:212:ASP:OD1  | 10:SE:213:ALA:N    | 2.30                     | 0.64              |
| 41:LB:291:G:O4'    | 61:LV:143:ARG:NH2  | 2.31                     | 0.64              |
| 44:LE:1387:G:O6    | 73:Lh:112:ASN:ND2  | 2.28                     | 0.64              |
| 55:LP:36:GLU:OE2   | 55:LP:163:ARG:NH1  | 2.27                     | 0.64              |
| 82:Lq:52:THR:OG1   | 82:Lq:54:ASP:OD1   | 2.14                     | 0.64              |
| 1:S1:1549:A2M:H5'' | 1:S1:1549:A2M:H8   | 1.80                     | 0.64              |
| 2:S2:28:G:OP1      | 36:Se:3:LYS:NZ     | 2.29                     | 0.64              |
| 16:SK:44:ARG:HB2   | 16:SK:60:LEU:O     | 1.96                     | 0.64              |
| 23:SR:24:LYS:HB3   | 32:Sa:50:VAL:HG21  | 1.80                     | 0.64              |
| 45:LF:1885:U:H4'   | 71:Lf:4:GLY:H      | 1.62                     | 0.64              |
| 54:LO:20:G:OP2     | 58:LS:14:LYS:NZ    | 2.31                     | 0.64              |
| 56:LQ:10:ARG:NH1   | 56:LQ:11:HIS:O     | 2.31                     | 0.64              |
| 69:Ld:106:ARG:HD2  | 69:Ld:246:ARG:HG3  | 1.79                     | 0.64              |
| 1:S1:2269:A:OP2    | 100:S1:2406:HOH:O  | 2.15                     | 0.64              |
| 45:LF:1929:A2M:H8  | 92:L1:44:TRP:HH2   | 1.62                     | 0.64              |
| 46:LG:2024:A:OP1   | 100:LG:2301:HOH:O  | 2.15                     | 0.64              |
| 1:S1:1256:A:OP2    | 14:SI:120:THR:OG1  | 2.14                     | 0.64              |
| 11:SF:37:THR:HG23  | 11:SF:40:GLY:H     | 1.62                     | 0.64              |
| 40:LA:77:G:H5'     | 81:Lp:41:ALA:HB3   | 1.80                     | 0.64              |
| 44:LE:880:G:O6     | 57:LR:290:ARG:NH1  | 2.30                     | 0.64              |
| 44:LE:1002:G:OP2   | 70:Le:173:ARG:NH1  | 2.27                     | 0.64              |
| 80:Lo:26:ILE:O     | 80:Lo:30:THR:OG1   | 2.16                     | 0.64              |
| 1:S1:61:C:O2       | 1:S1:357:G:O2'     | 2.16                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:1364:A:OP2    | 25:ST:124:ARG:NH2  | 2.28                     | 0.64              |
| 11:SF:100:LYS:HG2  | 11:SF:118:CYS:SG   | 2.36                     | 0.64              |
| 21:SP:14:ARG:NH2   | 26:SU:106:GLU:OE2  | 2.29                     | 0.64              |
| 67:Lb:114:ARG:NH1  | 67:Lb:151:ILE:O    | 2.31                     | 0.64              |
| 71:Lf:99:ARG:NH1   | 71:Lf:131:ASN:OD1  | 2.30                     | 0.64              |
| 86:Lu:89:LEU:HD11  | 86:Lu:115:ILE:HG23 | 1.80                     | 0.64              |
| 1:S1:1108:U:H4'    | 1:S1:1109:G:H3'    | 1.79                     | 0.64              |
| 43:LD:703:C:H2'    | 43:LD:704:A:C8     | 2.32                     | 0.64              |
| 55:LP:179:VAL:HG13 | 55:LP:184:ASN:HB2  | 1.80                     | 0.64              |
| 64:LY:50:ASN:OD1   | 100:LY:201:HOH:O   | 2.15                     | 0.64              |
| 73:Lh:17:LYS:NZ    | 73:Lh:47:SER:OG    | 2.27                     | 0.64              |
| 88:Lw:63:ARG:O     | 88:Lw:67:ARG:NH2   | 2.30                     | 0.64              |
| 90:Ly:59:MET:HE1   | 90:Ly:67:MET:HE2   | 1.79                     | 0.64              |
| 1:S1:1321:A:H2'    | 1:S1:1322:G:C8     | 2.34                     | 0.64              |
| 1:S1:1612:A:OP1    | 100:S1:2407:HOH:O  | 2.15                     | 0.64              |
| 1:S1:1872:U:H5''   | 27:SV:3:ARG:HG2    | 1.78                     | 0.64              |
| 10:SE:87:MET:HE3   | 10:SE:123:LEU:HD22 | 1.79                     | 0.64              |
| 46:LG:2022:A2M:H8  | 46:LG:2022:A2M:OP2 | 1.98                     | 0.64              |
| 54:LO:44:U:OP2     | 58:LS:147:ARG:NH2  | 2.31                     | 0.64              |
| 58:LS:33:VAL:HG23  | 58:LS:35:GLU:H     | 1.63                     | 0.64              |
| 58:LS:143:ARG:NH1  | 58:LS:162:HIS:O    | 2.30                     | 0.64              |
| 90:Ly:21:ARG:NH2   | 100:Ly:301:HOH:O   | 2.31                     | 0.64              |
| 2:S2:19:G:OP2      | 2:S2:56:C:N4       | 2.31                     | 0.63              |
| 40:LA:20:U:H5      | 57:LR:190:ARG:HH12 | 1.46                     | 0.63              |
| 46:LG:2014:U:H4'   | 88:Lw:29:PRO:HD2   | 1.79                     | 0.63              |
| 1:S1:94:G:HO2'     | 1:S1:561:A:HO2'    | 1.30                     | 0.63              |
| 1:S1:2190:G:H2'    | 1:S1:2191:G:H8     | 1.62                     | 0.63              |
| 44:LE:1059:G:H2'   | 44:LE:1060:U:C6    | 2.33                     | 0.63              |
| 45:LF:1575:A:H2'   | 45:LF:1576:A:C8    | 2.33                     | 0.63              |
| 45:LF:1728:C:N3    | 70:Le:37:ARG:NH2   | 2.46                     | 0.63              |
| 1:S1:16:G:H2'      | 1:S1:17:C:C6       | 2.34                     | 0.63              |
| 1:S1:78:C:OP1      | 12:SG:161:ARG:NH1  | 2.31                     | 0.63              |
| 1:S1:1579:G:OP1    | 100:S1:2409:HOH:O  | 2.15                     | 0.63              |
| 10:SE:52:LEU:O     | 10:SE:54:TYR:N     | 2.26                     | 0.63              |
| 11:SF:141:ARG:NH2  | 30:SY:10:ASP:OD2   | 2.31                     | 0.63              |
| 44:LE:1156:G:OP2   | 71:Lf:93:LYS:NZ    | 2.28                     | 0.63              |
| 45:LF:1916:C:H4'   | 45:LF:1917:A:H4'   | 1.79                     | 0.63              |
| 69:Ld:82:LEU:HB3   | 69:Ld:87:ALA:HB3   | 1.80                     | 0.63              |
| 1:S1:428:G:N7      | 16:SK:273:ARG:NH2  | 2.44                     | 0.63              |
| 1:S1:581:A:H2'     | 1:S1:582:A:H8      | 1.63                     | 0.63              |
| 1:S1:650:C:H2'     | 1:S1:651:C:C6      | 2.33                     | 0.63              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:S1:1508:G:N2      | 15:SJ:70:ASN:O     | 2.32                     | 0.63              |
| 12:SG:180:GLN:OE1   | 100:SG:301:HOH:O   | 2.15                     | 0.63              |
| 16:SK:91:GLU:O      | 16:SK:95:THR:HG22  | 1.98                     | 0.63              |
| 28:SW:65:LEU:HD23   | 28:SW:81:ILE:HD12  | 1.78                     | 0.63              |
| 47:LH:2602:OMC:HM22 | 47:LH:2603:U:H5''  | 1.80                     | 0.63              |
| 1:S1:745:G:H2'      | 1:S1:746:G:C8      | 2.33                     | 0.63              |
| 1:S1:831:U:N3       | 1:S1:832:G:O6      | 2.31                     | 0.63              |
| 4:S4:33:U:N3        | 4:S4:36:A:OP2      | 2.31                     | 0.63              |
| 29:SX:43:ALA:HB3    | 29:SX:46:LYS:HG2   | 1.81                     | 0.63              |
| 40:LA:59:U:O4       | 81:Lp:62:ASN:ND2   | 2.31                     | 0.63              |
| 77:Ll:68:LYS:H      | 77:Ll:82:ASP:HB2   | 1.63                     | 0.63              |
| 7:SB:147:PHE:O      | 7:SB:165:ASN:ND2   | 2.31                     | 0.63              |
| 13:SH:3:LYS:HD3     | 13:SH:4:THR:HG23   | 1.80                     | 0.63              |
| 38:Sg:84:ARG:HE     | 38:Sg:90:LEU:N     | 1.96                     | 0.63              |
| 44:LE:1420:G:H2'    | 44:LE:1421:A:H8    | 1.63                     | 0.63              |
| 57:LR:300:PRO:HG3   | 83:Lr:165:THR:HG22 | 1.80                     | 0.63              |
| 65:LZ:7:ASN:OD1     | 65:LZ:13:ARG:NH2   | 2.30                     | 0.63              |
| 68:Lc:41:LEU:HD23   | 68:Lc:45:THR:HG21  | 1.81                     | 0.63              |
| 1:S1:1252:C:O2'     | 1:S1:1253:G:O5'    | 2.16                     | 0.63              |
| 1:S1:1365:U:OP1     | 1:S1:1432:C:O2'    | 2.16                     | 0.63              |
| 2:S2:75:C:N4        | 48:LI:3509:OMG:HN1 | 1.96                     | 0.63              |
| 11:SF:88:GLN:HG2    | 11:SF:97:THR:HG22  | 1.80                     | 0.63              |
| 16:SK:112:ARG:NH2   | 16:SK:261:VAL:O    | 2.31                     | 0.63              |
| 46:LG:2165:G:O6     | 71:Lf:122:ARG:NH1  | 2.32                     | 0.63              |
| 56:LQ:17:LEU:O      | 56:LQ:19:ARG:N     | 2.31                     | 0.63              |
| 58:LS:71:ARG:NH1    | 58:LS:72:ASN:OD1   | 2.30                     | 0.63              |
| 74:Li:13:GLU:O      | 74:Li:107:LYS:NZ   | 2.31                     | 0.63              |
| 1:S1:1576:C:OP1     | 13:SH:65:HIS:HA    | 1.97                     | 0.63              |
| 23:SR:31:LEU:HD21   | 23:SR:68:LEU:HD11  | 1.81                     | 0.63              |
| 44:LE:811:G:OP2     | 44:LE:811:G:N2     | 2.31                     | 0.63              |
| 62:LW:123:CYS:HB2   | 72:Lg:169:PHE:O    | 1.98                     | 0.63              |
| 28:SW:72:ALA:HB3    | 28:SW:78:PRO:HA    | 1.80                     | 0.63              |
| 1:S1:72:G:O6        | 12:SG:173:ARG:NH2  | 2.27                     | 0.62              |
| 1:S1:573:A:H5''     | 9:SD:11:VAL:HG13   | 1.81                     | 0.62              |
| 1:S1:590:G:H2'      | 1:S1:591:G:H8      | 1.64                     | 0.62              |
| 1:S1:2232:G:OP2     | 1:S1:2232:G:N2     | 2.27                     | 0.62              |
| 47:LH:2685:OMC:H5   | 47:LH:2732:A:H62   | 1.47                     | 0.62              |
| 69:Ld:179:PRO:HD2   | 69:Ld:193:LEU:HD12 | 1.79                     | 0.62              |
| 83:Lr:139:TYR:CE2   | 83:Lr:231:GLU:HB2  | 2.34                     | 0.62              |
| 20:SO:99:ARG:HH21   | 20:SO:133:VAL:HG12 | 1.62                     | 0.62              |
| 48:LI:3398:C:H2'    | 48:LI:3399:A:C8    | 2.34                     | 0.62              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:S1:66:C:N4        | 12:SG:136:GLY:O   | 2.31                     | 0.62              |
| 1:S1:159:G:H2'      | 1:S1:160:G:C8     | 2.34                     | 0.62              |
| 1:S1:348:A:H5''     | 1:S1:349:G:C8     | 2.34                     | 0.62              |
| 1:S1:1424:A:OP2     | 100:S1:2410:HOH:O | 2.16                     | 0.62              |
| 1:S1:1581:A:H2'     | 1:S1:1582:G:C8    | 2.34                     | 0.62              |
| 8:SC:77:LYS:NZ      | 19:SN:20:VAL:O    | 2.32                     | 0.62              |
| 13:SH:96:GLN:NE2    | 13:SH:100:ASP:OD1 | 2.32                     | 0.62              |
| 41:LB:231:A:OP2     | 66:La:71:ARG:NH1  | 2.32                     | 0.62              |
| 45:LF:1945:C:OP1    | 100:LF:2006:HOH:O | 2.16                     | 0.62              |
| 48:LI:3488:G:O2'    | 49:LJ:3614:A:N1   | 2.32                     | 0.62              |
| 53:LN:4045:A:N7     | 100:LN:4102:HOH:O | 2.31                     | 0.62              |
| 55:LP:29:LEU:HG     | 55:LP:124:SER:HB2 | 1.81                     | 0.62              |
| 61:LV:276:LYS:HA    | 61:LV:279:LYS:HE2 | 1.82                     | 0.62              |
| 71:Lf:106:MET:HE1   | 71:Lf:140:MET:HB2 | 1.81                     | 0.62              |
| 1:S1:87:U:H3        | 1:S1:549:A:H62    | 1.47                     | 0.62              |
| 1:S1:1506:C:OP2     | 15:SJ:71:LYS:NZ   | 2.26                     | 0.62              |
| 46:LG:2032:G:OP1    | 91:Lz:42:LEU:N    | 2.31                     | 0.62              |
| 47:LH:2583:G:H2'    | 47:LH:2584:G:C8   | 2.34                     | 0.62              |
| 49:LJ:3592:G:OP1    | 56:LQ:26:ARG:NH1  | 2.32                     | 0.62              |
| 56:LQ:352:LYS:O     | 56:LQ:356:GLU:CB  | 2.44                     | 0.62              |
| 57:LR:324:ASN:OD1   | 57:LR:333:LYS:NZ  | 2.31                     | 0.62              |
| 59:LT:175:ARG:NH1   | 93:L2:123:LYS:O   | 2.33                     | 0.62              |
| 38:Sg:63:MET:HG3    | 38:Sg:64:SER:H    | 1.64                     | 0.62              |
| 47:LH:2625:OMU:H5   | 47:LH:2630:G:N7   | 2.15                     | 0.62              |
| 47:LH:2876:U:O2     | 74:Li:71:ARG:NH2  | 2.26                     | 0.62              |
| 56:LQ:378:GLU:OE2   | 56:LQ:381:ARG:NH2 | 2.33                     | 0.62              |
| 60:LU:32:CYS:HA     | 60:LU:43:VAL:HG12 | 1.81                     | 0.62              |
| 1:S1:681:G:N3       | 2:S2:35:A:O2'     | 2.30                     | 0.62              |
| 1:S1:858:U:H2'      | 1:S1:859:G:C8     | 2.35                     | 0.62              |
| 17:SL:21:LYS:O      | 17:SL:131:ARG:NH1 | 2.31                     | 0.62              |
| 47:LH:2953:G:H1     | 48:LI:2988:U:H4'  | 1.64                     | 0.62              |
| 50:LK:3802:U:O4     | 60:LU:187:ASN:ND2 | 2.32                     | 0.62              |
| 1:S1:1912:A:O2'     | 1:S1:1913:G:OP2   | 2.18                     | 0.62              |
| 4:S4:40:C:OP1       | 20:SO:64:LYS:NZ   | 2.28                     | 0.62              |
| 39:Sh:253:CYS:SG    | 39:Sh:295:TRP:NE1 | 2.70                     | 0.62              |
| 41:LB:181:G:OP2     | 41:LB:181:G:N2    | 2.28                     | 0.62              |
| 47:LH:2769:A2M:HM'1 | 48:LI:3547:C:H1'  | 1.82                     | 0.62              |
| 48:LI:3501:G:N3     | 48:LI:3521:A2M:H2 | 2.14                     | 0.62              |
| 63:LX:31:PHE:HE2    | 67:Lb:199:LYS:HB3 | 1.65                     | 0.62              |
| 2:S2:14:A:H61       | 2:S2:22:G:H1'     | 1.65                     | 0.62              |
| 10:SE:36:HIS:NE2    | 10:SE:143:ASP:OD1 | 2.33                     | 0.62              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 17:SL:21:LYS:HD3    | 17:SL:84:SER:HA    | 1.81                     | 0.62              |
| 20:SO:35:TYR:HB3    | 20:SO:42:PHE:HB2   | 1.81                     | 0.62              |
| 26:SU:93:ARG:HB2    | 26:SU:112:TRP:HZ3  | 1.65                     | 0.62              |
| 41:LB:247:OMU:HM21  | 66:La:72:LEU:HD11  | 1.81                     | 0.62              |
| 66:La:7:LYS:HG2     | 66:La:9:LYS:HE2    | 1.82                     | 0.62              |
| 1:S1:65:G:N2        | 1:S1:83:G:O6       | 2.19                     | 0.62              |
| 1:S1:485:OMG:OP2    | 1:S1:520:G:O2'     | 2.18                     | 0.62              |
| 1:S1:960:C:H2'      | 1:S1:961:A:C8      | 2.35                     | 0.62              |
| 44:LE:1023:PSU:H5'' | 70:Le:41:PRO:HB2   | 1.82                     | 0.62              |
| 44:LE:1371:A:N3     | 48:LI:3205:U:O2'   | 2.33                     | 0.62              |
| 47:LH:2844:A:OP1    | 74:Li:142:MET:N    | 2.33                     | 0.62              |
| 13:SH:59:VAL:CG1    | 13:SH:72:LYS:HE3   | 2.30                     | 0.62              |
| 29:SX:12:VAL:HG12   | 29:SX:142:LEU:HG   | 1.82                     | 0.62              |
| 44:LE:1114:G:H5''   | 90:Ly:16:HIS:HE1   | 1.64                     | 0.62              |
| 45:LF:1833:U:OP1    | 74:Li:84:ARG:NH2   | 2.32                     | 0.62              |
| 1:S1:1588:G:H5'     | 1:S1:1600:C:H41    | 1.65                     | 0.61              |
| 3:S3:24:G:O2'       | 47:LH:2754:PSU:OP1 | 2.18                     | 0.61              |
| 7:SB:63:ARG:NH1     | 30:SY:37:GLY:O     | 2.32                     | 0.61              |
| 11:SF:109:ASP:O     | 11:SF:142:ARG:NH2  | 2.32                     | 0.61              |
| 16:SK:22:ARG:NH1    | 16:SK:28:GLU:OE2   | 2.33                     | 0.61              |
| 42:LC:616:G:OP1     | 74:Li:64:ARG:NH1   | 2.33                     | 0.61              |
| 45:LF:1911:C:O2'    | 46:LG:2021:A:N3    | 2.32                     | 0.61              |
| 56:LQ:317:ARG:O     | 56:LQ:337:LYS:NZ   | 2.31                     | 0.61              |
| 70:Le:128:ILE:HG22  | 70:Le:129:THR:HG23 | 1.82                     | 0.61              |
| 84:Ls:34:LEU:HD22   | 84:Ls:62:TYR:HD2   | 1.64                     | 0.61              |
| 31:SZ:11:VAL:HG13   | 31:SZ:29:ILE:CG2   | 2.30                     | 0.61              |
| 47:LH:2701:A:H2'    | 47:LH:2702:A:C8    | 2.35                     | 0.61              |
| 48:LI:3291:C:O2     | 96:L4:18:LYS:NZ    | 2.33                     | 0.61              |
| 90:Ly:34:CYS:HB3    | 90:Ly:39:TYR:H     | 1.65                     | 0.61              |
| 1:S1:1506:C:OP1     | 15:SJ:12:LYS:NZ    | 2.32                     | 0.61              |
| 13:SH:122:ARG:HG3   | 13:SH:189:ASN:HD21 | 1.65                     | 0.61              |
| 14:SI:66:VAL:HB     | 14:SI:98:VAL:HG12  | 1.80                     | 0.61              |
| 39:Sh:278:LEU:CD2   | 39:Sh:288:PRO:HD2  | 2.30                     | 0.61              |
| 1:S1:342:G:H2'      | 1:S1:343:G:C8      | 2.35                     | 0.61              |
| 1:S1:429:U:OP2      | 16:SK:276:GLN:NE2  | 2.33                     | 0.61              |
| 25:ST:102:LEU:HD21  | 25:ST:115:LEU:HD22 | 1.81                     | 0.61              |
| 41:LB:246:G:O2'     | 41:LB:258:G:O6     | 2.16                     | 0.61              |
| 47:LH:2744:A2M:N6   | 100:LH:3028:HOH:O  | 2.31                     | 0.61              |
| 69:Ld:195:GLU:HG2   | 69:Ld:200:GLY:HA3  | 1.82                     | 0.61              |
| 81:Lp:95:LEU:HD22   | 81:Lp:100:ARG:HG3  | 1.81                     | 0.61              |
| 1:S1:1903:G:O2'     | 24:SS:55:ASN:OD1   | 2.16                     | 0.61              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 47:LH:2827:C:OP2    | 64:LY:48:ARG:NH1   | 2.33                     | 0.61              |
| 49:LJ:3711:U:OP2    | 93:L2:109:ARG:NH2  | 2.29                     | 0.61              |
| 76:Lk:109:ILE:HD12  | 76:Lk:141:LYS:HB2  | 1.81                     | 0.61              |
| 1:S1:952:G:H2'      | 1:S1:953:A:H8      | 1.65                     | 0.61              |
| 19:SN:31:HIS:NE2    | 19:SN:34:MET:SD    | 2.72                     | 0.61              |
| 38:Sg:82:ARG:HB2    | 38:Sg:91:ILE:HG23  | 1.82                     | 0.61              |
| 44:LE:1009:A:H5'    | 66:La:119:THR:HB   | 1.80                     | 0.61              |
| 47:LH:2947:A:N7     | 48:LI:2988:U:O2'   | 2.30                     | 0.61              |
| 76:Lk:80:GLN:HB2    | 76:Lk:123:MET:HG2  | 1.83                     | 0.61              |
| 7:SB:207:PRO:O      | 27:SV:81:ARG:NH2   | 2.33                     | 0.61              |
| 42:LC:350:G:C2      | 42:LC:459:U:O2     | 2.54                     | 0.61              |
| 45:LF:1800:U:O4     | 100:LF:2007:HOH:O  | 2.16                     | 0.61              |
| 58:LS:25:ALA:HB2    | 58:LS:142:GLU:HB3  | 1.81                     | 0.61              |
| 1:S1:1614:U:OP1     | 1:S1:1941:C:N4     | 2.34                     | 0.61              |
| 22:SQ:20:SER:HB3    | 22:SQ:25:ALA:HB2   | 1.81                     | 0.61              |
| 42:LC:569:G:OP1     | 57:LR:56:HIS:ND1   | 2.32                     | 0.61              |
| 44:LE:935:A2M:OP2   | 48:LI:3454:U:O2'   | 2.18                     | 0.61              |
| 47:LH:2583:G:H2'    | 47:LH:2584:G:H8    | 1.64                     | 0.61              |
| 57:LR:181:LYS:HG3   | 57:LR:197:VAL:HG22 | 1.83                     | 0.61              |
| 77:Ll:31:SER:HA     | 77:Ll:48:PRO:HA    | 1.83                     | 0.61              |
| 25:ST:25:TRP:CE3    | 25:ST:26:LEU:HG    | 2.36                     | 0.61              |
| 44:LE:1068:A:OP2    | 48:LI:3356:G:N2    | 2.34                     | 0.61              |
| 59:LT:1:MET:HG2     | 72:Lg:141:HIS:HB3  | 1.83                     | 0.61              |
| 63:LX:29:ARG:NE     | 67:Lb:197:LEU:HD21 | 2.16                     | 0.61              |
| 79:Ln:33:ASN:ND2    | 79:Ln:35:GLU:OE2   | 2.34                     | 0.61              |
| 88:Lw:16:LYS:O      | 88:Lw:21:ASN:ND2   | 2.33                     | 0.61              |
| 31:SZ:63:PHE:HB2    | 31:SZ:77:HIS:HB2   | 1.82                     | 0.61              |
| 44:LE:968:G:OP2     | 57:LR:111:ARG:NH2  | 2.33                     | 0.61              |
| 44:LE:1001:U:OP1    | 44:LE:1079:A:O2'   | 2.14                     | 0.61              |
| 45:LF:1795:C:H2'    | 45:LF:1796:G:H8    | 1.66                     | 0.61              |
| 47:LH:2361:PSU:O2   | 100:LI:3602:HOH:O  | 2.11                     | 0.61              |
| 50:LK:3798:U:OP2    | 72:Lg:175:SER:OG   | 2.19                     | 0.61              |
| 3:S3:2:C:N4         | 3:S3:71:G:O6       | 2.25                     | 0.60              |
| 3:S3:76:A:O2'       | 48:LI:3558:A:N7    | 2.31                     | 0.60              |
| 8:SC:66:ARG:NH1     | 19:SN:90:LEU:HD21  | 2.15                     | 0.60              |
| 11:SF:82:MET:HE1    | 11:SF:212:VAL:HG21 | 1.83                     | 0.60              |
| 14:SI:164:LYS:O     | 14:SI:168:GLU:HB3  | 1.99                     | 0.60              |
| 39:Sh:66:HIS:CE1    | 39:Sh:92:ARG:HG3   | 2.36                     | 0.60              |
| 45:LF:1822:OMC:HM22 | 45:LF:1823:U:H5'   | 1.83                     | 0.60              |
| 48:LI:3220:G:OP1    | 68:Lc:24:ARG:NH2   | 2.34                     | 0.60              |
| 57:LR:28:TYR:CE1    | 70:Le:22:PRO:HG3   | 2.36                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:1616:OMU:H6   | 1:S1:1616:OMU:O5'  | 2.00                     | 0.60              |
| 29:SX:117:GLU:OE1  | 29:SX:127:THR:OG1  | 2.16                     | 0.60              |
| 45:LF:1816:G:OP2   | 66:La:19:ARG:NH1   | 2.34                     | 0.60              |
| 47:LH:2601:G:O2'   | 47:LH:2602:OMC:OP2 | 2.15                     | 0.60              |
| 48:LI:3030:G:OP1   | 61:LV:287:ARG:NH1  | 2.34                     | 0.60              |
| 61:LV:241:ASN:HA   | 61:LV:244:LYS:HG3  | 1.83                     | 0.60              |
| 64:LY:94:THR:HG23  | 78:Lm:20:ARG:HD3   | 1.82                     | 0.60              |
| 68:Lc:36:CYS:SG    | 68:Lc:69:ARG:NH1   | 2.74                     | 0.60              |
| 72:Lg:38:VAL:HG22  | 83:Lr:231:GLU:CD   | 2.26                     | 0.60              |
| 1:S1:459:G:OP1     | 100:S1:2411:HOH:O  | 2.17                     | 0.60              |
| 1:S1:926:G:H2'     | 1:S1:927:G:C4      | 2.37                     | 0.60              |
| 13:SH:61:SER:CB    | 13:SH:141:THR:HG21 | 2.32                     | 0.60              |
| 14:SI:131:LEU:HD21 | 14:SI:157:ILE:HG12 | 1.83                     | 0.60              |
| 44:LE:950:U:H2'    | 44:LE:951:A:C8     | 2.35                     | 0.60              |
| 47:LH:2409:C:H2'   | 47:LH:2410:A:O4'   | 2.01                     | 0.60              |
| 47:LH:2669:U:H2'   | 47:LH:2670:G:C8    | 2.35                     | 0.60              |
| 48:LI:3574:C:O2'   | 56:LQ:261:ARG:HB3  | 2.01                     | 0.60              |
| 11:SF:188:LEU:HD22 | 11:SF:215:THR:HG23 | 1.83                     | 0.60              |
| 42:LC:352:U:O2     | 42:LC:456:G:N2     | 2.33                     | 0.60              |
| 44:LE:1239:U:OP1   | 100:LE:1507:HOH:O  | 2.17                     | 0.60              |
| 48:LI:3542:PSU:OP2 | 48:LI:3564:G:N1    | 2.29                     | 0.60              |
| 55:LP:26:GLN:OE1   | 55:LP:28:ARG:NH1   | 2.34                     | 0.60              |
| 90:Ly:30:GLN:NE2   | 100:Ly:302:HOH:O   | 2.34                     | 0.60              |
| 1:S1:65:G:OP1      | 12:SG:180:GLN:NE2  | 2.31                     | 0.60              |
| 6:SA:84:LEU:HB3    | 6:SA:96:THR:HB     | 1.83                     | 0.60              |
| 44:LE:835:C:H2'    | 44:LE:836:C:H6     | 1.66                     | 0.60              |
| 46:LG:2143:C:O2'   | 46:LG:2145:C:OP2   | 2.15                     | 0.60              |
| 60:LU:16:GLN:NE2   | 60:LU:65:THR:O     | 2.26                     | 0.60              |
| 88:Lw:45:PRO:HG2   | 88:Lw:59:VAL:HG21  | 1.84                     | 0.60              |
| 1:S1:583:C:H42     | 1:S1:610:C:H42     | 1.50                     | 0.60              |
| 1:S1:1161:G:C2     | 1:S1:1241:C:C2     | 2.90                     | 0.60              |
| 1:S1:2058:A:O2'    | 28:SW:87:ASN:ND2   | 2.34                     | 0.60              |
| 42:LC:632:U:H2'    | 42:LC:633:G:C8     | 2.37                     | 0.60              |
| 44:LE:1420:G:H2'   | 44:LE:1421:A:C8    | 2.36                     | 0.60              |
| 51:LL:3834:A:N6    | 62:LW:162:GLU:OE2  | 2.30                     | 0.60              |
| 57:LR:309:GLU:OE2  | 57:LR:313:GLN:NE2  | 2.35                     | 0.60              |
| 58:LS:100:GLU:HG3  | 58:LS:180:ILE:HB   | 1.83                     | 0.60              |
| 11:SF:98:ARG:HG2   | 11:SF:120:LYS:HA   | 1.83                     | 0.60              |
| 12:SG:235:VAL:HA   | 12:SG:239:ARG:HH21 | 1.65                     | 0.60              |
| 18:SM:22:ILE:HG21  | 18:SM:100:VAL:HG21 | 1.83                     | 0.60              |
| 39:Sh:38:ARG:HD3   | 39:Sh:69:PHE:HB3   | 1.83                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:LC:576:G:N1     | 42:LC:579:A:OP2    | 2.33                     | 0.60              |
| 48:LI:3387:A:OP1   | 100:LI:3605:HOH:O  | 2.16                     | 0.60              |
| 61:LV:191:HIS:CE1  | 61:LV:218:GLY:H    | 2.20                     | 0.60              |
| 1:S1:962:G:H2'     | 1:S1:963:G:H8      | 1.67                     | 0.60              |
| 18:SM:28:SER:HB3   | 18:SM:34:LEU:HD12  | 1.84                     | 0.60              |
| 42:LC:485:U:O2'    | 42:LC:487:G:N7     | 2.25                     | 0.60              |
| 44:LE:1386:C:O2'   | 73:Lh:108:ARG:NH2  | 2.35                     | 0.60              |
| 47:LH:2321:A:OP1   | 71:Lf:89:ARG:NH1   | 2.34                     | 0.60              |
| 56:LQ:113:GLN:HE22 | 56:LQ:167:GLN:HG2  | 1.67                     | 0.60              |
| 1:S1:435:A:H5'     | 16:SK:7:ASP:HB3    | 1.84                     | 0.60              |
| 1:S1:1113:U:O4'    | 1:S1:1135:G:N2     | 2.35                     | 0.60              |
| 1:S1:2276:U:O4     | 33:Sb:28:ARG:NH2   | 2.35                     | 0.60              |
| 13:SH:78:HIS:HD2   | 13:SH:155:PHE:CD2  | 2.19                     | 0.60              |
| 14:SI:97:GLN:HE22  | 14:SI:170:LYS:HG3  | 1.66                     | 0.60              |
| 15:SJ:55:ASN:H     | 15:SJ:59:ASN:HD22  | 1.48                     | 0.60              |
| 42:LC:303:C:H2'    | 42:LC:304:G:C8     | 2.37                     | 0.60              |
| 45:LF:1700:U:O4    | 100:LF:2002:HOH:O  | 2.11                     | 0.60              |
| 47:LH:2772:C:N4    | 47:LH:2796:C:OP2   | 2.33                     | 0.60              |
| 57:LR:135:GLY:O    | 57:LR:176:LYS:NZ   | 2.35                     | 0.60              |
| 60:LU:194:ARG:NH2  | 65:LZ:107:ASN:O    | 2.34                     | 0.60              |
| 66:La:152:ALA:HB3  | 89:Lx:17:ALA:HB2   | 1.84                     | 0.60              |
| 1:S1:261:C:H2'     | 1:S1:262:G:O4'     | 2.02                     | 0.60              |
| 10:SE:65:LEU:HD12  | 10:SE:80:ILE:HG13  | 1.83                     | 0.60              |
| 43:LD:700:G:O6     | 65:LZ:6:ARG:N      | 2.28                     | 0.60              |
| 44:LE:962:C:O2     | 70:Le:59:ARG:NH2   | 2.35                     | 0.60              |
| 54:LO:6:C:O3'      | 69:Ld:49:ARG:NH2   | 2.35                     | 0.60              |
| 62:LW:183:ARG:HD3  | 65:LZ:209:ILE:HD11 | 1.83                     | 0.60              |
| 69:Ld:41:ASN:ND2   | 73:Lh:67:VAL:O     | 2.34                     | 0.60              |
| 1:S1:1108:U:O2'    | 1:S1:1110:G:OP2    | 2.14                     | 0.59              |
| 45:LF:1514:G:O2'   | 86:Lu:52:ARG:O     | 2.17                     | 0.59              |
| 60:LU:24:ARG:NH1   | 60:LU:24:ARG:O     | 2.30                     | 0.59              |
| 35:Sd:51:ARG:NH1   | 35:Sd:70:ARG:O     | 2.35                     | 0.59              |
| 44:LE:948:U:H2'    | 44:LE:949:OMC:C6   | 2.37                     | 0.59              |
| 44:LE:962:C:N3     | 70:Le:59:ARG:HD2   | 2.17                     | 0.59              |
| 47:LH:2849:A2M:H2' | 47:LH:2850:C:C6    | 2.37                     | 0.59              |
| 48:LI:3028:G:H2'   | 48:LI:3029:A:C8    | 2.37                     | 0.59              |
| 50:LK:3781:U:OP1   | 65:LZ:3:LYS:NZ     | 2.34                     | 0.59              |
| 93:L2:76:MET:HE3   | 93:L2:81:GLN:HG2   | 1.84                     | 0.59              |
| 10:SE:11:ARG:NH2   | 10:SE:24:GLY:O     | 2.36                     | 0.59              |
| 11:SF:223:TYR:OH   | 100:SF:301:HOH:O   | 2.13                     | 0.59              |
| 12:SG:184:THR:HG22 | 12:SG:186:ALA:H    | 1.66                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LA:92:G:H5''    | 90:Ly:72:LYS:HB3   | 1.83                     | 0.59              |
| 44:LE:1179:G:OP2   | 74:Li:134:ALA:N    | 2.33                     | 0.59              |
| 47:LH:2933:A:H1'   | 48:LI:3003:C:N4    | 2.17                     | 0.59              |
| 66:La:66:ARG:NH2   | 96:L4:38:GLN:OE1   | 2.29                     | 0.59              |
| 75:Lj:60:THR:HA    | 75:Lj:118:ALA:O    | 2.03                     | 0.59              |
| 2:S2:28:G:H2'      | 2:S2:29:G:H8       | 1.67                     | 0.59              |
| 14:SI:59:ILE:HG23  | 14:SI:176:VAL:HG21 | 1.84                     | 0.59              |
| 18:SM:35:GLU:OE2   | 18:SM:89:ARG:NH1   | 2.35                     | 0.59              |
| 42:LC:512:U:H2'    | 42:LC:513:A:C8     | 2.37                     | 0.59              |
| 45:LF:1474:G:OP1   | 82:Lq:22:ARG:NH2   | 2.35                     | 0.59              |
| 47:LH:2363:G:O6    | 56:LQ:243:LYS:NZ   | 2.29                     | 0.59              |
| 53:LN:4011:G:N1    | 53:LN:4019:U:C2    | 2.70                     | 0.59              |
| 62:LW:82:ARG:HB2   | 62:LW:109:VAL:HG12 | 1.84                     | 0.59              |
| 73:Lh:57:PHE:HA    | 73:Lh:60:LYS:HG3   | 1.84                     | 0.59              |
| 75:Lj:127:LEU:O    | 75:Lj:131:THR:HG23 | 2.03                     | 0.59              |
| 79:Ln:82:PRO:HD2   | 84:Ls:62:TYR:CE1   | 2.37                     | 0.59              |
| 1:S1:1007:G:H2'    | 1:S1:1008:G:H8     | 1.68                     | 0.59              |
| 1:S1:1608:G:OP1    | 1:S1:1609:G:O2'    | 2.17                     | 0.59              |
| 23:SR:43:ILE:HD12  | 29:SX:48:LEU:HD11  | 1.85                     | 0.59              |
| 33:Sb:7:ASN:O      | 33:Sb:9:GLY:N      | 2.34                     | 0.59              |
| 48:LI:3499:G:H2'   | 48:LI:3500:A2M:H8  | 1.85                     | 0.59              |
| 57:LR:61:TRP:HB3   | 57:LR:65:ARG:HD3   | 1.83                     | 0.59              |
| 61:LV:175:VAL:HG21 | 61:LV:233:SER:O    | 2.02                     | 0.59              |
| 1:S1:981:G:H2'     | 1:S1:982:G:C8      | 2.37                     | 0.59              |
| 1:S1:1310:A:H1'    | 47:LH:2694:G:C6    | 2.38                     | 0.59              |
| 1:S1:1315:G:OP1    | 20:SO:99:ARG:NH1   | 2.33                     | 0.59              |
| 1:S1:1329:U:OP2    | 6:SA:153:TYR:OH    | 2.17                     | 0.59              |
| 6:SA:157:SER:OG    | 6:SA:161:ARG:NH1   | 2.36                     | 0.59              |
| 6:SA:185:LYS:O     | 6:SA:188:LEU:C     | 2.46                     | 0.59              |
| 14:SI:140:VAL:HG23 | 14:SI:157:ILE:HG23 | 1.83                     | 0.59              |
| 25:ST:4:MET:HE2    | 25:ST:121:ARG:HG2  | 1.84                     | 0.59              |
| 44:LE:1215:A:N3    | 44:LE:1216:G:H5''  | 2.18                     | 0.59              |
| 49:LJ:3593:A:OP1   | 56:LQ:26:ARG:NH2   | 2.36                     | 0.59              |
| 79:Ln:77:HIS:HB3   | 84:Ls:38:ARG:HD2   | 1.85                     | 0.59              |
| 1:S1:565:A2M:H8    | 1:S1:565:A2M:H5''  | 1.85                     | 0.59              |
| 1:S1:1638:G:OP1    | 22:SQ:43:LEU:N     | 2.33                     | 0.59              |
| 10:SE:66:LYS:HD2   | 10:SE:78:THR:HB    | 1.85                     | 0.59              |
| 22:SQ:26:LEU:HA    | 22:SQ:29:VAL:HG12  | 1.83                     | 0.59              |
| 29:SX:47:GLU:HG3   | 29:SX:87:ARG:HD2   | 1.83                     | 0.59              |
| 38:Sg:219:ARG:HE   | 38:Sg:220:ARG:HG3  | 1.67                     | 0.59              |
| 42:LC:315:G:H2'    | 42:LC:316:A:H8     | 1.67                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:LC:382:A:H2'    | 42:LC:383:G:C8     | 2.38                     | 0.59              |
| 42:LC:474:G:OP2    | 67:Lb:44:ARG:NH2   | 2.33                     | 0.59              |
| 44:LE:937:G:O2'    | 45:LF:1820:A:OP1   | 2.20                     | 0.59              |
| 47:LH:2606:G:O6    | 71:Lf:83:ARG:NH1   | 2.36                     | 0.59              |
| 65:LZ:97:ARG:HB2   | 65:LZ:214:LEU:HD22 | 1.84                     | 0.59              |
| 78:Lm:4:GLU:HG3    | 78:Lm:20:ARG:HH21  | 1.68                     | 0.59              |
| 1:S1:348:A:H3'     | 1:S1:349:G:H8      | 1.67                     | 0.59              |
| 1:S1:641:OMG:C5    | 9:SD:171:ARG:HD3   | 2.36                     | 0.59              |
| 11:SF:236:PHE:HB2  | 30:SY:51:THR:HG21  | 1.85                     | 0.59              |
| 46:LG:2034:C:H2'   | 46:LG:2035:A:C8    | 2.37                     | 0.59              |
| 47:LH:2907:A:H2'   | 47:LH:2908:C:C6    | 2.38                     | 0.59              |
| 48:LI:3457:G:N7    | 100:LI:3625:HOH:O  | 2.32                     | 0.59              |
| 1:S1:1676:C:O2     | 100:S1:2405:HOH:O  | 2.14                     | 0.59              |
| 7:SB:200:ASP:OD2   | 7:SB:205:ARG:NH2   | 2.33                     | 0.59              |
| 45:LF:1560:U:OP2   | 62:LW:54:ARG:NH1   | 2.30                     | 0.59              |
| 1:S1:1958:U:H5     | 13:SH:62:LEU:O     | 1.85                     | 0.59              |
| 7:SB:57:LYS:NZ     | 30:SY:69:ASN:OD1   | 2.35                     | 0.59              |
| 9:SD:112:ILE:HD12  | 9:SD:148:VAL:HB    | 1.85                     | 0.59              |
| 13:SH:122:ARG:O    | 13:SH:189:ASN:ND2  | 2.35                     | 0.59              |
| 14:SI:106:ILE:HG12 | 14:SI:126:VAL:HG21 | 1.85                     | 0.59              |
| 38:Sg:173:PHE:CD1  | 38:Sg:214:LYS:HE3  | 2.38                     | 0.59              |
| 42:LC:466:A:H1'    | 42:LC:467:U:H5'    | 1.85                     | 0.59              |
| 44:LE:1252:A:H4'   | 44:LE:1268:G:N2    | 2.17                     | 0.59              |
| 44:LE:1264:G:OP1   | 100:LE:1508:HOH:O  | 2.17                     | 0.59              |
| 55:LP:147:ARG:HH21 | 55:LP:155:LYS:HD3  | 1.67                     | 0.59              |
| 59:LT:122:LEU:HD23 | 59:LT:124:ARG:HE   | 1.68                     | 0.59              |
| 33:Sb:39:PHE:HA    | 33:Sb:71:LYS:HA    | 1.84                     | 0.58              |
| 48:LI:3254:U:H5'   | 58:LS:75:ILE:HD11  | 1.83                     | 0.58              |
| 57:LR:108:LYS:NZ   | 67:Lb:204:ARG:O    | 2.35                     | 0.58              |
| 59:LT:69:CYS:HA    | 59:LT:72:THR:HG22  | 1.85                     | 0.58              |
| 62:LW:56:LYS:NZ    | 62:LW:149:ASP:OD2  | 2.34                     | 0.58              |
| 76:Lk:84:LEU:HD12  | 76:Lk:123:MET:HG3  | 1.83                     | 0.58              |
| 1:S1:1074:U:H3'    | 1:S1:1075:C:H5''   | 1.85                     | 0.58              |
| 7:SB:145:ILE:HG12  | 7:SB:159:LEU:HB3   | 1.85                     | 0.58              |
| 9:SD:139:GLN:NE2   | 31:SZ:69:PHE:O     | 2.35                     | 0.58              |
| 17:SL:47:LEU:HD12  | 17:SL:56:VAL:HG21  | 1.85                     | 0.58              |
| 23:SR:37:ILE:O     | 23:SR:41:PHE:HB3   | 2.03                     | 0.58              |
| 25:ST:40:LEU:HD21  | 25:ST:50:ILE:HG23  | 1.85                     | 0.58              |
| 40:LA:163:G:O6     | 48:LI:3142:C:O2'   | 2.18                     | 0.58              |
| 61:LV:118:THR:HG21 | 61:LV:217:LYS:HG2  | 1.85                     | 0.58              |
| 66:La:2:THR:HG22   | 66:La:3:TYR:H      | 1.67                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:Lf:168:LEU:HA   | 71:Lf:171:ARG:HG2  | 1.83                     | 0.58              |
| 1:S1:1585:U:H2'    | 1:S1:1586:G:C8     | 2.38                     | 0.58              |
| 9:SD:71:ILE:HD11   | 10:SE:249:ILE:HD12 | 1.82                     | 0.58              |
| 14:SI:192:THR:HG23 | 14:SI:200:GLN:HB3  | 1.83                     | 0.58              |
| 44:LE:1435:C:H2'   | 44:LE:1436:A:H8    | 1.67                     | 0.58              |
| 51:LL:3838:G:OP2   | 62:LW:119:LYS:NZ   | 2.33                     | 0.58              |
| 52:LM:3949:U:H4'   | 52:LM:3950:A:H5'   | 1.84                     | 0.58              |
| 65:LZ:56:ILE:O     | 72:Lg:157:ARG:NH2  | 2.28                     | 0.58              |
| 68:Lc:46:PHE:HB2   | 68:Lc:139:ARG:HD2  | 1.85                     | 0.58              |
| 80:Lo:59:PRO:HA    | 80:Lo:66:LYS:HA    | 1.86                     | 0.58              |
| 1:S1:34:U:H2'      | 1:S1:35:G:H8       | 1.69                     | 0.58              |
| 54:LO:110:G:H2'    | 54:LO:111:C:C6     | 2.38                     | 0.58              |
| 57:LR:40:LYS:HD2   | 57:LR:107:ALA:HB2  | 1.85                     | 0.58              |
| 60:LU:82:GLN:HB3   | 60:LU:124:ARG:HD3  | 1.84                     | 0.58              |
| 70:Le:42:PHE:CD2   | 70:Le:132:GLY:HA3  | 2.38                     | 0.58              |
| 1:S1:661:G:OP2     | 36:Se:57:GLN:NE2   | 2.36                     | 0.58              |
| 1:S1:1448:A:H5''   | 34:Sc:72:LYS:HG3   | 1.86                     | 0.58              |
| 7:SB:15:ILE:HG13   | 27:SV:115:MET:HG3  | 1.83                     | 0.58              |
| 20:SO:118:ARG:NH1  | 35:Sd:69:GLU:O     | 2.34                     | 0.58              |
| 29:SX:30:LYS:O     | 29:SX:112:LYS:NZ   | 2.31                     | 0.58              |
| 40:LA:70:A:N1      | 40:LA:81:C:O2'     | 2.34                     | 0.58              |
| 41:LB:227:A:O2'    | 42:LC:520:A:N3     | 2.35                     | 0.58              |
| 44:LE:1114:G:H5''  | 90:Ly:16:HIS:CE1   | 2.38                     | 0.58              |
| 44:LE:1281:G:O6    | 45:LF:1745:C:O2'   | 2.17                     | 0.58              |
| 53:LN:3986:C:O2'   | 53:LN:3990:G:OP2   | 2.21                     | 0.58              |
| 54:LO:112:U:H2'    | 54:LO:113:G:H8     | 1.69                     | 0.58              |
| 56:LQ:161:ARG:NH1  | 56:LQ:182:GLU:OE2  | 2.35                     | 0.58              |
| 56:LQ:220:ILE:HG23 | 56:LQ:278:VAL:HG22 | 1.85                     | 0.58              |
| 1:S1:321:U:O2'     | 1:S1:323:A:N7      | 2.33                     | 0.58              |
| 1:S1:729:C:H2'     | 1:S1:730:U:C6      | 2.39                     | 0.58              |
| 45:LF:1566:G:H2'   | 45:LF:1567:A:C8    | 2.39                     | 0.58              |
| 56:LQ:122:TRP:CZ2  | 56:LQ:127:LYS:HG2  | 2.38                     | 0.58              |
| 4:S4:27:G:H2'      | 4:S4:28:G:H8       | 1.68                     | 0.58              |
| 11:SF:89:LYS:HD3   | 11:SF:96:ARG:HD3   | 1.84                     | 0.58              |
| 44:LE:832:U:H2'    | 44:LE:833:C:C6     | 2.39                     | 0.58              |
| 45:LF:1725:U:H5    | 70:Le:36:ARG:HH22  | 1.52                     | 0.58              |
| 49:LJ:3726:A:O2'   | 49:LJ:3728:A:OP2   | 2.20                     | 0.58              |
| 56:LQ:92:TYR:HB2   | 56:LQ:159:VAL:HB   | 1.86                     | 0.58              |
| 56:LQ:94:LYS:HE3   | 62:LW:157:THR:HG23 | 1.85                     | 0.58              |
| 61:LV:82:ASP:HB2   | 76:Lk:44:ILE:HD11  | 1.84                     | 0.58              |
| 66:La:25:GLY:O     | 100:La:201:HOH:O   | 2.16                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:Ld:39:ASP:OD1   | 73:Lh:70:ARG:NH1   | 2.36                     | 0.58              |
| 91:Lz:23:VAL:HG22  | 91:Lz:36:VAL:HG22  | 1.86                     | 0.58              |
| 1:S1:17:C:O2'      | 1:S1:1547:A:N1     | 2.32                     | 0.58              |
| 1:S1:490:C:H2'     | 1:S1:491:C:C6      | 2.38                     | 0.58              |
| 1:S1:830:C:H2'     | 1:S1:831:U:C2      | 2.38                     | 0.58              |
| 1:S1:2078:7MG:H2'  | 1:S1:2079:A:C8     | 2.39                     | 0.58              |
| 11:SF:81:VAL:HG22  | 11:SF:103:VAL:HG22 | 1.86                     | 0.58              |
| 11:SF:103:VAL:HG11 | 11:SF:130:ILE:HG12 | 1.85                     | 0.58              |
| 11:SF:119:SER:HG   | 11:SF:124:THR:HG1  | 1.51                     | 0.58              |
| 96:L4:8:ARG:O      | 96:L4:23:HIS:HB2   | 2.04                     | 0.58              |
| 7:SB:158:ASP:HB3   | 30:SY:34:PHE:HZ    | 1.69                     | 0.58              |
| 11:SF:72:PRO:HD2   | 11:SF:76:LYS:HB2   | 1.85                     | 0.58              |
| 14:SI:90:GLU:O     | 14:SI:93:PHE:C     | 2.46                     | 0.58              |
| 27:SV:94:GLN:HE21  | 27:SV:98:GLN:HE21  | 1.50                     | 0.58              |
| 39:Sh:93:LEU:HD21  | 39:Sh:117:PHE:HZ   | 1.69                     | 0.58              |
| 47:LH:2383:U:H5''  | 47:LH:2384:U:H5    | 1.69                     | 0.58              |
| 55:LP:242:ARG:NH1  | 55:LP:243:THR:O    | 2.36                     | 0.58              |
| 58:LS:64:ILE:HD12  | 58:LS:69:ILE:HD11  | 1.86                     | 0.58              |
| 59:LT:115:ARG:HE   | 59:LT:123:ILE:HD13 | 1.67                     | 0.58              |
| 1:S1:68:A:O2'      | 1:S1:70:C:OP2      | 2.18                     | 0.58              |
| 1:S1:1260:A:OP2    | 100:S1:2412:HOH:O  | 2.17                     | 0.58              |
| 9:SD:83:TYR:O      | 9:SD:85:LEU:N      | 2.34                     | 0.58              |
| 13:SH:139:LEU:HD22 | 13:SH:178:LYS:HG2  | 1.86                     | 0.58              |
| 44:LE:1229:A:O2'   | 90:Ly:49:TRP:O     | 2.15                     | 0.58              |
| 48:LI:3141:A:H2'   | 48:LI:3142:C:C6    | 2.38                     | 0.58              |
| 56:LQ:154:LYS:HG2  | 56:LQ:191:ALA:HA   | 1.85                     | 0.58              |
| 95:L5:14:TYR:OH    | 95:L5:30:GLU:OE1   | 2.20                     | 0.58              |
| 1:S1:980:U:H2'     | 1:S1:981:G:C8      | 2.39                     | 0.57              |
| 1:S1:2156:C:H4'    | 94:L3:30:ARG:HD2   | 1.85                     | 0.57              |
| 10:SE:11:ARG:HD2   | 10:SE:20:MET:HB3   | 1.86                     | 0.57              |
| 14:SI:25:GLU:HA    | 14:SI:28:VAL:HG22  | 1.86                     | 0.57              |
| 33:Sb:43:ASN:OD1   | 33:Sb:67:LYS:NZ    | 2.36                     | 0.57              |
| 40:LA:5:G:H2'      | 40:LA:6:U:C6       | 2.39                     | 0.57              |
| 53:LN:4011:G:C2    | 53:LN:4019:U:O2    | 2.56                     | 0.57              |
| 90:Ly:91:THR:O     | 90:Ly:95:ARG:HG3   | 2.03                     | 0.57              |
| 3:S3:34:C:O2'      | 3:S3:35:A:OP1      | 2.22                     | 0.57              |
| 3:S3:75:C:H2'      | 3:S3:76:A:C2       | 2.39                     | 0.57              |
| 44:LE:835:C:H1'    | 97:L6:54:GLN:HE21  | 1.69                     | 0.57              |
| 44:LE:1116:A:OP2   | 100:LE:1509:HOH:O  | 2.17                     | 0.57              |
| 45:LF:1697:G:H2'   | 45:LF:1704:C:O2    | 2.04                     | 0.57              |
| 58:LS:48:GLU:HB2   | 58:LS:55:PRO:HD3   | 1.85                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:LX:49:ALA:O    | 63:LX:53:PHE:HA    | 2.04                     | 0.57              |
| 87:Lv:83:HIS:ND1  | 87:Lv:90:LYS:HE3   | 2.19                     | 0.57              |
| 1:S1:1653:G:H1    | 28:SW:60:ALA:HB2   | 1.68                     | 0.57              |
| 1:S1:1962:A:O2'   | 29:SX:50:PRO:O     | 2.21                     | 0.57              |
| 34:Sc:76:THR:OG1  | 34:Sc:79:CYS:SG    | 2.62                     | 0.57              |
| 41:LB:278:U:H2'   | 41:LB:279:C:H6     | 1.67                     | 0.57              |
| 44:LE:973:C:OP2   | 63:LX:42:ARG:NH2   | 2.35                     | 0.57              |
| 44:LE:992:G:O6    | 57:LR:111:ARG:NH2  | 2.32                     | 0.57              |
| 45:LF:1722:A:OP1  | 70:Le:11:ASN:ND2   | 2.37                     | 0.57              |
| 45:LF:1770:C:OP2  | 57:LR:198:ARG:NH1  | 2.33                     | 0.57              |
| 1:S1:2179:C:OP1   | 16:SK:44:ARG:NH1   | 2.37                     | 0.57              |
| 19:SN:24:LYS:HG3  | 19:SN:26:ASP:H     | 1.68                     | 0.57              |
| 22:SQ:25:ALA:HB3  | 22:SQ:131:MET:HE3  | 1.86                     | 0.57              |
| 54:LO:1:G:H5'     | 97:L6:37:LYS:HG2   | 1.86                     | 0.57              |
| 54:LO:75:G:H3'    | 72:Lg:50:LYS:HA    | 1.86                     | 0.57              |
| 55:LP:227:ARG:O   | 55:LP:234:LYS:NZ   | 2.24                     | 0.57              |
| 61:LV:90:PRO:HD2  | 61:LV:93:ILE:HD12  | 1.85                     | 0.57              |
| 67:Lb:191:ASN:O   | 67:Lb:195:ARG:HG2  | 2.03                     | 0.57              |
| 69:Ld:20:ARG:NH2  | 69:Ld:24:GLU:OE2   | 2.37                     | 0.57              |
| 1:S1:1588:G:O6    | 23:SR:138:LYS:NZ   | 2.38                     | 0.57              |
| 2:S2:63:G:H2'     | 2:S2:64:A:H8       | 1.69                     | 0.57              |
| 11:SF:246:ASP:OD1 | 11:SF:247:PHE:N    | 2.38                     | 0.57              |
| 22:SQ:101:SER:H   | 22:SQ:109:LYS:HE3  | 1.70                     | 0.57              |
| 39:Sh:47:ILE:HG23 | 39:Sh:55:VAL:HG13  | 1.86                     | 0.57              |
| 44:LE:813:U:H2'   | 97:L6:62:LYS:HE2   | 1.87                     | 0.57              |
| 48:LI:3424:A:OP1  | 68:Lc:154:ARG:NH1  | 2.37                     | 0.57              |
| 48:LI:3532:G:O2'  | 48:LI:3535:OMC:OP2 | 2.18                     | 0.57              |
| 68:Lc:50:TYR:OH   | 68:Lc:145:GLU:OE2  | 2.19                     | 0.57              |
| 77:LI:58:LYS:O    | 77:LI:59:ARG:NH1   | 2.34                     | 0.57              |
| 1:S1:858:U:N3     | 1:S1:859:G:O6      | 2.38                     | 0.57              |
| 13:SH:81:ALA:O    | 13:SH:85:ILE:HG22  | 2.03                     | 0.57              |
| 40:LA:50:G:N1     | 92:L1:35:GLN:OE1   | 2.27                     | 0.57              |
| 54:LO:99:G:N7     | 72:Lg:55:LYS:NZ    | 2.50                     | 0.57              |
| 1:S1:258:U:O2'    | 1:S1:292:C:OP1     | 2.20                     | 0.57              |
| 1:S1:1581:A:O2'   | 1:S1:2073:A:N3     | 2.35                     | 0.57              |
| 1:S1:2067:C:O2    | 23:SR:88:LYS:NZ    | 2.25                     | 0.57              |
| 4:S4:75:A:H1'     | 96:L4:55:LYS:HB2   | 1.86                     | 0.57              |
| 22:SQ:64:CYS:SG   | 22:SQ:65:THR:N     | 2.73                     | 0.57              |
| 23:SR:28:ALA:HB1  | 23:SR:43:ILE:HG12  | 1.87                     | 0.57              |
| 33:Sb:10:ARG:HH22 | 33:Sb:31:PRO:HG2   | 1.69                     | 0.57              |
| 44:LE:798:G:O6    | 44:LE:845:U:O2     | 2.22                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:LE:835:C:H2'    | 44:LE:836:C:C6     | 2.39                     | 0.57              |
| 44:LE:918:U:O2     | 87:Lv:24:GLN:NE2   | 2.37                     | 0.57              |
| 44:LE:1263:G:OP1   | 100:LE:1510:HOH:O  | 2.17                     | 0.57              |
| 47:LH:2960:G:H1    | 47:LH:2965:C:H42   | 1.52                     | 0.57              |
| 59:LT:94:PHE:HB2   | 59:LT:144:ASP:HB3  | 1.85                     | 0.57              |
| 69:Ld:50:LEU:HD22  | 69:Ld:164:VAL:HG21 | 1.85                     | 0.57              |
| 73:Lh:117:ARG:NH1  | 98:L7:36:ARG:HG2   | 2.18                     | 0.57              |
| 1:S1:723:A2M:OP2   | 100:S1:2413:HOH:O  | 2.17                     | 0.57              |
| 1:S1:1570:A:H2'    | 1:S1:1571:C:C6     | 2.39                     | 0.57              |
| 1:S1:1628:G:OP2    | 100:S1:2405:HOH:O  | 2.18                     | 0.57              |
| 1:S1:1706:A:OP1    | 7:SB:139:TYR:OH    | 2.16                     | 0.57              |
| 15:SJ:38:LEU:HD23  | 15:SJ:41:MET:HE3   | 1.86                     | 0.57              |
| 29:SX:45:PHE:O     | 29:SX:87:ARG:NH1   | 2.37                     | 0.57              |
| 1:S1:1357:U:H1'    | 25:ST:52:ILE:HG13  | 1.87                     | 0.57              |
| 7:SB:200:ASP:O     | 7:SB:205:ARG:NH2   | 2.38                     | 0.57              |
| 10:SE:19:MET:SD    | 10:SE:108:ARG:NH1  | 2.78                     | 0.57              |
| 19:SN:73:GLU:OE2   | 19:SN:76:ARG:NH1   | 2.37                     | 0.57              |
| 44:LE:1445:C:OP1   | 98:L7:31:LYS:NZ    | 2.37                     | 0.57              |
| 47:LH:2250:C:H2'   | 47:LH:2251:A:C8    | 2.40                     | 0.57              |
| 47:LH:2631:A:OP2   | 47:LH:2812:A2M:H8  | 2.04                     | 0.57              |
| 48:LI:3356:G:H2'   | 48:LI:3357:A:C8    | 2.39                     | 0.57              |
| 48:LI:3579:C:OP1   | 56:LQ:21:ARG:NH1   | 2.38                     | 0.57              |
| 57:LR:28:TYR:HE1   | 70:Le:22:PRO:HG3   | 1.70                     | 0.57              |
| 58:LS:170:ILE:HG23 | 58:LS:181:VAL:HG21 | 1.87                     | 0.57              |
| 67:Lb:104:GLY:HA2  | 67:Lb:160:GLU:HG3  | 1.87                     | 0.57              |
| 73:Lh:14:LEU:HD11  | 73:Lh:58:GLN:HG2   | 1.86                     | 0.57              |
| 1:S1:723:A2M:OP1   | 100:S1:2414:HOH:O  | 2.18                     | 0.57              |
| 11:SF:114:LEU:HD11 | 11:SF:212:VAL:HG13 | 1.86                     | 0.57              |
| 44:LE:994:G:H2'    | 44:LE:995:G:H8     | 1.70                     | 0.57              |
| 45:LF:1711:G:O2'   | 83:Lr:207:LEU:O    | 2.23                     | 0.57              |
| 54:LO:106:G:H2'    | 54:LO:107:G:C8     | 2.39                     | 0.57              |
| 80:Lo:58:VAL:HG12  | 80:Lo:69:LYS:HG3   | 1.87                     | 0.57              |
| 84:Ls:30:TYR:OH    | 84:Ls:58:GLU:OE1   | 2.22                     | 0.57              |
| 1:S1:100:U:OP2     | 100:S1:2401:HOH:O  | 2.17                     | 0.56              |
| 1:S1:672:G:N7      | 21:SP:67:ARG:NH1   | 2.50                     | 0.56              |
| 11:SF:181:ALA:HB1  | 11:SF:185:PRO:HB2  | 1.86                     | 0.56              |
| 12:SG:75:LEU:HD12  | 12:SG:99:ILE:HD11  | 1.85                     | 0.56              |
| 21:SP:41:PHE:O     | 21:SP:43:GLY:N     | 2.38                     | 0.56              |
| 36:Se:59:ASN:OD1   | 36:Se:61:GLN:NE2   | 2.37                     | 0.56              |
| 45:LF:1725:U:O3'   | 57:LR:285:LYS:NZ   | 2.37                     | 0.56              |
| 47:LH:2890:A:H2'   | 57:LR:63:THR:HG21  | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:LI:3468:U:H2'   | 48:LI:3469:U:C6    | 2.40                     | 0.56              |
| 60:LU:81:ALA:O     | 60:LU:120:SER:OG   | 2.23                     | 0.56              |
| 61:LV:256:LEU:O    | 61:LV:261:LYS:NZ   | 2.38                     | 0.56              |
| 83:Lr:176:TYR:HB3  | 83:Lr:194:ARG:HD3  | 1.87                     | 0.56              |
| 1:S1:270:G:N2      | 1:S1:348:A:OP2     | 2.29                     | 0.56              |
| 1:S1:1581:A:H2'    | 1:S1:1582:G:H8     | 1.71                     | 0.56              |
| 2:S2:56:C:H2'      | 2:S2:57:G:H8       | 1.70                     | 0.56              |
| 2:S2:62:C:H2'      | 2:S2:63:G:C8       | 2.40                     | 0.56              |
| 38:Sg:135:THR:HG22 | 38:Sg:214:LYS:HB3  | 1.87                     | 0.56              |
| 41:LB:260:A:H2'    | 41:LB:261:C:C6     | 2.40                     | 0.56              |
| 44:LE:942:A:H2'    | 44:LE:943:A:C8     | 2.40                     | 0.56              |
| 45:LF:1735:G:OP2   | 80:Lo:44:ARG:NH1   | 2.38                     | 0.56              |
| 46:LG:2152:U:H2'   | 46:LG:2153:A:C8    | 2.40                     | 0.56              |
| 47:LH:2635:C:OP2   | 55:LP:200:ARG:NH1  | 2.38                     | 0.56              |
| 56:LQ:19:ARG:NH2   | 56:LQ:234:ARG:O    | 2.35                     | 0.56              |
| 58:LS:89:LEU:HG    | 58:LS:137:PHE:HE2  | 1.70                     | 0.56              |
| 59:LT:57:CYS:HB3   | 59:LT:70:ILE:HG23  | 1.86                     | 0.56              |
| 1:S1:958:A:H2'     | 1:S1:959:A:C8      | 2.38                     | 0.56              |
| 1:S1:1456:A:OP1    | 6:SA:193:LYS:CE    | 2.52                     | 0.56              |
| 1:S1:2147:C:O2'    | 47:LH:2743:A:N1    | 2.36                     | 0.56              |
| 6:SA:109:ARG:NH2   | 20:SO:136:ILE:HG12 | 2.20                     | 0.56              |
| 6:SA:142:LYS:HE2   | 6:SA:204:PRO:HB2   | 1.87                     | 0.56              |
| 10:SE:30:LYS:O     | 10:SE:81:LYS:HD2   | 2.05                     | 0.56              |
| 11:SF:171:VAL:HB   | 11:SF:198:PHE:HB2  | 1.86                     | 0.56              |
| 12:SG:7:SER:HA     | 12:SG:115:ILE:HG12 | 1.86                     | 0.56              |
| 28:SW:86:ARG:NH1   | 28:SW:102:TYR:O    | 2.34                     | 0.56              |
| 33:Sb:34:LYS:HG2   | 33:Sb:76:ILE:HD11  | 1.87                     | 0.56              |
| 39:Sh:169:ILE:HB   | 39:Sh:181:TRP:HB2  | 1.86                     | 0.56              |
| 40:LA:92:G:O2'     | 40:LA:93:A:O5'     | 2.18                     | 0.56              |
| 41:LB:201:G:OP1    | 100:LB:301:HOH:O   | 2.18                     | 0.56              |
| 45:LF:1788:U:O3'   | 86:Lu:71:ARG:NH1   | 2.38                     | 0.56              |
| 47:LH:2857:G:H2'   | 47:LH:2858:G:C8    | 2.40                     | 0.56              |
| 47:LH:2943:U:H4'   | 48:LI:2982:G:H22   | 1.69                     | 0.56              |
| 48:LI:3340:C:OP1   | 66:La:62:LYS:NZ    | 2.37                     | 0.56              |
| 54:LO:51:G:N7      | 100:LO:203:HOH:O   | 2.32                     | 0.56              |
| 54:LO:69:C:H2'     | 54:LO:70:A:C8      | 2.39                     | 0.56              |
| 64:LY:57:VAL:O     | 64:LY:125:ALA:HB2  | 2.06                     | 0.56              |
| 66:La:118:GLY:O    | 66:La:140:LYS:NZ   | 2.29                     | 0.56              |
| 77:LI:50:ARG:HB2   | 77:LI:114:ARG:HH22 | 1.69                     | 0.56              |
| 1:S1:1309:U:OP1    | 1:S1:1310:A:O2'    | 2.20                     | 0.56              |
| 1:S1:1981:G:H2'    | 1:S1:1982:C:C6     | 2.40                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:S3:57:G:N2        | 58:LS:70:ARG:HH22  | 2.03                     | 0.56              |
| 7:SB:155:VAL:HG13   | 7:SB:156:TYR:H     | 1.70                     | 0.56              |
| 45:LF:1488:C:H2'    | 45:LF:1489:A:C8    | 2.40                     | 0.56              |
| 45:LF:1585:C:H4'    | 72:Lg:93:VAL:HG13  | 1.87                     | 0.56              |
| 45:LF:1751:G:N2     | 45:LF:1752:U:O4    | 2.39                     | 0.56              |
| 47:LH:2799:G:OP1    | 100:LH:3007:HOH:O  | 2.17                     | 0.56              |
| 59:LT:93:ARG:NH2    | 93:L2:77:GLU:OE2   | 2.38                     | 0.56              |
| 65:LZ:93:THR:O      | 65:LZ:97:ARG:HG3   | 2.06                     | 0.56              |
| 68:Lc:30:LYS:HG3    | 68:Lc:63:GLU:HG2   | 1.87                     | 0.56              |
| 83:Lr:85:ALA:HB2    | 83:Lr:120:LEU:HD11 | 1.87                     | 0.56              |
| 1:S1:335:C:H2'      | 1:S1:336:C:C6      | 2.40                     | 0.56              |
| 1:S1:1919:U:O2'     | 1:S1:1920:G:OP1    | 2.20                     | 0.56              |
| 3:S3:61:C:H2'       | 3:S3:62:C:C6       | 2.40                     | 0.56              |
| 5:S5:9:U:O2'        | 21:SP:61:GLN:NE2   | 2.37                     | 0.56              |
| 12:SG:161:ARG:NH2   | 12:SG:174:SER:O    | 2.39                     | 0.56              |
| 17:SL:102:GLN:HB3   | 17:SL:110:LYS:HG3  | 1.87                     | 0.56              |
| 21:SP:96:GLU:N      | 21:SP:96:GLU:OE1   | 2.38                     | 0.56              |
| 39:Sh:290:CYS:HA    | 39:Sh:306:TYR:HB3  | 1.87                     | 0.56              |
| 42:LC:333:G:OP2     | 67:Lb:54:LYS:NZ    | 2.38                     | 0.56              |
| 44:LE:812:C:N4      | 44:LE:828:G:O6     | 2.38                     | 0.56              |
| 44:LE:974:U:H5      | 63:LX:42:ARG:HH12  | 1.53                     | 0.56              |
| 44:LE:1029:U:O2'    | 44:LE:1031:G:OP2   | 2.20                     | 0.56              |
| 45:LF:1822:OMC:HM23 | 57:LR:89:MET:HG3   | 1.88                     | 0.56              |
| 45:LF:1844:C:OP1    | 85:Lt:77:ARG:NH2   | 2.26                     | 0.56              |
| 46:LG:2093:U:H5'    | 88:Lw:19:ARG:HH12  | 1.69                     | 0.56              |
| 64:LY:16:ILE:HD11   | 64:LY:124:GLU:HG2  | 1.87                     | 0.56              |
| 67:Lb:73:ARG:HH21   | 67:Lb:92:LEU:HD21  | 1.69                     | 0.56              |
| 1:S1:132:G:OP1      | 1:S1:202:U:O2'     | 2.21                     | 0.56              |
| 1:S1:421:C:OP1      | 26:SU:138:LYS:NZ   | 2.34                     | 0.56              |
| 44:LE:944:G:OP2     | 100:LE:1511:HOH:O  | 2.17                     | 0.56              |
| 45:LF:1659:A:H2'    | 45:LF:1660:G:C8    | 2.40                     | 0.56              |
| 47:LH:2941:C:N3     | 47:LH:2942:G:N2    | 2.54                     | 0.56              |
| 75:Lj:81:LEU:HD21   | 75:Lj:109:ILE:HG12 | 1.86                     | 0.56              |
| 1:S1:110:A2M:H2     | 1:S1:402:U:O2      | 2.06                     | 0.56              |
| 1:S1:380:U:H2'      | 1:S1:381:G:N7      | 2.20                     | 0.56              |
| 1:S1:1663:U:OP1     | 22:SQ:48:LYS:NZ    | 2.39                     | 0.56              |
| 1:S1:2114:A:O2'     | 13:SH:60:ASN:HB3   | 2.04                     | 0.56              |
| 7:SB:49:LEU:HD12    | 7:SB:162:PRO:HB3   | 1.86                     | 0.56              |
| 13:SH:59:VAL:HG11   | 13:SH:72:LYS:HE3   | 1.87                     | 0.56              |
| 39:Sh:161:ASN:OD1   | 39:Sh:168:LEU:N    | 2.27                     | 0.56              |
| 44:LE:1059:G:H2'    | 44:LE:1060:U:H6    | 1.69                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 48:LI:3551:G:N2     | 48:LI:3554:A:OP2   | 2.30                     | 0.56              |
| 55:LP:200:ARG:NH2   | 55:LP:217:GLN:OE1  | 2.39                     | 0.56              |
| 64:LY:88:TRP:HH2    | 64:LY:98:PHE:HE1   | 1.53                     | 0.56              |
| 91:Lz:24:LYS:HD3    | 91:Lz:69:ILE:HD11  | 1.87                     | 0.56              |
| 1:S1:495:G:OP1      | 16:SK:49:ARG:NH1   | 2.37                     | 0.56              |
| 1:S1:941:C:OP2      | 38:Sg:137:TRP:NE1  | 2.38                     | 0.56              |
| 1:S1:1768:C:OP1     | 29:SX:132:ARG:NH2  | 2.39                     | 0.56              |
| 1:S1:2068:C:OP1     | 23:SR:40:ARG:HD3   | 2.06                     | 0.56              |
| 8:SC:64:LYS:O       | 8:SC:69:ARG:NH1    | 2.33                     | 0.56              |
| 11:SF:119:SER:OG    | 11:SF:124:THR:OG1  | 2.21                     | 0.56              |
| 27:SV:75:GLU:OE2    | 27:SV:78:ARG:NH2   | 2.39                     | 0.56              |
| 27:SV:102:VAL:HG12  | 27:SV:107:LEU:HD22 | 1.88                     | 0.56              |
| 35:Sd:51:ARG:NH2    | 35:Sd:67:GLU:O     | 2.39                     | 0.56              |
| 39:Sh:88:ASP:O      | 39:Sh:90:THR:N     | 2.39                     | 0.56              |
| 44:LE:810:G:OP1     | 68:Lc:208:ARG:NH1  | 2.39                     | 0.56              |
| 44:LE:1314:G:O2'    | 44:LE:1377:G:O6    | 2.22                     | 0.56              |
| 45:LF:1759:G:OP2    | 66:La:7:LYS:NZ     | 2.26                     | 0.56              |
| 81:Lp:91:GLU:HA     | 81:Lp:94:ALA:HB2   | 1.87                     | 0.56              |
| 1:S1:751:C:N4       | 1:S1:858:U:O4      | 2.39                     | 0.56              |
| 1:S1:1588:G:O2'     | 28:SW:139:GLY:O    | 2.18                     | 0.56              |
| 2:S2:59:U:H2'       | 2:S2:60:U:C6       | 2.41                     | 0.56              |
| 17:SL:101:TYR:HA    | 17:SL:105:VAL:HG22 | 1.88                     | 0.56              |
| 39:Sh:43:LEU:HD22   | 39:Sh:59:PRO:HB3   | 1.88                     | 0.56              |
| 40:LA:35:A:OP1      | 81:Lp:92:ARG:NH2   | 2.38                     | 0.56              |
| 40:LA:107:U:H2'     | 40:LA:108:C:C6     | 2.41                     | 0.56              |
| 41:LB:258:G:N7      | 63:LX:13:HIS:NE2   | 2.52                     | 0.56              |
| 44:LE:1438:U:OP2    | 82:Lq:75:TYR:OH    | 2.23                     | 0.56              |
| 48:LI:3546:OMC:HM22 | 48:LI:3547:C:O4'   | 2.06                     | 0.56              |
| 73:Lh:40:VAL:HB     | 73:Lh:96:VAL:HG22  | 1.87                     | 0.56              |
| 4:S4:1:G:H2'        | 4:S4:2:C:H6        | 1.71                     | 0.56              |
| 14:SI:146:ARG:HB3   | 14:SI:154:GLN:HB2  | 1.88                     | 0.56              |
| 41:LB:229:C:O2      | 63:LX:68:LYS:NZ    | 2.33                     | 0.56              |
| 41:LB:239:U:H2'     | 41:LB:240:G:H8     | 1.71                     | 0.56              |
| 46:LG:2115:G:OP2    | 75:Lj:128:LYS:NZ   | 2.39                     | 0.56              |
| 53:LN:3991:C:H4'    | 56:LQ:319:GLY:HA2  | 1.87                     | 0.56              |
| 1:S1:214:C:H2'      | 1:S1:215:A:H8      | 1.71                     | 0.55              |
| 40:LA:150:G:H5''    | 67:Lb:60:VAL:HG11  | 1.88                     | 0.55              |
| 42:LC:588:G:N2      | 42:LC:591:A:OP2    | 2.33                     | 0.55              |
| 48:LI:3388:A:C8     | 96:L4:56:PRO:HB3   | 2.41                     | 0.55              |
| 49:LJ:3677:A:OP1    | 100:LJ:3801:HOH:O  | 2.18                     | 0.55              |
| 55:LP:137:ILE:HD13  | 55:LP:155:LYS:HE3  | 1.87                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 94:L3:2:GLY:N      | 100:L3:102:HOH:O   | 2.39                     | 0.55              |
| 1:S1:2256:A:H4'    | 94:L3:22:LEU:HD21  | 1.88                     | 0.55              |
| 2:S2:63:G:H2'      | 2:S2:64:A:C8       | 2.41                     | 0.55              |
| 7:SB:117:MET:O     | 7:SB:119:PRO:HD3   | 2.06                     | 0.55              |
| 11:SF:153:HIS:ND1  | 11:SF:196:ASP:OD2  | 2.36                     | 0.55              |
| 12:SG:150:THR:HG23 | 12:SG:152:GLU:HG3  | 1.87                     | 0.55              |
| 13:SH:112:THR:O    | 13:SH:122:ARG:HA   | 2.06                     | 0.55              |
| 22:SQ:28:GLU:HB3   | 22:SQ:32:ARG:HH22  | 1.70                     | 0.55              |
| 42:LC:582:A:N6     | 42:LC:604:G:O2'    | 2.40                     | 0.55              |
| 46:LG:2154:PSU:H5' | 79:Ln:38:TYR:HB3   | 1.86                     | 0.55              |
| 55:LP:130:SER:OG   | 55:LP:171:GLY:O    | 2.16                     | 0.55              |
| 82:Lq:64:SER:O     | 82:Lq:71:ARG:NH2   | 2.39                     | 0.55              |
| 42:LC:580:A:O2'    | 77:Ll:86:ARG:NH1   | 2.39                     | 0.55              |
| 44:LE:1073:G:H2'   | 44:LE:1074:U:H5''  | 1.87                     | 0.55              |
| 47:LH:2617:PSU:H2' | 47:LH:2618:G:C8    | 2.42                     | 0.55              |
| 56:LQ:29:ILE:HD11  | 56:LQ:341:THR:HG21 | 1.88                     | 0.55              |
| 1:S1:970:A:N1      | 1:S1:980:U:C4      | 2.74                     | 0.55              |
| 1:S1:1542:A:H2'    | 1:S1:1543:A:H8     | 1.71                     | 0.55              |
| 1:S1:1851:A:HO2'   | 1:S1:1852:G:H8     | 1.54                     | 0.55              |
| 4:S4:75:A:H4'      | 96:L4:57:VAL:HG12  | 1.88                     | 0.55              |
| 9:SD:63:GLU:O      | 9:SD:69:ARG:NH1    | 2.40                     | 0.55              |
| 11:SF:89:LYS:HB3   | 11:SF:96:ARG:HH11  | 1.72                     | 0.55              |
| 28:SW:89:VAL:HG22  | 28:SW:120:TYR:CE1  | 2.40                     | 0.55              |
| 45:LF:1545:C:H4'   | 62:LW:94:PRO:HD3   | 1.89                     | 0.55              |
| 57:LR:5:PRO:HB3    | 80:Lo:13:LYS:HG2   | 1.89                     | 0.55              |
| 1:S1:301:G:H2'     | 1:S1:302:G:C8      | 2.42                     | 0.55              |
| 1:S1:2049:G:H2'    | 1:S1:2050:A:C8     | 2.41                     | 0.55              |
| 1:S1:2277:G:H1'    | 94:L3:3:SER:HB3    | 1.89                     | 0.55              |
| 14:SI:46:LEU:HG    | 14:SI:81:ILE:HD11  | 1.87                     | 0.55              |
| 14:SI:125:SER:O    | 14:SI:129:ASN:ND2  | 2.28                     | 0.55              |
| 47:LH:2950:G:N7    | 47:LH:2951:G:N2    | 2.53                     | 0.55              |
| 48:LI:3008:U:H2'   | 48:LI:3009:U:C6    | 2.41                     | 0.55              |
| 48:LI:3528:A:H8    | 48:LI:3528:A:OP2   | 1.90                     | 0.55              |
| 55:LP:105:SER:HB3  | 55:LP:160:SER:HB3  | 1.87                     | 0.55              |
| 65:LZ:59:ILE:O     | 72:Lg:157:ARG:NH2  | 2.24                     | 0.55              |
| 85:Lt:119:ARG:HG3  | 85:Lt:127:LYS:HE3  | 1.88                     | 0.55              |
| 1:S1:1062:G:O6     | 31:SZ:47:LYS:NZ    | 2.36                     | 0.55              |
| 1:S1:2067:C:H2'    | 1:S1:2068:C:C6     | 2.42                     | 0.55              |
| 2:S2:24:G:H2'      | 2:S2:25:C:O4'      | 2.06                     | 0.55              |
| 12:SG:124:GLU:HA   | 12:SG:128:ASP:OD2  | 2.07                     | 0.55              |
| 40:LA:113:G:H4'    | 40:LA:146:G:H5'    | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:LI:3466:U:H1'   | 56:LQ:252:ALA:HB3  | 1.89                     | 0.55              |
| 49:LJ:3687:U:OP1   | 56:LQ:329:LYS:NZ   | 2.40                     | 0.55              |
| 52:LM:3913:C:H2'   | 52:LM:3914:A:C8    | 2.42                     | 0.55              |
| 1:S1:996:G:O2'     | 1:S1:997:G:OP2     | 2.24                     | 0.55              |
| 8:SC:30:GLU:O      | 8:SC:67:ARG:NH2    | 2.39                     | 0.55              |
| 15:SJ:75:ILE:HG13  | 15:SJ:93:LEU:HD21  | 1.88                     | 0.55              |
| 41:LB:239:U:H2'    | 41:LB:240:G:C8     | 2.42                     | 0.55              |
| 43:LD:691:C:H2'    | 43:LD:692:C:C6     | 2.42                     | 0.55              |
| 44:LE:815:C:H2'    | 44:LE:816:A:H8     | 1.70                     | 0.55              |
| 44:LE:1045:C:H2'   | 44:LE:1047:A:C8    | 2.41                     | 0.55              |
| 47:LH:2246:U:H2'   | 55:LP:50:HIS:CD2   | 2.42                     | 0.55              |
| 48:LI:3183:U:H2'   | 48:LI:3184:U:C6    | 2.41                     | 0.55              |
| 67:Lb:165:THR:HG22 | 67:Lb:166:SER:H    | 1.71                     | 0.55              |
| 81:Lp:7:HIS:CE1    | 81:Lp:8:GLU:HG3    | 2.42                     | 0.55              |
| 84:Ls:34:LEU:HD22  | 84:Ls:62:TYR:CD2   | 2.42                     | 0.55              |
| 1:S1:211:C:H3'     | 1:S1:212:A:H8      | 1.72                     | 0.55              |
| 1:S1:695:G:H2'     | 1:S1:696:A:C8      | 2.41                     | 0.55              |
| 1:S1:1161:G:C2     | 1:S1:1241:C:O2     | 2.59                     | 0.55              |
| 1:S1:1499:C:OP1    | 33:Sb:6:ARG:NH1    | 2.40                     | 0.55              |
| 1:S1:2099:C:H3'    | 24:SS:31:ARG:NH2   | 2.21                     | 0.55              |
| 6:SA:34:THR:HA     | 6:SA:39:ARG:NH2    | 2.22                     | 0.55              |
| 18:SM:80:ASP:OD2   | 24:SS:43:ARG:NE    | 2.36                     | 0.55              |
| 42:LC:339:U:H4'    | 42:LC:340:G:H5''   | 1.89                     | 0.55              |
| 46:LG:2016:C:O2'   | 46:LG:2017:G:N7    | 2.40                     | 0.55              |
| 73:Lh:81:ARG:NH2   | 82:Lq:16:ASP:OD1   | 2.40                     | 0.55              |
| 79:Ln:99:ILE:HG13  | 79:Ln:100:THR:HG23 | 1.88                     | 0.55              |
| 1:S1:107:A:H2'     | 1:S1:108:G:C8      | 2.41                     | 0.55              |
| 1:S1:785:G:H2'     | 1:S1:786:G:C8      | 2.41                     | 0.55              |
| 1:S1:899:A:H3'     | 1:S1:900:A:H8      | 1.72                     | 0.55              |
| 1:S1:1248:C:N4     | 1:S1:1249:G:O6     | 2.40                     | 0.55              |
| 1:S1:1271:C:H2'    | 1:S1:1272:G:C8     | 2.42                     | 0.55              |
| 1:S1:2285:U:O4     | 94:L3:21:ARG:NH1   | 2.39                     | 0.55              |
| 21:SP:63:ASN:HD22  | 21:SP:114:ASP:CG   | 2.15                     | 0.55              |
| 29:SX:31:ILE:HG22  | 29:SX:113:MET:SD   | 2.47                     | 0.55              |
| 45:LF:1751:G:OP1   | 100:LF:2008:HOH:O  | 2.18                     | 0.55              |
| 45:LF:1959:G:H1'   | 47:LH:2655:G:H21   | 1.72                     | 0.55              |
| 48:LI:3469:U:H2'   | 48:LI:3470:C:H6    | 1.72                     | 0.55              |
| 53:LN:4003:A:H2'   | 53:LN:4004:G:H8    | 1.72                     | 0.55              |
| 53:LN:4007:A:H2'   | 53:LN:4008:G:C8    | 2.41                     | 0.55              |
| 56:LQ:220:ILE:HG13 | 56:LQ:278:VAL:HG13 | 1.89                     | 0.55              |
| 70:Le:40:THR:OG1   | 70:Le:43:ASN:OD1   | 2.24                     | 0.55              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:S1:691:C:OP2     | 36:Se:23:LYS:NZ      | 2.40                     | 0.55              |
| 1:S1:1259:G:H5''   | 15:SJ:57:ARG:HH11    | 1.72                     | 0.55              |
| 1:S1:2108:A:OP2    | 17:SL:135:LYS:NZ     | 2.31                     | 0.55              |
| 8:SC:144:LEU:HD12  | 8:SC:150:LYS:HB2     | 1.89                     | 0.55              |
| 8:SC:212:ILE:HG12  | 27:SV:16:ILE:HG13    | 1.89                     | 0.55              |
| 44:LE:1068:A:H2'   | 44:LE:1069:C:O4'     | 2.06                     | 0.55              |
| 44:LE:1256:U:H2'   | 44:LE:1257:C:C6      | 2.42                     | 0.55              |
| 45:LF:1570:C:OP2   | 45:LF:1571:C:O2'     | 2.23                     | 0.55              |
| 46:LG:2186:U:H2'   | 46:LG:2187:U:C6      | 2.42                     | 0.55              |
| 54:LO:7:G:OP1      | 69:Ld:32:ARG:NH1     | 2.40                     | 0.55              |
| 1:S1:615:A:OP2     | 9:SD:176:LYS:NZ      | 2.30                     | 0.54              |
| 1:S1:617:U:H2'     | 1:S1:618:G:H8        | 1.70                     | 0.54              |
| 1:S1:977:A:N1      | 38:Sg:129:ARG:HD3    | 2.22                     | 0.54              |
| 1:S1:1542:A:H2'    | 1:S1:1543:A:C8       | 2.42                     | 0.54              |
| 1:S1:1638:G:H22    | 22:SQ:113:ALA:HB3    | 1.72                     | 0.54              |
| 2:S2:23:A:H2'      | 2:S2:24:G:C8         | 2.42                     | 0.54              |
| 44:LE:946:A:OP2    | 100:LF:2001:HOH:O    | 2.18                     | 0.54              |
| 47:LH:2895:C:H2'   | 47:LH:2896:U:H6      | 1.72                     | 0.54              |
| 48:LI:3295:G:H2'   | 48:LI:3296:A:C8      | 2.42                     | 0.54              |
| 56:LQ:245:HIS:O    | 56:LQ:246[B]:LYS:HG2 | 2.07                     | 0.54              |
| 77:Ll:68:LYS:N     | 77:Ll:82:ASP:HB2     | 2.22                     | 0.54              |
| 83:Lr:127:MET:O    | 83:Lr:131:VAL:HG22   | 2.08                     | 0.54              |
| 1:S1:106:C:H2'     | 1:S1:107:A:C8        | 2.42                     | 0.54              |
| 13:SH:41:ARG:HG2   | 13:SH:44:LYS:HG2     | 1.89                     | 0.54              |
| 26:SU:18:PHE:O     | 26:SU:37:ARG:NH2     | 2.34                     | 0.54              |
| 28:SW:101:VAL:HB   | 28:SW:125:SER:HB2    | 1.88                     | 0.54              |
| 44:LE:806:C:H2'    | 44:LE:807:G:C8       | 2.42                     | 0.54              |
| 44:LE:868:C:H2'    | 44:LE:869:A:C8       | 2.43                     | 0.54              |
| 48:LI:3145:PSU:H2' | 48:LI:3146:C:C6      | 2.42                     | 0.54              |
| 55:LP:137:ILE:HD11 | 55:LP:149:LYS:HB2    | 1.89                     | 0.54              |
| 62:LW:8:LYS:O      | 62:LW:10:ARG:NH2     | 2.40                     | 0.54              |
| 69:Ld:29:TYR:O     | 69:Ld:33:ARG:HG3     | 2.07                     | 0.54              |
| 6:SA:30:VAL:HB     | 6:SA:42:CYS:HB2      | 1.89                     | 0.54              |
| 7:SB:58:LEU:HD21   | 7:SB:177:MET:HB3     | 1.90                     | 0.54              |
| 22:SQ:58:CYS:SG    | 22:SQ:59:VAL:N       | 2.80                     | 0.54              |
| 40:LA:20:U:H5      | 57:LR:190:ARG:NH1    | 2.04                     | 0.54              |
| 41:LB:247:OMU:H5'' | 70:Le:170:SER:HA     | 1.89                     | 0.54              |
| 42:LC:430:A:H2'    | 42:LC:431:C:O4'      | 2.07                     | 0.54              |
| 45:LF:1470:A:H5''  | 83:Lr:108:ARG:HD2    | 1.88                     | 0.54              |
| 45:LF:1518:G:OP2   | 87:Lv:22:ARG:NH1     | 2.39                     | 0.54              |
| 46:LG:2034:C:H2'   | 46:LG:2035:A:H8      | 1.71                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:LT:66:ASP:O     | 59:LT:70:ILE:HG12  | 2.07                     | 0.54              |
| 93:L2:92:MET:HE3   | 93:L2:103:LEU:O    | 2.08                     | 0.54              |
| 1:S1:254:G:H2'     | 1:S1:255:U:C6      | 2.42                     | 0.54              |
| 1:S1:270:G:H1      | 1:S1:348:A:P       | 2.30                     | 0.54              |
| 1:S1:573:A:O2'     | 1:S1:1049:A:N3     | 2.35                     | 0.54              |
| 6:SA:171:SER:O     | 6:SA:175:THR:HG22  | 2.07                     | 0.54              |
| 11:SF:164:GLY:O    | 11:SF:167:ARG:NH2  | 2.37                     | 0.54              |
| 26:SU:129:VAL:CG1  | 26:SU:146:GLN:HB2  | 2.38                     | 0.54              |
| 45:LF:1526:G:H2'   | 45:LF:1527:A:O4'   | 2.08                     | 0.54              |
| 54:LO:6:C:O2'      | 69:Ld:71:ASP:OD2   | 2.23                     | 0.54              |
| 79:Ln:75:VAL:HG13  | 79:Ln:80:LEU:HD21  | 1.87                     | 0.54              |
| 87:Lv:81:ARG:HG3   | 87:Lv:90:LYS:HB2   | 1.89                     | 0.54              |
| 93:L2:92:MET:HB2   | 93:L2:120:ARG:O    | 2.07                     | 0.54              |
| 96:L4:17:CYS:SG    | 96:L4:76:SER:OG    | 2.66                     | 0.54              |
| 98:L7:13:HIS:O     | 98:L7:17:GLU:HG3   | 2.06                     | 0.54              |
| 1:S1:4:C:O2'       | 9:SD:17:ARG:NH2    | 2.39                     | 0.54              |
| 1:S1:43:G:O2'      | 1:S1:98:C:OP1      | 2.17                     | 0.54              |
| 1:S1:429:U:OP1     | 16:SK:58:ARG:NH2   | 2.32                     | 0.54              |
| 1:S1:574:C:H5'     | 1:S1:1049:A:H1'    | 1.90                     | 0.54              |
| 1:S1:978:G:O6      | 38:Sg:134:ARG:NH1  | 2.40                     | 0.54              |
| 1:S1:1073:G:H2'    | 1:S1:1074:U:C6     | 2.42                     | 0.54              |
| 8:SC:11:ARG:HA     | 8:SC:14:VAL:HG12   | 1.90                     | 0.54              |
| 22:SQ:26:LEU:HD22  | 22:SQ:85:ILE:HG21  | 1.89                     | 0.54              |
| 32:Sa:63:GLU:OE2   | 32:Sa:67:TYR:OH    | 2.22                     | 0.54              |
| 35:Sd:16:LEU:HD12  | 35:Sd:62:ILE:HG21  | 1.89                     | 0.54              |
| 44:LE:877:A:H1'    | 44:LE:1284:G:N3    | 2.23                     | 0.54              |
| 44:LE:1182:A:OP1   | 100:LE:1512:HOH:O  | 2.19                     | 0.54              |
| 48:LI:3544:G:OP1   | 100:LI:3606:HOH:O  | 2.18                     | 0.54              |
| 55:LP:133:TYR:HB3  | 55:LP:168:LEU:HD23 | 1.89                     | 0.54              |
| 58:LS:27:LEU:HD13  | 58:LS:139:VAL:HG22 | 1.88                     | 0.54              |
| 59:LT:110:LYS:HA   | 59:LT:128:VAL:HG22 | 1.89                     | 0.54              |
| 66:La:108:LEU:HD11 | 66:La:116:LEU:HD13 | 1.89                     | 0.54              |
| 69:Ld:41:ASN:ND2   | 82:Lq:36:GLU:OE1   | 2.40                     | 0.54              |
| 83:Lr:238:ILE:O    | 83:Lr:242:ILE:HG13 | 2.08                     | 0.54              |
| 1:S1:31:C:O2'      | 1:S1:651:C:OP1     | 2.24                     | 0.54              |
| 1:S1:182:C:OP1     | 12:SG:133:ARG:NH1  | 2.40                     | 0.54              |
| 1:S1:590:G:H2'     | 1:S1:591:G:C8      | 2.42                     | 0.54              |
| 1:S1:2023:U:OP1    | 29:SX:80:LYS:NZ    | 2.40                     | 0.54              |
| 11:SF:115:GLY:O    | 11:SF:129:SER:OG   | 2.26                     | 0.54              |
| 12:SG:32:LEU:HD22  | 12:SG:65:GLN:HB2   | 1.90                     | 0.54              |
| 32:Sa:99:ILE:CG2   | 32:Sa:111:TYR:HB3  | 2.37                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LD:712:C:H5     | 43:LD:714:A:H62    | 1.56                     | 0.54              |
| 47:LH:2894:C:H2'   | 47:LH:2895:C:C6    | 2.43                     | 0.54              |
| 48:LI:3135:C:H2'   | 48:LI:3136:G:C8    | 2.43                     | 0.54              |
| 63:LX:160:ASP:O    | 63:LX:162:PHE:N    | 2.39                     | 0.54              |
| 1:S1:262:G:H2'     | 1:S1:263:G:C8      | 2.43                     | 0.54              |
| 1:S1:332:G:O2'     | 16:SK:74:THR:O     | 2.24                     | 0.54              |
| 1:S1:963:G:H1      | 1:S1:993:U:H3      | 1.54                     | 0.54              |
| 1:S1:2302:C:O2'    | 33:Sb:96:ARG:NE    | 2.40                     | 0.54              |
| 11:SF:43:VAL:HG11  | 11:SF:66:ILE:HG23  | 1.90                     | 0.54              |
| 29:SX:17:PHE:HZ    | 29:SX:134:LEU:HD22 | 1.73                     | 0.54              |
| 41:LB:219:G:OP2    | 81:Lp:90:LYS:NZ    | 2.27                     | 0.54              |
| 44:LE:850:C:C6     | 73:Lh:140:ARG:HG3  | 2.43                     | 0.54              |
| 44:LE:933:A:O2'    | 44:LE:935:A2M:OP1  | 2.25                     | 0.54              |
| 44:LE:960:G:P      | 57:LR:27:ARG:HH12  | 2.29                     | 0.54              |
| 44:LE:1454:A:H4'   | 69:Ld:43:TYR:CD2   | 2.43                     | 0.54              |
| 48:LI:3342:U:H2'   | 48:LI:3343:U:C6    | 2.43                     | 0.54              |
| 60:LU:111:GLN:O    | 60:LU:111:GLN:NE2  | 2.40                     | 0.54              |
| 1:S1:28:A2M:HM'3   | 21:SP:46:HIS:CD2   | 2.42                     | 0.54              |
| 1:S1:2282:A:OP2    | 94:L3:20:LYS:NZ    | 2.39                     | 0.54              |
| 12:SG:64:LYS:HD2   | 12:SG:99:ILE:HD12  | 1.90                     | 0.54              |
| 18:SM:37:VAL:HG21  | 18:SM:108:ILE:HG23 | 1.89                     | 0.54              |
| 38:Sg:50:ILE:HD12  | 38:Sg:58:LEU:HD13  | 1.88                     | 0.54              |
| 38:Sg:153:HIS:CE1  | 38:Sg:193:PHE:HA   | 2.43                     | 0.54              |
| 44:LE:815:C:N3     | 44:LE:831:G:N2     | 2.56                     | 0.54              |
| 45:LF:1923:JMC:OP1 | 74:Li:129:ARG:NH1  | 2.29                     | 0.54              |
| 48:LI:3580:A:H2'   | 48:LI:3581:C:C6    | 2.43                     | 0.54              |
| 50:LK:3761:C:O5'   | 59:LT:42:LYS:NZ    | 2.41                     | 0.54              |
| 1:S1:561:A:H3'     | 1:S1:562:G:H8      | 1.73                     | 0.54              |
| 1:S1:1073:G:H4'    | 9:SD:68:ARG:HH22   | 1.73                     | 0.54              |
| 1:S1:2094:U:H2'    | 1:S1:2095:G:H8     | 1.72                     | 0.54              |
| 4:S4:8:U:O4        | 4:S4:14:A:N7       | 2.40                     | 0.54              |
| 16:SK:89:ASN:ND2   | 16:SK:92:LEU:HG    | 2.23                     | 0.54              |
| 39:Sh:205:SER:HA   | 39:Sh:245:PHE:HD2  | 1.72                     | 0.54              |
| 42:LC:590:G:H2'    | 42:LC:591:A:C8     | 2.43                     | 0.54              |
| 44:LE:1061:C:H2'   | 44:LE:1062:C:C6    | 2.43                     | 0.54              |
| 45:LF:1510:U:OP1   | 100:LF:2009:HOH:O  | 2.19                     | 0.54              |
| 45:LF:1526:G:OP1   | 83:Lr:91:ARG:NH1   | 2.31                     | 0.54              |
| 57:LR:309:GLU:O    | 57:LR:313:GLN:HG2  | 2.08                     | 0.54              |
| 82:Lq:54:ASP:OD1   | 82:Lq:55:VAL:N     | 2.41                     | 0.54              |
| 94:L3:19:MET:O     | 94:L3:23:GLN:HG3   | 2.07                     | 0.54              |
| 1:S1:1409:U:H2'    | 1:S1:1410:A:H8     | 1.73                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:S1:1977:A:N1     | 24:SS:13:ARG:NH1    | 2.47                     | 0.54              |
| 1:S1:2303:A:H5'    | 33:Sb:96:ARG:HG2    | 1.90                     | 0.54              |
| 3:S3:26:A:N6       | 3:S3:44:G:H1        | 2.04                     | 0.54              |
| 47:LH:2600:U:H4'   | 47:LH:2601:G:O5'    | 2.06                     | 0.54              |
| 47:LH:2668:G:H2'   | 47:LH:2669:U:O4'    | 2.08                     | 0.54              |
| 57:LR:206:SER:OG   | 57:LR:207:LYS:NZ    | 2.41                     | 0.54              |
| 57:LR:208:ARG:HG3  | 57:LR:212:GLN:HE22  | 1.72                     | 0.54              |
| 67:Lb:168:GLY:HA2  | 67:Lb:171:HIS:CE1   | 2.43                     | 0.54              |
| 88:Lw:39:LYS:HD2   | 88:Lw:63:ARG:HH22   | 1.72                     | 0.54              |
| 95:L5:51:ALA:HB3   | 95:L5:54:ILE:HD12   | 1.90                     | 0.54              |
| 1:S1:498:A:OP2     | 100:S1:2415:HOH:O   | 2.18                     | 0.53              |
| 1:S1:725:A:OP2     | 100:S1:2413:HOH:O   | 2.18                     | 0.53              |
| 1:S1:1353:C:OP1    | 1:S1:1471:C:O2'     | 2.24                     | 0.53              |
| 1:S1:1896:U:P      | 17:SL:122:ARG:HH12  | 2.31                     | 0.53              |
| 1:S1:1939:G:N7     | 100:S1:2450:HOH:O   | 2.33                     | 0.53              |
| 1:S1:2036:C:H4'    | 1:S1:2042:G:C6      | 2.42                     | 0.53              |
| 2:S2:62:C:H2'      | 2:S2:63:G:H8        | 1.73                     | 0.53              |
| 7:SB:73:ASP:HB3    | 7:SB:120:ARG:HB2    | 1.90                     | 0.53              |
| 13:SH:37:HIS:O     | 17:SL:55:LYS:HE3    | 2.07                     | 0.53              |
| 42:LC:315:G:H2'    | 42:LC:316:A:C8      | 2.43                     | 0.53              |
| 44:LE:806:C:H2'    | 44:LE:807:G:H8      | 1.74                     | 0.53              |
| 45:LF:1740:A:H4'   | 66:La:3:TYR:HB2     | 1.90                     | 0.53              |
| 45:LF:1911:C:H2'   | 45:LF:1912:A:C8     | 2.43                     | 0.53              |
| 49:LJ:3636:OMU:H5' | 56:LQ:223:THR:HG21  | 1.90                     | 0.53              |
| 54:LO:106:G:H2'    | 54:LO:107:G:H8      | 1.73                     | 0.53              |
| 1:S1:965:G:P       | 38:Sg:129:ARG:HH21  | 2.31                     | 0.53              |
| 1:S1:1871:C:O2'    | 27:SV:52:GLY:HA3    | 2.09                     | 0.53              |
| 2:S2:7:A:H5'       | 2:S2:8:U:C5         | 2.43                     | 0.53              |
| 11:SF:219:LEU:O    | 11:SF:222:THR:OG1   | 2.20                     | 0.53              |
| 13:SH:85:ILE:HG13  | 32:Sa:69:VAL:HG11   | 1.91                     | 0.53              |
| 14:SI:47:GLN:N     | 14:SI:48:PRO:HD2    | 2.23                     | 0.53              |
| 24:SS:39:ARG:HG3   | 24:SS:40:ARG:HD3    | 1.89                     | 0.53              |
| 27:SV:111:ALA:HA   | 27:SV:116:ALA:HB2   | 1.90                     | 0.53              |
| 38:Sg:84:ARG:HH21  | 38:Sg:89:THR:C      | 2.16                     | 0.53              |
| 40:LA:37:G:O2'     | 40:LA:111:A:N1      | 2.42                     | 0.53              |
| 40:LA:65:C:H5'     | 81:Lp:10:ARG:HH22   | 1.73                     | 0.53              |
| 42:LC:435:G:H2'    | 42:LC:436:U:O4'     | 2.09                     | 0.53              |
| 45:LF:1705:C:O2'   | 87:Lv:84:GLY:HA2    | 2.09                     | 0.53              |
| 47:LH:2397:G:H5'   | 47:LH:2602:OMC:HM23 | 1.89                     | 0.53              |
| 50:LK:3794:C:H4'   | 65:LZ:63:HIS:CG     | 2.44                     | 0.53              |
| 61:LV:134:TYR:OH   | 61:LV:239:ILE:HG23  | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:Ld:42:LYS:HB3   | 69:Ld:45:THR:HB    | 1.90                     | 0.53              |
| 72:Lg:99:ASP:OD1   | 72:Lg:100:THR:N    | 2.41                     | 0.53              |
| 1:S1:610:C:H2'     | 1:S1:611:U:C6      | 2.43                     | 0.53              |
| 1:S1:1585:U:H2'    | 1:S1:1586:G:H8     | 1.73                     | 0.53              |
| 1:S1:1920:G:H4'    | 1:S1:1921:A:H5'    | 1.90                     | 0.53              |
| 1:S1:2100:A:OP2    | 24:SS:31:ARG:NH2   | 2.33                     | 0.53              |
| 4:S4:2:C:H2'       | 4:S4:3:G:C8        | 2.43                     | 0.53              |
| 21:SP:11:ARG:HB2   | 26:SU:106:GLU:HG2  | 1.91                     | 0.53              |
| 39:Sh:180:VAL:HG23 | 39:Sh:189:LEU:HB2  | 1.91                     | 0.53              |
| 45:LF:1954:A:H62   | 45:LF:1969:C:H5    | 1.54                     | 0.53              |
| 48:LI:3257:C:H2'   | 48:LI:3258:C:C6    | 2.43                     | 0.53              |
| 48:LI:3408:U:H4'   | 48:LI:3529:C:OP2   | 2.08                     | 0.53              |
| 91:Lz:33:LYS:HE2   | 91:Lz:46:VAL:HG22  | 1.91                     | 0.53              |
| 1:S1:285:A:OP2     | 1:S1:1120:U:O2'    | 2.15                     | 0.53              |
| 1:S1:696:A:O2'     | 1:S1:700:C:OP1     | 2.24                     | 0.53              |
| 1:S1:1591:PSU:H1'  | 28:SW:131:VAL:HG13 | 1.91                     | 0.53              |
| 1:S1:2044:G:OP2    | 100:S1:2417:HOH:O  | 2.18                     | 0.53              |
| 4:S4:19:G:H22      | 47:LH:2940:G:N2    | 2.06                     | 0.53              |
| 6:SA:101:MET:HE3   | 6:SA:186:PHE:HB3   | 1.89                     | 0.53              |
| 10:SE:98:LYS:HB3   | 10:SE:119:VAL:HG11 | 1.91                     | 0.53              |
| 13:SH:6:PRO:HB3    | 13:SH:34:TYR:CE2   | 2.43                     | 0.53              |
| 28:SW:92:PRO:HA    | 28:SW:95:ILE:HG13  | 1.89                     | 0.53              |
| 40:LA:5:G:O2'      | 40:LA:6:U:H5'      | 2.09                     | 0.53              |
| 40:LA:37:G:H1'     | 40:LA:110:A:N6     | 2.23                     | 0.53              |
| 44:LE:877:A:O2'    | 44:LE:886:A:N3     | 2.39                     | 0.53              |
| 44:LE:909:G:H1'    | 86:Lu:12:ARG:HH12  | 1.72                     | 0.53              |
| 55:LP:107:MET:HE1  | 55:LP:164:ALA:HB3  | 1.90                     | 0.53              |
| 56:LQ:242:ARG:HA   | 56:LQ:248:LEU:HD21 | 1.89                     | 0.53              |
| 57:LR:208:ARG:HG3  | 57:LR:212:GLN:NE2  | 2.24                     | 0.53              |
| 73:Lh:93:THR:HA    | 73:Lh:96:VAL:HG12  | 1.91                     | 0.53              |
| 86:Lu:10:VAL:HG13  | 86:Lu:14:GLU:HG3   | 1.90                     | 0.53              |
| 1:S1:58:U:OP1      | 1:S1:557:U:O2'     | 2.26                     | 0.53              |
| 1:S1:342:G:H2'     | 1:S1:343:G:H8      | 1.73                     | 0.53              |
| 1:S1:1150:C:O2'    | 1:S1:1253:G:OP1    | 2.26                     | 0.53              |
| 1:S1:1514:U:O4     | 21:SP:2:GLY:N      | 2.42                     | 0.53              |
| 1:S1:1756:U:H3     | 18:SM:90:LEU:HD11  | 1.74                     | 0.53              |
| 7:SB:74:VAL:O      | 7:SB:97:GLN:HG2    | 2.09                     | 0.53              |
| 10:SE:151:ASP:OD1  | 12:SG:219:ARG:NH1  | 2.34                     | 0.53              |
| 11:SF:217:ALA:O    | 11:SF:221:LYS:HG2  | 2.08                     | 0.53              |
| 14:SI:135:LEU:HD12 | 14:SI:138:VAL:HG13 | 1.90                     | 0.53              |
| 17:SL:21:LYS:HG2   | 17:SL:22:LYS:HG3   | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:Sh:176:LYS:HD2  | 39:Sh:197:GLY:H    | 1.72                     | 0.53              |
| 39:Sh:256:THR:HG22 | 39:Sh:258:SER:H    | 1.73                     | 0.53              |
| 43:LD:734:G:H4'    | 43:LD:736:A:H62    | 1.73                     | 0.53              |
| 44:LE:1322:A:N1    | 44:LE:1373:C:O2'   | 2.38                     | 0.53              |
| 45:LF:1840:U:H1'   | 85:Lt:66:LYS:HE2   | 1.91                     | 0.53              |
| 46:LG:2023:G:H4'   | 47:LH:2291:A:H4'   | 1.90                     | 0.53              |
| 61:LV:61:VAL:HG12  | 79:Ln:55:ARG:HH22  | 1.72                     | 0.53              |
| 68:Lc:193:ASP:H    | 68:Lc:197:THR:HA   | 1.73                     | 0.53              |
| 95:L5:23:ARG:HA    | 95:L5:26:VAL:HG22  | 1.90                     | 0.53              |
| 1:S1:1978:C:O2     | 24:SS:13:ARG:NH1   | 2.35                     | 0.53              |
| 1:S1:2036:C:OP2    | 32:Sa:87:ARG:NH1   | 2.36                     | 0.53              |
| 2:S2:28:G:H2'      | 2:S2:29:G:C8       | 2.43                     | 0.53              |
| 4:S4:9:A:O2'       | 4:S4:10:G:N7       | 2.28                     | 0.53              |
| 44:LE:815:C:H2'    | 44:LE:816:A:C8     | 2.44                     | 0.53              |
| 44:LE:1133:U:H2'   | 44:LE:1134:G:O4'   | 2.09                     | 0.53              |
| 44:LE:1141:U:H2'   | 44:LE:1142:G:C8    | 2.43                     | 0.53              |
| 44:LE:1431:A:O2'   | 44:LE:1432:C:OP2   | 2.27                     | 0.53              |
| 46:LG:2093:U:H5'   | 88:Lw:19:ARG:NH1   | 2.23                     | 0.53              |
| 49:LJ:3639:C:H4'   | 56:LQ:368:LYS:HD2  | 1.90                     | 0.53              |
| 59:LT:45:MET:HG2   | 59:LT:57:CYS:SG    | 2.49                     | 0.53              |
| 60:LU:129:LYS:HA   | 60:LU:137:PHE:CZ   | 2.44                     | 0.53              |
| 61:LV:123:LEU:HD21 | 61:LV:254:VAL:HG12 | 1.90                     | 0.53              |
| 1:S1:167:A:C2      | 1:S1:180:OMG:C6    | 2.93                     | 0.53              |
| 1:S1:579:G:N2      | 1:S1:614:G:H22     | 2.06                     | 0.53              |
| 1:S1:649:A2M:O3'   | 1:S1:650:C:O2      | 2.27                     | 0.53              |
| 1:S1:940:G:H2'     | 38:Sg:212:LYS:HD2  | 1.90                     | 0.53              |
| 1:S1:1355:C:O2'    | 25:ST:55:ARG:NH1   | 2.42                     | 0.53              |
| 1:S1:2218:U:H2'    | 1:S1:2219:C:C6     | 2.44                     | 0.53              |
| 8:SC:122:TYR:OH    | 11:SF:121:GLU:OE1  | 2.26                     | 0.53              |
| 23:SR:128:TRP:CH2  | 28:SW:130:PRO:HG3  | 2.44                     | 0.53              |
| 28:SW:103:ASN:OD1  | 28:SW:125:SER:OG   | 2.20                     | 0.53              |
| 46:LG:2063:G:N2    | 46:LG:2066:A:OP2   | 2.33                     | 0.53              |
| 47:LH:2315:U:H1'   | 88:Lw:7:ARG:HD3    | 1.89                     | 0.53              |
| 57:LR:131:VAL:HG12 | 57:LR:136:HIS:HB2  | 1.90                     | 0.53              |
| 1:S1:221:C:O2'     | 1:S1:222:A:N7      | 2.41                     | 0.53              |
| 1:S1:586:C:H2'     | 1:S1:587:G:C8      | 2.43                     | 0.53              |
| 1:S1:1584:A:OP2    | 23:SR:140:THR:HG21 | 2.09                     | 0.53              |
| 4:S4:9:A:O4'       | 4:S4:46:G:O2'      | 2.26                     | 0.53              |
| 12:SG:90:ARG:NH1   | 100:SG:302:HOH:O   | 2.29                     | 0.53              |
| 46:LG:2186:U:H4'   | 88:Lw:41:LEU:HD21  | 1.90                     | 0.53              |
| 59:LT:92:MET:HE2   | 59:LT:181:ILE:HG22 | 1.91                     | 0.53              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 60:LU:17:VAL:HB     | 60:LU:67:THR:HB    | 1.91                     | 0.53              |
| 82:Lq:23:LEU:HB3    | 82:Lq:26:ARG:HG2   | 1.91                     | 0.53              |
| 88:Lw:47:THR:OG1    | 88:Lw:52:GLY:O     | 2.24                     | 0.53              |
| 1:S1:1980:U:H3      | 19:SN:29:SER:HG    | 1.53                     | 0.53              |
| 9:SD:31:CYS:HA      | 9:SD:36:LEU:HD12   | 1.91                     | 0.53              |
| 11:SF:166:CYS:HA    | 11:SF:203:GLY:HA3  | 1.89                     | 0.53              |
| 25:ST:52:ILE:CG2    | 34:Sc:53:ALA:HB3   | 2.39                     | 0.53              |
| 39:Sh:16:HIS:ND1    | 39:Sh:37:SER:HB2   | 2.24                     | 0.53              |
| 40:LA:103:A:H5''    | 81:Lp:66:LYS:HG3   | 1.90                     | 0.53              |
| 47:LH:2347:G:H5''   | 56:LQ:247:GLY:HA2  | 1.90                     | 0.53              |
| 48:LI:3107:A:H2'    | 48:LI:3108:G:H8    | 1.74                     | 0.53              |
| 59:LT:49:GLY:HA3    | 59:LT:53:LYS:HA    | 1.89                     | 0.53              |
| 1:S1:429:U:O2'      | 16:SK:5:ARG:NH2    | 2.42                     | 0.53              |
| 1:S1:1100:A:N1      | 71:Lf:170:LYS:HG3  | 2.24                     | 0.53              |
| 2:S2:61:C:H2'       | 2:S2:62:C:C6       | 2.43                     | 0.53              |
| 3:S3:58:A:O2'       | 3:S3:60:U:OP2      | 2.26                     | 0.53              |
| 6:SA:124:ASP:OD2    | 6:SA:134:ARG:NH1   | 2.43                     | 0.53              |
| 9:SD:57:ARG:O       | 9:SD:61:THR:HG23   | 2.09                     | 0.53              |
| 9:SD:84:GLY:N       | 9:SD:107:ARG:HD2   | 2.22                     | 0.53              |
| 45:LF:1880:U:H4'    | 45:LF:1881:G:H5''  | 1.91                     | 0.53              |
| 48:LI:3270:A:H2'    | 48:LI:3271:G:C8    | 2.44                     | 0.53              |
| 51:LL:3868:A:H2'    | 51:LL:3869:G:O4'   | 2.09                     | 0.53              |
| 52:LM:3952:G:H2'    | 52:LM:3953:PSU:O4' | 2.09                     | 0.53              |
| 57:LR:18:LEU:HD21   | 57:LR:22:PHE:HB2   | 1.91                     | 0.53              |
| 76:Lk:125:ASP:OD1   | 76:Lk:125:ASP:N    | 2.42                     | 0.53              |
| 1:S1:726:A:N7       | 100:S1:2456:HOH:O  | 2.34                     | 0.52              |
| 1:S1:924:G:H2'      | 1:S1:925:C:C6      | 2.44                     | 0.52              |
| 1:S1:1355:C:OP2     | 34:Sc:22:LYS:NZ    | 2.30                     | 0.52              |
| 1:S1:1376:A:OP2     | 100:S1:2418:HOH:O  | 2.19                     | 0.52              |
| 1:S1:2262:A:H4'     | 5:S5:8:U:O2'       | 2.08                     | 0.52              |
| 15:SJ:55:ASN:OD1    | 34:Sc:28:GLN:NE2   | 2.41                     | 0.52              |
| 40:LA:69:G:O2'      | 40:LA:86:G:N2      | 2.40                     | 0.52              |
| 42:LC:553:C:O2      | 42:LC:557:A:O2'    | 2.27                     | 0.52              |
| 45:LF:1891:A2M:OP1  | 49:LJ:3665:C:O2'   | 2.27                     | 0.52              |
| 48:LI:3269:A:H2'    | 48:LI:3270:A:C8    | 2.44                     | 0.52              |
| 48:LI:3352:G:O6     | 63:LX:213:LYS:NZ   | 2.32                     | 0.52              |
| 48:LI:3465:OMC:HM21 | 56:LQ:241:PRO:HD3  | 1.90                     | 0.52              |
| 54:LO:27:A:H2'      | 54:LO:28:C:C6      | 2.45                     | 0.52              |
| 62:LW:59:LEU:O      | 62:LW:63:MET:HG3   | 2.09                     | 0.52              |
| 71:Lf:162:ALA:O     | 71:Lf:164:LYS:HG2  | 2.09                     | 0.52              |
| 1:S1:214:C:H2'      | 1:S1:215:A:C8      | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:694:C:H2'     | 1:S1:695:G:H8      | 1.73                     | 0.52              |
| 8:SC:25:GLU:OE2    | 8:SC:29:ARG:HD2    | 2.08                     | 0.52              |
| 22:SQ:103:ASP:HB2  | 22:SQ:108:VAL:O    | 2.09                     | 0.52              |
| 42:LC:439:U:H2'    | 42:LC:440:G:C8     | 2.45                     | 0.52              |
| 44:LE:1264:G:H4'   | 66:La:37:SER:HB3   | 1.90                     | 0.52              |
| 47:LH:2939:G:H4'   | 47:LH:2940:G:OP2   | 2.10                     | 0.52              |
| 50:LK:3809:U:H2'   | 50:LK:3810:G:C8    | 2.44                     | 0.52              |
| 68:Lc:44:ASP:OD1   | 68:Lc:181:TYR:OH   | 2.13                     | 0.52              |
| 71:Lf:103:LEU:HD22 | 71:Lf:139:LEU:HD13 | 1.91                     | 0.52              |
| 72:Lg:5:SER:HB3    | 72:Lg:104:GLY:HA2  | 1.91                     | 0.52              |
| 76:Lk:112:ASN:HB2  | 76:Lk:115:GLN:HG3  | 1.91                     | 0.52              |
| 86:Lu:39:TRP:O     | 86:Lu:40:ARG:NH1   | 2.43                     | 0.52              |
| 90:Ly:67:MET:HA    | 90:Ly:70:VAL:HG22  | 1.91                     | 0.52              |
| 1:S1:695:G:P       | 36:Se:43:ARG:HH22  | 2.33                     | 0.52              |
| 1:S1:1152:U:H3     | 1:S1:1249:G:H1     | 1.57                     | 0.52              |
| 1:S1:1259:G:H4'    | 15:SJ:57:ARG:HG2   | 1.91                     | 0.52              |
| 1:S1:1302:A:N1     | 1:S1:1395:A:O2'    | 2.43                     | 0.52              |
| 1:S1:1571:C:C2     | 1:S1:1572:A:C8     | 2.98                     | 0.52              |
| 4:S4:13:C:H2'      | 4:S4:14:A:C8       | 2.45                     | 0.52              |
| 10:SE:71:LYS:HE2   | 10:SE:74:GLY:HA2   | 1.91                     | 0.52              |
| 11:SF:52:GLU:HB2   | 30:SY:12:TYR:HB2   | 1.90                     | 0.52              |
| 16:SK:269:ARG:HB2  | 16:SK:285:LEU:HD21 | 1.91                     | 0.52              |
| 44:LE:838:U:H2'    | 44:LE:839:G:C8     | 2.44                     | 0.52              |
| 45:LF:1495:G:O2'   | 68:Lc:118:ALA:O    | 2.27                     | 0.52              |
| 45:LF:1981:G:N7    | 76:Lk:52:ARG:NH2   | 2.53                     | 0.52              |
| 47:LH:2669:U:OP1   | 55:LP:192:LYS:NZ   | 2.36                     | 0.52              |
| 48:LI:3266:G:H1'   | 48:LI:3279:G:H5'   | 1.90                     | 0.52              |
| 57:LR:281:VAL:HG11 | 70:Le:131:LYS:HG2  | 1.91                     | 0.52              |
| 83:Lr:176:TYR:CZ   | 83:Lr:197:GLU:HG2  | 2.43                     | 0.52              |
| 91:Lz:23:VAL:HG23  | 91:Lz:64:ILE:HG21  | 1.91                     | 0.52              |
| 95:L5:49:ARG:NE    | 95:L5:68:ALA:O     | 2.39                     | 0.52              |
| 1:S1:403:PSU:H2'   | 1:S1:404:C:C6      | 2.45                     | 0.52              |
| 1:S1:438:A:H2      | 16:SK:88:THR:HG21  | 1.75                     | 0.52              |
| 1:S1:1777:U:H3'    | 1:S1:1778:A:C8     | 2.44                     | 0.52              |
| 18:SM:66:THR:HG23  | 18:SM:81:ARG:HG2   | 1.90                     | 0.52              |
| 36:Se:23:LYS:HB2   | 36:Se:26:LYS:HZ1   | 1.74                     | 0.52              |
| 41:LB:213:G:OP1    | 90:Ly:48:ASN:N     | 2.39                     | 0.52              |
| 42:LC:318:U:H2'    | 42:LC:319:C:C6     | 2.44                     | 0.52              |
| 42:LC:481:G:OP2    | 42:LC:481:G:N2     | 2.34                     | 0.52              |
| 43:LD:655:G:P      | 87:Lv:78:ARG:HH22  | 2.32                     | 0.52              |
| 44:LE:1215:A:OP2   | 100:LE:1513:HOH:O  | 2.19                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 83:Lr:89:ARG:NH2   | 83:Lr:92:GLY:O     | 2.41                     | 0.52              |
| 1:S1:1116:G:H21    | 1:S1:1133:G:H1'    | 1.75                     | 0.52              |
| 1:S1:1869:U:OP1    | 27:SV:32:LYS:NZ    | 2.41                     | 0.52              |
| 10:SE:116:GLY:O    | 10:SE:119:VAL:HG22 | 2.10                     | 0.52              |
| 13:SH:58:LEU:O     | 13:SH:62:LEU:HG    | 2.10                     | 0.52              |
| 39:Sh:160:PHE:CE1  | 39:Sh:169:ILE:HG12 | 2.45                     | 0.52              |
| 41:LB:168:C:H5'    | 61:LV:229:LYS:HG3  | 1.91                     | 0.52              |
| 42:LC:496:U:H2'    | 42:LC:497:U:C6     | 2.44                     | 0.52              |
| 44:LE:949:OMC:HM21 | 57:LR:100:LYS:HB2  | 1.92                     | 0.52              |
| 47:LH:2260:G:OP1   | 79:Ln:65:ARG:NH1   | 2.42                     | 0.52              |
| 47:LH:2932:C:H3'   | 47:LH:2933:A:C8    | 2.44                     | 0.52              |
| 48:LI:3424:A:H2'   | 48:LI:3425:G:O4'   | 2.08                     | 0.52              |
| 55:LP:173:GLY:O    | 95:L5:69:TRP:NE1   | 2.43                     | 0.52              |
| 69:Ld:51:CYS:HA    | 69:Ld:145:ASP:HB3  | 1.91                     | 0.52              |
| 76:Lk:124:TYR:O    | 76:Lk:126:ILE:N    | 2.42                     | 0.52              |
| 84:Ls:61:TYR:O     | 84:Ls:64:MET:HG3   | 2.09                     | 0.52              |
| 90:Ly:21:ARG:CD    | 90:Ly:39:TYR:HD1   | 2.22                     | 0.52              |
| 1:S1:1430:U:H4'    | 1:S1:1431:G:OP2    | 2.10                     | 0.52              |
| 10:SE:195:LEU:HD13 | 10:SE:208:ILE:HG23 | 1.92                     | 0.52              |
| 16:SK:59:ALA:HB1   | 16:SK:62:LEU:HG    | 1.91                     | 0.52              |
| 16:SK:118:TRP:CE2  | 16:SK:243:ARG:HD3  | 2.45                     | 0.52              |
| 57:LR:22:PHE:CD1   | 57:LR:126:ALA:HB2  | 2.45                     | 0.52              |
| 72:Lg:12:ILE:HG12  | 72:Lg:64:ILE:HG13  | 1.92                     | 0.52              |
| 74:Li:24:LEU:HD12  | 74:Li:148:LEU:HD12 | 1.91                     | 0.52              |
| 1:S1:423:G:H2'     | 1:S1:424:U:C6      | 2.44                     | 0.52              |
| 1:S1:1116:G:H4'    | 1:S1:1117:A:H5'    | 1.92                     | 0.52              |
| 1:S1:1763:A:H2'    | 1:S1:1764:G:H8     | 1.75                     | 0.52              |
| 10:SE:122:LYS:HE3  | 10:SE:162:ILE:HD11 | 1.92                     | 0.52              |
| 16:SK:85:TYR:HD2   | 16:SK:103:ILE:HD13 | 1.74                     | 0.52              |
| 41:LB:237:A:H2'    | 41:LB:238:U:O4'    | 2.10                     | 0.52              |
| 46:LG:2165:G:H21   | 46:LG:2169:G:N2    | 2.08                     | 0.52              |
| 54:LO:83:G:H4'     | 83:Lr:218:LYS:HB3  | 1.91                     | 0.52              |
| 55:LP:45:VAL:HG22  | 55:LP:61:VAL:HG22  | 1.92                     | 0.52              |
| 65:LZ:38:ILE:HD11  | 65:LZ:59:ILE:HG21  | 1.91                     | 0.52              |
| 67:Lb:68:ARG:HA    | 67:Lb:98:MET:HE1   | 1.90                     | 0.52              |
| 73:Lh:4:SER:O      | 73:Lh:10:ARG:NH1   | 2.42                     | 0.52              |
| 74:Li:38:LEU:HD11  | 74:Li:50:LEU:HD21  | 1.92                     | 0.52              |
| 88:Lw:34:THR:HG22  | 88:Lw:35:VAL:H     | 1.75                     | 0.52              |
| 1:S1:31:C:O2'      | 21:SP:135:ARG:NH2  | 2.43                     | 0.52              |
| 1:S1:1414:C:H2'    | 1:S1:1415:G:H8     | 1.75                     | 0.52              |
| 29:SX:140:GLN:HG2  | 29:SX:147:PHE:HB2  | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:Sh:42:LEU:HD12  | 39:Sh:63:LEU:HB2   | 1.92                     | 0.52              |
| 42:LC:335:G:OP1    | 81:Lp:109:LYS:NZ   | 2.42                     | 0.52              |
| 44:LE:1276:C:H2'   | 44:LE:1277:C:O4'   | 2.09                     | 0.52              |
| 45:LF:1935:G:N3    | 46:LG:2022:A2M:H2  | 2.25                     | 0.52              |
| 48:LI:3006:U:H2'   | 48:LI:3007:G:C8    | 2.45                     | 0.52              |
| 58:LS:20:ARG:HA    | 58:LS:143:ARG:HD3  | 1.91                     | 0.52              |
| 73:Lh:44:THR:HA    | 73:Lh:95:HIS:HB3   | 1.91                     | 0.52              |
| 74:Li:72:THR:HG22  | 74:Li:74:GLN:H     | 1.74                     | 0.52              |
| 83:Lr:207:LEU:HB3  | 83:Lr:241:MET:HB3  | 1.92                     | 0.52              |
| 1:S1:1014:A:H5''   | 10:SE:200:ARG:HH21 | 1.75                     | 0.52              |
| 12:SG:239:ARG:O    | 12:SG:240:LYS:NZ   | 2.32                     | 0.52              |
| 13:SH:24:LEU:HD11  | 13:SH:132:ARG:HD2  | 1.91                     | 0.52              |
| 41:LB:198:U:H4'    | 66:La:39:ARG:HD2   | 1.91                     | 0.52              |
| 42:LC:353:G:O6     | 42:LC:455:U:O4     | 2.27                     | 0.52              |
| 45:LF:1856:OMG:H3' | 74:Li:47:PHE:CG    | 2.45                     | 0.52              |
| 60:LU:53:PRO:HA    | 60:LU:156:GLN:NE2  | 2.25                     | 0.52              |
| 60:LU:87:ARG:HG3   | 60:LU:126:LYS:HD3  | 1.91                     | 0.52              |
| 1:S1:172:A:H2'     | 1:S1:173:A:O4'     | 2.10                     | 0.52              |
| 1:S1:215:A:H2'     | 1:S1:216:C:C6      | 2.44                     | 0.52              |
| 1:S1:650:C:H5      | 1:S1:696:A:H61     | 1.57                     | 0.52              |
| 1:S1:1316:C:H2'    | 1:S1:1317:U:C6     | 2.44                     | 0.52              |
| 1:S1:1983:C:H2'    | 1:S1:1984:C:C6     | 2.45                     | 0.52              |
| 3:S3:51:U:N3       | 3:S3:52:G:N7       | 2.58                     | 0.52              |
| 4:S4:76:A:C2       | 48:LI:3379:OMG:H2' | 2.45                     | 0.52              |
| 6:SA:64:PHE:O      | 6:SA:83:ARG:HA     | 2.10                     | 0.52              |
| 8:SC:52:ILE:HD11   | 8:SC:88:LEU:HD23   | 1.92                     | 0.52              |
| 10:SE:159:THR:HG22 | 10:SE:173:VAL:HB   | 1.92                     | 0.52              |
| 17:SL:44:ILE:HD12  | 17:SL:57:MET:HG2   | 1.91                     | 0.52              |
| 23:SR:65:ILE:O     | 23:SR:69:VAL:HG13  | 2.10                     | 0.52              |
| 38:Sg:192:LEU:C    | 38:Sg:192:LEU:HD12 | 2.35                     | 0.52              |
| 42:LC:536:A:H2'    | 42:LC:537:OMC:C6   | 2.45                     | 0.52              |
| 45:LF:1849:U:N3    | 45:LF:1852:A:OP2   | 2.24                     | 0.52              |
| 47:LH:2864:G:H2'   | 47:LH:2865:G:C8    | 2.44                     | 0.52              |
| 48:LI:3235:U:H2'   | 48:LI:3236:G:H8    | 1.71                     | 0.52              |
| 60:LU:132:LYS:HB3  | 60:LU:136:ALA:HB3  | 1.90                     | 0.52              |
| 63:LX:127:TYR:C    | 63:LX:129:SER:H    | 2.18                     | 0.52              |
| 72:Lg:17:TYR:OH    | 83:Lr:81:GLU:OE2   | 2.14                     | 0.52              |
| 72:Lg:27:VAL:HG21  | 73:Lh:139:LEU:HD21 | 1.92                     | 0.52              |
| 84:Ls:27:CYS:HB2   | 84:Ls:94:SER:HB3   | 1.92                     | 0.52              |
| 85:Lt:56:LEU:O     | 85:Lt:60:VAL:HG22  | 2.10                     | 0.52              |
| 88:Lw:62:LEU:HB3   | 88:Lw:66:GLN:HB2   | 1.90                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 95:L5:86:LEU:O    | 95:L5:90:THR:HG22  | 2.09                     | 0.52              |
| 1:S1:1559:G:H1'   | 1:S1:2271:A:C4     | 2.46                     | 0.51              |
| 8:SC:73:SER:O     | 8:SC:77:LYS:HG3    | 2.11                     | 0.51              |
| 9:SD:110:GLN:NE2  | 9:SD:126:ARG:HB2   | 2.25                     | 0.51              |
| 27:SV:94:GLN:HE21 | 27:SV:98:GLN:NE2   | 2.08                     | 0.51              |
| 33:Sb:44:MET:HG3  | 33:Sb:66:PRO:HG2   | 1.90                     | 0.51              |
| 44:LE:1100:A:OP1  | 66:La:34:LYS:NZ    | 2.23                     | 0.51              |
| 45:LF:1862:C:H2'  | 45:LF:1863:A:C8    | 2.45                     | 0.51              |
| 48:LI:3256:U:H2'  | 48:LI:3257:C:C6    | 2.45                     | 0.51              |
| 76:Lk:138:ASP:OD1 | 76:Lk:138:ASP:N    | 2.40                     | 0.51              |
| 85:Lt:48:LEU:HD11 | 85:Lt:148:LYS:HE3  | 1.92                     | 0.51              |
| 1:S1:1923:G:H2'   | 1:S1:1924:C:C6     | 2.45                     | 0.51              |
| 3:S3:2:C:H2'      | 3:S3:3:G:H8        | 1.73                     | 0.51              |
| 7:SB:176:TRP:CG   | 7:SB:199:VAL:HG12  | 2.46                     | 0.51              |
| 13:SH:160:ALA:O   | 13:SH:164:ILE:HG12 | 2.10                     | 0.51              |
| 14:SI:82:HIS:CE1  | 14:SI:100:VAL:HG22 | 2.45                     | 0.51              |
| 17:SL:121:ASP:OD1 | 17:SL:123:THR:OG1  | 2.25                     | 0.51              |
| 18:SM:82:TYR:HB3  | 24:SS:51:PHE:HB3   | 1.91                     | 0.51              |
| 25:ST:74:VAL:O    | 25:ST:78:ASN:ND2   | 2.37                     | 0.51              |
| 33:Sb:25:ASN:OD1  | 33:Sb:26:CYS:N     | 2.43                     | 0.51              |
| 38:Sg:56:ARG:HE   | 38:Sg:91:ILE:HB    | 1.75                     | 0.51              |
| 44:LE:792:G:H2'   | 44:LE:793:U:C6     | 2.45                     | 0.51              |
| 44:LE:837:U:H2'   | 44:LE:838:U:C6     | 2.45                     | 0.51              |
| 45:LF:1539:C:H2'  | 45:LF:1540:A:O4'   | 2.10                     | 0.51              |
| 45:LF:1679:G:OP2  | 62:LW:64:ARG:NH2   | 2.44                     | 0.51              |
| 45:LF:1773:C:P    | 86:Lu:85:ASN:HD21  | 2.34                     | 0.51              |
| 46:LG:2061:U:H2'  | 46:LG:2062:G:H8    | 1.76                     | 0.51              |
| 47:LH:2626:A:OP1  | 100:LH:3003:HOH:O  | 2.19                     | 0.51              |
| 47:LH:2862:C:N4   | 48:LI:3528:A:O4'   | 2.42                     | 0.51              |
| 56:LQ:106:TRP:HB2 | 56:LQ:133:TYR:CZ   | 2.46                     | 0.51              |
| 56:LQ:122:TRP:O   | 56:LQ:127:LYS:HD2  | 2.10                     | 0.51              |
| 1:S1:12:U:H2'     | 1:S1:13:C:C6       | 2.45                     | 0.51              |
| 1:S1:106:C:H2'    | 1:S1:107:A:H8      | 1.75                     | 0.51              |
| 1:S1:671:A:OP1    | 21:SP:68:LYS:NZ    | 2.43                     | 0.51              |
| 1:S1:952:G:H2'    | 1:S1:953:A:C8      | 2.44                     | 0.51              |
| 1:S1:1116:G:N2    | 1:S1:1133:G:O2'    | 2.44                     | 0.51              |
| 1:S1:1697:G:H2'   | 1:S1:1723:A:H4'    | 1.92                     | 0.51              |
| 1:S1:1970:G:OP2   | 1:S1:1970:G:N2     | 2.32                     | 0.51              |
| 10:SE:124:CYS:HG  | 10:SE:142:HIS:CE1  | 2.28                     | 0.51              |
| 47:LH:2927:A:H2'  | 47:LH:2928:A:C8    | 2.45                     | 0.51              |
| 50:LK:3759:G:OP1  | 62:LW:42:ARG:NH1   | 2.37                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:LM:3950:A:C8    | 53:LN:3981:A:H8    | 2.28                     | 0.51              |
| 71:Lf:36:ALA:O     | 71:Lf:41:ASN:ND2   | 2.19                     | 0.51              |
| 82:Lq:4:SER:OG     | 82:Lq:6:ASN:OD1    | 2.25                     | 0.51              |
| 83:Lr:109:LEU:HD21 | 83:Lr:116:VAL:HG22 | 1.92                     | 0.51              |
| 83:Lr:226:ASP:HB3  | 83:Lr:230:ARG:NH2  | 2.25                     | 0.51              |
| 87:Lv:44:PHE:O     | 87:Lv:48:LYS:NZ    | 2.33                     | 0.51              |
| 44:LE:859:G:H2'    | 44:LE:860:C:H6     | 1.75                     | 0.51              |
| 44:LE:1415:G:H2'   | 44:LE:1416:A:H8    | 1.76                     | 0.51              |
| 45:LF:1542:A:H61   | 45:LF:1704:C:H5    | 1.57                     | 0.51              |
| 45:LF:1937:U:OP1   | 76:Lk:144:TYR:OH   | 2.28                     | 0.51              |
| 46:LG:2013:G:H2'   | 46:LG:2014:U:C6    | 2.46                     | 0.51              |
| 47:LH:2297:U:H4'   | 47:LH:2298:C:H5''  | 1.91                     | 0.51              |
| 48:LI:3534:G:N3    | 56:LQ:252:ALA:HB1  | 2.25                     | 0.51              |
| 52:LM:3950:A:H2'   | 52:LM:3951:A:C8    | 2.45                     | 0.51              |
| 57:LR:187:LYS:HD2  | 57:LR:190:ARG:HH21 | 1.75                     | 0.51              |
| 60:LU:10:VAL:O     | 60:LU:59:ARG:NH2   | 2.35                     | 0.51              |
| 83:Lr:219:LYS:HB2  | 83:Lr:225:GLY:HA3  | 1.92                     | 0.51              |
| 1:S1:368:A:H2'     | 1:S1:369:U:C6      | 2.45                     | 0.51              |
| 1:S1:380:U:N3      | 1:S1:381:G:O6      | 2.44                     | 0.51              |
| 1:S1:1749:C:H2'    | 1:S1:1750:U:H6     | 1.75                     | 0.51              |
| 2:S2:67:C:H2'      | 2:S2:68:C:C6       | 2.46                     | 0.51              |
| 12:SG:137:PRO:HD2  | 12:SG:160:ILE:HD13 | 1.93                     | 0.51              |
| 14:SI:59:ILE:HD11  | 14:SI:65:ALA:HB2   | 1.91                     | 0.51              |
| 16:SK:112:ARG:HH22 | 16:SK:262:PRO:HA   | 1.76                     | 0.51              |
| 29:SX:9:VAL:O      | 29:SX:10:LYS:HB2   | 2.10                     | 0.51              |
| 40:LA:29:G:N2      | 90:Ly:78:GLN:OE1   | 2.38                     | 0.51              |
| 42:LC:512:U:H2'    | 42:LC:513:A:H8     | 1.73                     | 0.51              |
| 43:LD:698:C:H5''   | 59:LT:50:LYS:HB2   | 1.92                     | 0.51              |
| 44:LE:1075:PSU:N1  | 48:LI:3312:C:N3    | 2.49                     | 0.51              |
| 48:LI:3398:C:H2'   | 48:LI:3399:A:H8    | 1.76                     | 0.51              |
| 49:LJ:3654:G:H2'   | 49:LJ:3655:A:H8    | 1.75                     | 0.51              |
| 51:LL:3854:A:C2    | 51:LL:3855:G:H1'   | 2.45                     | 0.51              |
| 66:La:116:LEU:HD23 | 66:La:137:ALA:HB1  | 1.92                     | 0.51              |
| 67:Lb:64:VAL:HG13  | 67:Lb:102:ALA:HB1  | 1.91                     | 0.51              |
| 1:S1:1457:A:H1'    | 1:S1:1458:U:H2'    | 1.93                     | 0.51              |
| 8:SC:96:ARG:HD3    | 8:SC:127:PHE:CZ    | 2.45                     | 0.51              |
| 10:SE:134:LYS:O    | 12:SG:209:ARG:NH1  | 2.39                     | 0.51              |
| 13:SH:7:LEU:HB2    | 13:SH:10:LYS:HA    | 1.93                     | 0.51              |
| 13:SH:28:ILE:HG23  | 13:SH:54:ILE:HD13  | 1.92                     | 0.51              |
| 36:Se:25:GLU:OE1   | 36:Se:27:LYS:HE3   | 2.09                     | 0.51              |
| 39:Sh:169:ILE:HD11 | 39:Sh:183:LEU:HB3  | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LD:650:A:C8     | 60:LU:94:LYS:HE3   | 2.44                     | 0.51              |
| 44:LE:833:C:H2'    | 44:LE:834:C:C6     | 2.46                     | 0.51              |
| 45:LF:1529:A:C6    | 45:LF:1750:U:H1'   | 2.46                     | 0.51              |
| 100:LG:2301:HOH:O  | 47:LH:2291:A:OP1   | 2.19                     | 0.51              |
| 47:LH:2235:A:H5''  | 88:Lw:22:LYS:HD2   | 1.91                     | 0.51              |
| 47:LH:2832:OMC:H2' | 47:LH:2833:G:C8    | 2.45                     | 0.51              |
| 100:LI:3621:HOH:O  | 68:Lc:7:LYS:NZ     | 2.31                     | 0.51              |
| 59:LT:106:SER:OG   | 59:LT:111:ALA:HB3  | 2.11                     | 0.51              |
| 64:LY:9:GLY:HA3    | 64:LY:128:ILE:HG23 | 1.93                     | 0.51              |
| 65:LZ:90:TRP:O     | 65:LZ:93:THR:OG1   | 2.23                     | 0.51              |
| 1:S1:927:G:H2'     | 1:S1:928:U:C6      | 2.46                     | 0.51              |
| 1:S1:1844:A:OP1    | 17:SL:74:ARG:NH2   | 2.44                     | 0.51              |
| 4:S4:51:U:O2       | 4:S4:63:G:C6       | 2.64                     | 0.51              |
| 19:SN:81:LEU:HD22  | 19:SN:85:ILE:HG21  | 1.93                     | 0.51              |
| 39:Sh:223:TRP:HB3  | 39:Sh:230:HIS:HA   | 1.92                     | 0.51              |
| 45:LF:1499:A:H61   | 68:Lc:114:GLY:HA2  | 1.75                     | 0.51              |
| 48:LI:3140:C:O5'   | 76:Lk:34:LYS:HE2   | 2.11                     | 0.51              |
| 48:LI:3439:G:H5'   | 68:Lc:63:GLU:HB3   | 1.93                     | 0.51              |
| 48:LI:3530:G:N2    | 56:LQ:253:CYS:SG   | 2.84                     | 0.51              |
| 54:LO:38:U:N3      | 54:LO:41:G:OP2     | 2.29                     | 0.51              |
| 65:LZ:103:LYS:O    | 65:LZ:107:ASN:ND2  | 2.43                     | 0.51              |
| 1:S1:1642:U:H2'    | 1:S1:1643:G:C8     | 2.46                     | 0.51              |
| 2:S2:37:MIA:H2'    | 2:S2:38:A:C8       | 2.46                     | 0.51              |
| 3:S3:33:U:OP2      | 17:SL:151:ARG:NH1  | 2.33                     | 0.51              |
| 8:SC:181:GLN:HG3   | 36:Se:67:GLY:HA2   | 1.92                     | 0.51              |
| 28:SW:61:LEU:HD13  | 28:SW:83:THR:HG21  | 1.92                     | 0.51              |
| 35:Sd:51:ARG:HG3   | 35:Sd:65:LEU:HD21  | 1.93                     | 0.51              |
| 42:LC:555:C:O2'    | 42:LC:572:G:N2     | 2.43                     | 0.51              |
| 44:LE:868:C:H2'    | 44:LE:869:A:H8     | 1.76                     | 0.51              |
| 44:LE:1095:U:H4'   | 63:LX:3:LYS:HG2    | 1.93                     | 0.51              |
| 45:LF:1908:U:OP1   | 92:L1:42:ARG:NH2   | 2.27                     | 0.51              |
| 46:LG:2218:G:H5''  | 75:Lj:151:LYS:HE3  | 1.93                     | 0.51              |
| 47:LH:2366:A:OP2   | 100:LH:3008:HOH:O  | 2.19                     | 0.51              |
| 49:LJ:3593:A:H2'   | 49:LJ:3594:C:C6    | 2.45                     | 0.51              |
| 56:LQ:57:VAL:HG22  | 56:LQ:73:VAL:HG22  | 1.91                     | 0.51              |
| 64:LY:99:GLU:HB3   | 78:Lm:24:THR:HG23  | 1.93                     | 0.51              |
| 66:La:43:GLY:HA3   | 66:La:47:HIS:CE1   | 2.46                     | 0.51              |
| 69:Ld:105:ALA:HB2  | 69:Ld:164:VAL:HA   | 1.92                     | 0.51              |
| 78:Lm:20:ARG:HG3   | 78:Lm:34:THR:HG22  | 1.92                     | 0.51              |
| 1:S1:497:G:H5''    | 16:SK:25:ARG:HA    | 1.92                     | 0.51              |
| 1:S1:549:A:OP2     | 100:S1:2416:HOH:O  | 2.18                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:644:U:O2      | 36:Se:27:LYS:NZ    | 2.37                     | 0.51              |
| 1:S1:727:C:N4      | 1:S1:1367:A:OP1    | 2.32                     | 0.51              |
| 1:S1:1981:G:H2'    | 1:S1:1982:C:H6     | 1.76                     | 0.51              |
| 7:SB:156:TYR:O     | 30:SY:59:ARG:NH2   | 2.42                     | 0.51              |
| 14:SI:77:LYS:HA    | 14:SI:80:ARG:HG2   | 1.92                     | 0.51              |
| 16:SK:64:GLY:HA2   | 16:SK:80:ILE:HG13  | 1.92                     | 0.51              |
| 18:SM:22:ILE:HD13  | 18:SM:100:VAL:HG11 | 1.92                     | 0.51              |
| 25:ST:64:LYS:O     | 25:ST:68:GLY:HA2   | 2.10                     | 0.51              |
| 28:SW:21:THR:HG23  | 28:SW:24:GLY:HA2   | 1.92                     | 0.51              |
| 28:SW:77:LYS:NZ    | 28:SW:96:GLY:O     | 2.39                     | 0.51              |
| 29:SX:67:ILE:HG21  | 29:SX:116:VAL:HG12 | 1.93                     | 0.51              |
| 42:LC:437:G:H2'    | 42:LC:438:C:C6     | 2.46                     | 0.51              |
| 45:LF:1885:U:H5''  | 71:Lf:6:LYS:HE3    | 1.93                     | 0.51              |
| 47:LH:2894:C:H2'   | 47:LH:2895:C:H6    | 1.75                     | 0.51              |
| 47:LH:2909:OMU:H2' | 47:LH:2910:C:O4'   | 2.11                     | 0.51              |
| 73:Lh:11:THR:HG22  | 73:Lh:14:LEU:HD23  | 1.93                     | 0.51              |
| 83:Lr:215:LYS:N    | 83:Lr:226:ASP:OD2  | 2.44                     | 0.51              |
| 1:S1:1401:C:OP1    | 100:S1:2421:HOH:O  | 2.20                     | 0.51              |
| 13:SH:8:LEU:N      | 13:SH:12:TRP:O     | 2.34                     | 0.51              |
| 34:Sc:36:ASP:HB2   | 34:Sc:82:ARG:HG3   | 1.92                     | 0.51              |
| 46:LG:2152:U:H2'   | 46:LG:2153:A:H8    | 1.75                     | 0.51              |
| 47:LH:2397:G:N2    | 100:LH:3033:HOH:O  | 2.35                     | 0.51              |
| 47:LH:2672:G:OP2   | 55:LP:198:ARG:NH1  | 2.42                     | 0.51              |
| 63:LX:52:VAL:HG23  | 63:LX:55:ARG:HH11  | 1.75                     | 0.51              |
| 71:Lf:163:LYS:HG2  | 71:Lf:166:LYS:HE3  | 1.93                     | 0.51              |
| 83:Lr:111:GLN:HB3  | 83:Lr:114:ASN:ND2  | 2.26                     | 0.51              |
| 1:S1:1496:A:OP1    | 100:S1:2419:HOH:O  | 2.19                     | 0.50              |
| 1:S1:1899:U:OP2    | 27:SV:2:GLY:N      | 2.45                     | 0.50              |
| 1:S1:2133:U:HO2'   | 1:S1:2270:C:HO2'   | 1.48                     | 0.50              |
| 3:S3:9:A:O2'       | 3:S3:10:G:N7       | 2.44                     | 0.50              |
| 3:S3:16:U:O3'      | 3:S3:60:U:O2'      | 2.25                     | 0.50              |
| 10:SE:221:ARG:HB2  | 10:SE:224:ASN:HB2  | 1.92                     | 0.50              |
| 13:SH:22:LEU:HA    | 13:SH:25:GLN:HG2   | 1.92                     | 0.50              |
| 25:ST:54:LEU:HG    | 25:ST:60:ILE:HB    | 1.92                     | 0.50              |
| 28:SW:38:LEU:HA    | 28:SW:41:ILE:HG22  | 1.94                     | 0.50              |
| 32:Sa:70:ILE:HG22  | 32:Sa:90:LEU:HD21  | 1.93                     | 0.50              |
| 39:Sh:278:LEU:HD12 | 39:Sh:278:LEU:C    | 2.36                     | 0.50              |
| 40:LA:157:A:H2'    | 40:LA:158:G:C8     | 2.46                     | 0.50              |
| 41:LB:286:A:O2'    | 41:LB:289:A:N6     | 2.43                     | 0.50              |
| 47:LH:2919:U:H2'   | 47:LH:2920:A2M:C8  | 2.41                     | 0.50              |
| 64:LY:65:VAL:HB    | 64:LY:73:ARG:HA    | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:LY:107:ASN:OD1  | 64:LY:111:GLU:N    | 2.45                     | 0.50              |
| 68:Lc:53:ILE:HB    | 68:Lc:164:VAL:HG13 | 1.92                     | 0.50              |
| 74:Li:35:VAL:HB    | 74:Li:119:ILE:HG12 | 1.93                     | 0.50              |
| 79:Ln:8:GLY:N      | 79:Ln:25:ILE:O     | 2.42                     | 0.50              |
| 1:S1:1270:U:O2     | 1:S1:1445:G:O2'    | 2.28                     | 0.50              |
| 1:S1:1293:C:O2     | 20:SO:56:ARG:NH1   | 2.36                     | 0.50              |
| 1:S1:1749:C:H2'    | 1:S1:1750:U:C6     | 2.47                     | 0.50              |
| 1:S1:2008:G:N2     | 1:S1:2052:G:O2'    | 2.45                     | 0.50              |
| 42:LC:593:G:H2'    | 42:LC:594:A2M:H8   | 1.92                     | 0.50              |
| 44:LE:1160:C:OP1   | 47:LH:2621:PSU:O2' | 2.24                     | 0.50              |
| 45:LF:1555:G:OP1   | 65:LZ:35:HIS:NE2   | 2.35                     | 0.50              |
| 45:LF:1681:OMU:O4  | 100:LF:2010:HOH:O  | 2.19                     | 0.50              |
| 45:LF:1921:A:OP2   | 74:Li:129:ARG:NH2  | 2.45                     | 0.50              |
| 49:LJ:3601:A:N1    | 49:LJ:3633:C:O2'   | 2.36                     | 0.50              |
| 50:LK:3797:C:OP2   | 72:Lg:178:ARG:HD2  | 2.11                     | 0.50              |
| 75:Lj:124:LYS:HG2  | 75:Lj:154:TYR:CE2  | 2.46                     | 0.50              |
| 76:Lk:150:ASP:OD1  | 76:Lk:151:ASN:N    | 2.44                     | 0.50              |
| 77:LI:100:PRO:HA   | 77:LI:103:VAL:HG22 | 1.92                     | 0.50              |
| 1:S1:65:G:O5'      | 12:SG:138:LYS:NZ   | 2.44                     | 0.50              |
| 1:S1:128:G:C6      | 1:S1:193:U:N3      | 2.79                     | 0.50              |
| 1:S1:694:C:H2'     | 1:S1:695:G:C8      | 2.47                     | 0.50              |
| 1:S1:2027:A:H2'    | 1:S1:2028:G:C8     | 2.46                     | 0.50              |
| 4:S4:37:A:H2'      | 4:S4:38:A:H8       | 1.76                     | 0.50              |
| 6:SA:224:ASN:O     | 6:SA:228:GLN:HG3   | 2.12                     | 0.50              |
| 7:SB:50:ASP:OD1    | 7:SB:50:ASP:N      | 2.44                     | 0.50              |
| 12:SG:149:LEU:HD12 | 12:SG:155:VAL:HG12 | 1.92                     | 0.50              |
| 13:SH:155:PHE:HB3  | 13:SH:156:PRO:HD3  | 1.93                     | 0.50              |
| 21:SP:122:VAL:HG12 | 21:SP:130:LEU:HD22 | 1.92                     | 0.50              |
| 44:LE:1340:C:N4    | 100:LE:1532:HOH:O  | 2.44                     | 0.50              |
| 49:LJ:3700:C:H2'   | 49:LJ:3701:PSU:C6  | 2.47                     | 0.50              |
| 52:LM:3943:C:H2'   | 52:LM:3944:G:C8    | 2.47                     | 0.50              |
| 56:LQ:116:ARG:HB3  | 56:LQ:177:LYS:HG3  | 1.93                     | 0.50              |
| 62:LW:89:VAL:HG11  | 62:LW:107:LEU:HD22 | 1.93                     | 0.50              |
| 65:LZ:85:ASP:OD1   | 65:LZ:88:ASN:ND2   | 2.29                     | 0.50              |
| 67:Lb:73:ARG:HD2   | 67:Lb:80:CYS:SG    | 2.52                     | 0.50              |
| 70:Le:123:ASP:OD1  | 70:Le:124:GLN:N    | 2.44                     | 0.50              |
| 71:Lf:131:ASN:O    | 71:Lf:131:ASN:ND2  | 2.44                     | 0.50              |
| 90:Ly:54:LYS:O     | 90:Ly:58:THR:HG23  | 2.10                     | 0.50              |
| 96:L4:3:GLN:HB3    | 96:L4:94:ALA:HB2   | 1.94                     | 0.50              |
| 1:S1:1934:U:H2'    | 1:S1:1935:C:C6     | 2.46                     | 0.50              |
| 1:S1:1973:G:O2'    | 1:S1:1997:C:O2     | 2.22                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:S2:76:A:O2'      | 48:LI:3541:U:O4    | 2.24                     | 0.50              |
| 9:SD:92:LYS:HB2    | 9:SD:95:TYR:CD2    | 2.46                     | 0.50              |
| 11:SF:228:PRO:HA   | 11:SF:231:TRP:CG   | 2.46                     | 0.50              |
| 22:SQ:90:ARG:HH21  | 22:SQ:90:ARG:HB2   | 1.77                     | 0.50              |
| 44:LE:983:A:OP1    | 57:LR:41:ASN:ND2   | 2.36                     | 0.50              |
| 49:LJ:3632:G:OP2   | 49:LJ:3682:C:N4    | 2.29                     | 0.50              |
| 51:LL:3829:A:O3'   | 65:LZ:148:LYS:NZ   | 2.28                     | 0.50              |
| 56:LQ:240:LEU:HB3  | 56:LQ:244:THR:HG21 | 1.94                     | 0.50              |
| 57:LR:4:ARG:NH2    | 57:LR:19:PRO:O     | 2.43                     | 0.50              |
| 1:S1:784:U:H2'     | 1:S1:785:G:C8      | 2.47                     | 0.50              |
| 1:S1:1277:G:OP1    | 25:ST:107:LYS:HE2  | 2.12                     | 0.50              |
| 1:S1:1281:G:H2'    | 1:S1:1282:A:C8     | 2.45                     | 0.50              |
| 1:S1:1302:A:H2'    | 1:S1:1303:A:O4'    | 2.11                     | 0.50              |
| 1:S1:1563:U:OP1    | 33:Sb:83:ARG:NH1   | 2.45                     | 0.50              |
| 10:SE:122:LYS:HG2  | 10:SE:123:LEU:H    | 1.76                     | 0.50              |
| 16:SK:243:ARG:O    | 16:SK:246:GLN:NE2  | 2.45                     | 0.50              |
| 42:LC:396:C:H2'    | 42:LC:397:C:C6     | 2.46                     | 0.50              |
| 44:LE:817:C:N4     | 44:LE:818:C:N4     | 2.60                     | 0.50              |
| 44:LE:966:C:H2'    | 44:LE:967:G:O4'    | 2.12                     | 0.50              |
| 48:LI:2982:G:N7    | 48:LI:2984:G:N2    | 2.50                     | 0.50              |
| 54:LO:42:A:O2'     | 58:LS:150:ARG:NH1  | 2.45                     | 0.50              |
| 60:LU:53:PRO:HA    | 60:LU:156:GLN:HE22 | 1.76                     | 0.50              |
| 71:Lf:137:ARG:HE   | 71:Lf:138:LEU:HD22 | 1.77                     | 0.50              |
| 84:Ls:44:LEU:HD23  | 84:Ls:95:ILE:HD12  | 1.93                     | 0.50              |
| 1:S1:93:U:H4'      | 10:SE:6:LYS:HA     | 1.92                     | 0.50              |
| 1:S1:962:G:H2'     | 1:S1:963:G:C8      | 2.46                     | 0.50              |
| 1:S1:1096:A2M:HM'3 | 25:ST:77:HIS:HA    | 1.92                     | 0.50              |
| 1:S1:1289:A:H2'    | 1:S1:1290:G:C8     | 2.46                     | 0.50              |
| 1:S1:1876:U:H2'    | 1:S1:1877:C:C6     | 2.46                     | 0.50              |
| 6:SA:41:ILE:HD12   | 6:SA:66:LEU:HD13   | 1.93                     | 0.50              |
| 7:SB:173:MET:HE1   | 7:SB:199:VAL:HG11  | 1.94                     | 0.50              |
| 9:SD:37:ARG:N      | 9:SD:41:GLU:OE1    | 2.41                     | 0.50              |
| 10:SE:43:PRO:HD2   | 10:SE:46:LEU:HD22  | 1.93                     | 0.50              |
| 45:LF:1678:G:N2    | 45:LF:1679:G:N7    | 2.57                     | 0.50              |
| 46:LG:2086:C:H2'   | 46:LG:2087:C:C6    | 2.46                     | 0.50              |
| 47:LH:2642:PSU:H2' | 47:LH:2643:G:C8    | 2.47                     | 0.50              |
| 62:LW:42:ARG:HD2   | 62:LW:113:ILE:HD11 | 1.93                     | 0.50              |
| 69:Ld:102:LEU:HD11 | 69:Ld:246:ARG:HH21 | 1.75                     | 0.50              |
| 78:Lm:7:LEU:HD22   | 78:Lm:33:LEU:HD22  | 1.94                     | 0.50              |
| 83:Lr:87:VAL:O     | 83:Lr:115:GLY:HA2  | 2.10                     | 0.50              |
| 1:S1:1304:A:H2'    | 1:S1:1305:U:H6     | 1.77                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:S1:1741:A:OP1   | 27:SV:45:ARG:NH1   | 2.44                     | 0.50              |
| 1:S1:2007:A:N3    | 1:S1:2066:G:O2'    | 2.37                     | 0.50              |
| 38:Sg:103:LEU:O   | 38:Sg:111:LYS:NZ   | 2.43                     | 0.50              |
| 41:LB:244:C:OP2   | 41:LB:245:A:O2'    | 2.30                     | 0.50              |
| 43:LD:691:C:H2'   | 43:LD:692:C:H6     | 1.75                     | 0.50              |
| 45:LF:1801:G:OP2  | 45:LF:1801:G:N2    | 2.35                     | 0.50              |
| 45:LF:1924:C:O2'  | 45:LF:1925:G:O4'   | 2.26                     | 0.50              |
| 47:LH:2353:A:O2'  | 49:LJ:3643:G:H4'   | 2.12                     | 0.50              |
| 48:LI:3139:U:O2'  | 48:LI:3141:A:N6    | 2.35                     | 0.50              |
| 61:LV:251:THR:HA  | 61:LV:254:VAL:HG22 | 1.94                     | 0.50              |
| 62:LW:175:LYS:HD2 | 65:LZ:200:TRP:HB3  | 1.92                     | 0.50              |
| 76:Lk:87:PRO:HD2  | 81:Lp:33:VAL:HG22  | 1.93                     | 0.50              |
| 1:S1:115:U:H2'    | 1:S1:116:C:C6      | 2.46                     | 0.50              |
| 1:S1:1156:G:H2'   | 1:S1:1157:G:C8     | 2.46                     | 0.50              |
| 1:S1:1266:C:H2'   | 1:S1:1267:U:H6     | 1.76                     | 0.50              |
| 1:S1:1518:G:N1    | 21:SP:20:GLN:OE1   | 2.34                     | 0.50              |
| 4:S4:5:G:H2'      | 4:S4:6:G:H8        | 1.76                     | 0.50              |
| 8:SC:125:LEU:HD23 | 8:SC:136:CYS:HB3   | 1.93                     | 0.50              |
| 10:SE:36:HIS:CG   | 10:SE:85:GLY:HA3   | 2.47                     | 0.50              |
| 31:SZ:9:PHE:HD1   | 31:SZ:36:ARG:NH2   | 2.10                     | 0.50              |
| 42:LC:467:U:O2'   | 42:LC:468:C:H5'    | 2.12                     | 0.50              |
| 44:LE:1082:G:OP2  | 70:Le:144:ARG:NH1  | 2.45                     | 0.50              |
| 52:LM:3950:A:H8   | 53:LN:3981:A:H8    | 1.60                     | 0.50              |
| 67:Lb:158:HIS:HB3 | 67:Lb:161:ALA:HB3  | 1.94                     | 0.50              |
| 1:S1:68:A:OP1     | 12:SG:162:ARG:NH2  | 2.31                     | 0.50              |
| 1:S1:970:A:H2'    | 1:S1:971:G:C8      | 2.47                     | 0.50              |
| 1:S1:982:G:H2'    | 1:S1:983:G:C8      | 2.47                     | 0.50              |
| 1:S1:1837:U:H2'   | 1:S1:1838:C:C6     | 2.47                     | 0.50              |
| 2:S2:28:G:O2'     | 2:S2:29:G:H5'      | 2.12                     | 0.50              |
| 3:S3:50:U:O2'     | 3:S3:51:U:O4'      | 2.30                     | 0.50              |
| 4:S4:27:G:H2'     | 4:S4:28:G:C8       | 2.45                     | 0.50              |
| 8:SC:107:LEU:HB2  | 8:SC:124:VAL:HG21  | 1.94                     | 0.50              |
| 16:SK:252:GLU:HG2 | 16:SK:255:LEU:HB2  | 1.94                     | 0.50              |
| 22:SQ:98:GLY:O    | 22:SQ:99:LEU:HD23  | 2.12                     | 0.50              |
| 26:SU:14:GLN:NE2  | 26:SU:39:TRP:O     | 2.45                     | 0.50              |
| 32:Sa:52:TRP:CH2  | 32:Sa:60:LEU:HD22  | 2.47                     | 0.50              |
| 40:LA:78:A:O2'    | 40:LA:80:U:H5''    | 2.12                     | 0.50              |
| 41:LB:279:C:H4'   | 67:Lb:147:GLU:OE2  | 2.12                     | 0.50              |
| 44:LE:1212:G:H2'  | 44:LE:1214:A:N7    | 2.27                     | 0.50              |
| 44:LE:1310:U:H2'  | 44:LE:1311:C:C6    | 2.46                     | 0.50              |
| 45:LF:1924:C:HO2' | 45:LF:1925:G:C1'   | 2.25                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:LH:2592:G:OP2   | 71:Lf:82:ARG:NH1   | 2.32                     | 0.50              |
| 47:LH:2701:A:H2'   | 47:LH:2702:A:H8    | 1.75                     | 0.50              |
| 48:LI:3083:C:H2'   | 48:LI:3084:C:C6    | 2.46                     | 0.50              |
| 49:LJ:3711:U:H4'   | 49:LJ:3712:U:H5''  | 1.93                     | 0.50              |
| 55:LP:34:TYR:CE1   | 55:LP:38:LYS:HG3   | 2.46                     | 0.50              |
| 58:LS:126:TYR:HD2  | 58:LS:129:ASN:CG   | 2.20                     | 0.50              |
| 60:LU:47:TYR:HB2   | 60:LU:156:GLN:NE2  | 2.27                     | 0.50              |
| 60:LU:189:LYS:HD3  | 87:Lv:35:ASN:HB3   | 1.94                     | 0.50              |
| 62:LW:41:VAL:HG22  | 62:LW:112:GLY:O    | 2.11                     | 0.50              |
| 62:LW:179:LEU:HD12 | 65:LZ:204:VAL:HG22 | 1.93                     | 0.50              |
| 64:LY:100:ASP:HB2  | 78:Lm:24:THR:HG21  | 1.93                     | 0.50              |
| 74:Li:41:MET:HE1   | 74:Li:49:TYR:HB2   | 1.94                     | 0.50              |
| 1:S1:1639:G:O6     | 22:SQ:44:HIS:HB3   | 2.11                     | 0.49              |
| 2:S2:74:C:O2'      | 2:S2:75:C:H5''     | 2.12                     | 0.49              |
| 14:SI:78:PHE:O     | 14:SI:82:HIS:HB2   | 2.12                     | 0.49              |
| 17:SL:144:ALA:O    | 17:SL:145:ARG:NE   | 2.35                     | 0.49              |
| 44:LE:850:C:H2'    | 73:Lh:138:LYS:HB2  | 1.93                     | 0.49              |
| 44:LE:967:G:H3'    | 57:LR:111:ARG:HH21 | 1.76                     | 0.49              |
| 44:LE:1045:C:H2'   | 44:LE:1047:A:H8    | 1.76                     | 0.49              |
| 44:LE:1127:C:H2'   | 44:LE:1128:U:C6    | 2.47                     | 0.49              |
| 44:LE:1412:C:H3'   | 44:LE:1413:A:H2'   | 1.94                     | 0.49              |
| 47:LH:2295:C:N4    | 47:LH:2312:U:OP2   | 2.45                     | 0.49              |
| 48:LI:3203:U:H2'   | 48:LI:3204:PSU:H6  | 1.77                     | 0.49              |
| 48:LI:3416:G:H1    | 48:LI:3444:PSU:HN3 | 1.60                     | 0.49              |
| 54:LO:110:G:OP1    | 97:L6:42:ARG:NH2   | 2.44                     | 0.49              |
| 56:LQ:108:GLN:HA   | 56:LQ:137:LEU:HD23 | 1.94                     | 0.49              |
| 1:S1:826:A:O2'     | 1:S1:827:C:OP1     | 2.27                     | 0.49              |
| 1:S1:1320:C:H2'    | 1:S1:1321:A:C8     | 2.47                     | 0.49              |
| 1:S1:1350:G:H2'    | 1:S1:1351:U:C6     | 2.48                     | 0.49              |
| 15:SJ:91:THR:HB    | 15:SJ:97:ARG:HH12  | 1.76                     | 0.49              |
| 39:Sh:25:THR:HG23  | 39:Sh:294:GLN:HG2  | 1.94                     | 0.49              |
| 39:Sh:222:LEU:HD11 | 39:Sh:265:LEU:HD22 | 1.94                     | 0.49              |
| 42:LC:353:G:H2'    | 42:LC:354:U:H4'    | 1.93                     | 0.49              |
| 44:LE:1113:U:H3    | 44:LE:1226:G:H1    | 1.60                     | 0.49              |
| 45:LF:1789:U:H1'   | 86:Lu:61:GLY:O     | 2.12                     | 0.49              |
| 48:LI:3148:G:C2    | 48:LI:3149:A:H1'   | 2.46                     | 0.49              |
| 48:LI:3234:U:H2'   | 48:LI:3235:U:O4'   | 2.11                     | 0.49              |
| 48:LI:3460:G:OP2   | 100:LI:3608:HOH:O  | 2.19                     | 0.49              |
| 56:LQ:122:TRP:CH2  | 56:LQ:127:LYS:HG2  | 2.46                     | 0.49              |
| 63:LX:6:ASN:ND2    | 70:Le:152:GLY:O    | 2.46                     | 0.49              |
| 67:Lb:6:TYR:O      | 67:Lb:10:VAL:HG23  | 2.12                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:Lg:118:HIS:O    | 72:Lg:120:ARG:NH1  | 2.45                     | 0.49              |
| 83:Lr:89:ARG:NH1   | 83:Lr:109:LEU:O    | 2.45                     | 0.49              |
| 95:L5:67:GLY:HA3   | 95:L5:70:THR:O     | 2.12                     | 0.49              |
| 1:S1:167:A:N1      | 1:S1:180:OMG:C5    | 2.76                     | 0.49              |
| 1:S1:636:G:OP1     | 9:SD:132:ARG:NH2   | 2.42                     | 0.49              |
| 1:S1:2260:A:H5''   | 21:SP:60:LYS:HG2   | 1.94                     | 0.49              |
| 7:SB:12:GLU:OE2    | 27:SV:118:ILE:HB   | 2.13                     | 0.49              |
| 13:SH:35:LEU:HD12  | 17:SL:55:LYS:HB2   | 1.94                     | 0.49              |
| 16:SK:235:ASN:OD1  | 16:SK:238:ARG:NH1  | 2.45                     | 0.49              |
| 16:SK:278:GLY:O    | 16:SK:279:ARG:NH2  | 2.44                     | 0.49              |
| 20:SO:32:CYS:HB2   | 20:SO:94:LEU:HD22  | 1.92                     | 0.49              |
| 37:Sf:103:VAL:HG13 | 37:Sf:107:TYR:HE1  | 1.77                     | 0.49              |
| 38:Sg:219:ARG:O    | 38:Sg:223:THR:HG23 | 2.12                     | 0.49              |
| 41:LB:263:A:OP1    | 63:LX:77:ARG:NH2   | 2.42                     | 0.49              |
| 44:LE:874:G:H4'    | 57:LR:307:LYS:HD3  | 1.94                     | 0.49              |
| 45:LF:1832:G:C8    | 74:Li:29:LYS:HB2   | 2.47                     | 0.49              |
| 45:LF:1911:C:H2'   | 45:LF:1912:A:H8    | 1.77                     | 0.49              |
| 48:LI:3351:U:H2'   | 48:LI:3352:G:O4'   | 2.11                     | 0.49              |
| 49:LJ:3662:C:H2'   | 49:LJ:3663:G:O4'   | 2.12                     | 0.49              |
| 53:LN:4011:G:C2    | 53:LN:4019:U:C2    | 3.00                     | 0.49              |
| 66:La:103:LEU:HD13 | 66:La:146:GLY:HA2  | 1.94                     | 0.49              |
| 68:Lc:31:ILE:HA    | 68:Lc:66:GLU:OE2   | 2.11                     | 0.49              |
| 69:Ld:40:LYS:NZ    | 73:Lh:32:ALA:O     | 2.44                     | 0.49              |
| 79:Ln:82:PRO:HD2   | 84:Ls:62:TYR:HE1   | 1.75                     | 0.49              |
| 1:S1:269:U:H2'     | 1:S1:270:G:H8      | 1.76                     | 0.49              |
| 1:S1:727:C:OP1     | 100:S1:2420:HOH:O  | 2.19                     | 0.49              |
| 1:S1:968:C:H2'     | 1:S1:969:C:C6      | 2.47                     | 0.49              |
| 1:S1:1947:G:OP2    | 23:SR:142:ARG:NH1  | 2.46                     | 0.49              |
| 15:SJ:104:LEU:HD23 | 15:SJ:125:ILE:HA   | 1.94                     | 0.49              |
| 27:SV:91:VAL:O     | 27:SV:95:ILE:HG23  | 2.11                     | 0.49              |
| 32:Sa:72:VAL:HG13  | 32:Sa:86:ALA:HB3   | 1.94                     | 0.49              |
| 38:Sg:153:HIS:HE1  | 38:Sg:193:PHE:HA   | 1.78                     | 0.49              |
| 42:LC:465:U:O2'    | 42:LC:466:A:OP1    | 2.29                     | 0.49              |
| 42:LC:488:G:OP2    | 42:LC:490:C:O2'    | 2.23                     | 0.49              |
| 44:LE:1313:G:N3    | 48:LI:3209:A:H2'   | 2.26                     | 0.49              |
| 45:LF:1774:U:O2'   | 45:LF:1802:A:N1    | 2.40                     | 0.49              |
| 46:LG:2037:G:H2'   | 46:LG:2038:G:H8    | 1.78                     | 0.49              |
| 46:LG:2070:C:HO2'  | 46:LG:2071:C:P     | 2.35                     | 0.49              |
| 48:LI:3321:C:H5'   | 69:Ld:177:ARG:HG2  | 1.95                     | 0.49              |
| 49:LJ:3631:G:H2'   | 49:LJ:3632:G:C8    | 2.47                     | 0.49              |
| 59:LT:41:VAL:HG21  | 59:LT:73:ILE:HD11  | 1.94                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 62:LW:51:SER:HB2    | 62:LW:139:LYS:HE3  | 1.94                     | 0.49              |
| 64:LY:37:LEU:O      | 64:LY:63:ALA:HB1   | 2.12                     | 0.49              |
| 71:Lf:135:ASN:HB2   | 71:Lf:138:LEU:HD23 | 1.95                     | 0.49              |
| 74:Li:111:PRO:HA    | 74:Li:114:MET:HG3  | 1.94                     | 0.49              |
| 95:L5:77:THR:HG22   | 95:L5:80:ARG:HH12  | 1.77                     | 0.49              |
| 1:S1:216:C:H2'      | 1:S1:217:U:O4'     | 2.12                     | 0.49              |
| 1:S1:779:U:N3       | 1:S1:820:G:O6      | 2.42                     | 0.49              |
| 1:S1:1243:C:O2'     | 1:S1:1244:C:OP1    | 2.27                     | 0.49              |
| 1:S1:2238:U:H2'     | 1:S1:2239:G:H8     | 1.78                     | 0.49              |
| 23:SR:15:ARG:NH1    | 58:LS:118:GLU:OE1  | 2.46                     | 0.49              |
| 38:Sg:84:ARG:HE     | 38:Sg:90:LEU:H     | 1.59                     | 0.49              |
| 40:LA:123:A:H2'     | 40:LA:124:G:H8     | 1.76                     | 0.49              |
| 42:LC:644:U:H2'     | 44:LE:896:A:H61    | 1.77                     | 0.49              |
| 44:LE:1435:C:H2'    | 44:LE:1436:A:C8    | 2.45                     | 0.49              |
| 45:LF:1542:A:N3     | 45:LF:1548:A:H2'   | 2.28                     | 0.49              |
| 47:LH:2771:G:H1'    | 47:LH:2773:C:N4    | 2.28                     | 0.49              |
| 48:LI:3561:U:H2'    | 48:LI:3562:PSU:C6  | 2.47                     | 0.49              |
| 51:LL:3857:U:H2'    | 51:LL:3858:G:H8    | 1.77                     | 0.49              |
| 69:Ld:43:TYR:CD2    | 73:Lh:35:LYS:HG2   | 2.48                     | 0.49              |
| 69:Ld:81:GLU:OE2    | 69:Ld:107:ARG:NH1  | 2.44                     | 0.49              |
| 75:Lj:109:ILE:HG22  | 75:Lj:111:GLY:H    | 1.76                     | 0.49              |
| 89:Lx:80:THR:HG22   | 89:Lx:82:ARG:H     | 1.78                     | 0.49              |
| 1:S1:5:U:H2'        | 1:S1:6:G:H8        | 1.78                     | 0.49              |
| 1:S1:27:PSU:H2'     | 1:S1:28:A2M:H8     | 1.95                     | 0.49              |
| 1:S1:204:A:OP1      | 16:SK:236:HIS:HB2  | 2.13                     | 0.49              |
| 1:S1:269:U:H3       | 1:S1:349:G:H1      | 1.60                     | 0.49              |
| 1:S1:711:A:H5'      | 1:S1:717:G:N2      | 2.26                     | 0.49              |
| 1:S1:852:C:H2'      | 1:S1:853:G:C8      | 2.48                     | 0.49              |
| 1:S1:1589:G:O2'     | 28:SW:136:PRO:O    | 2.17                     | 0.49              |
| 8:SC:46:GLN:O       | 8:SC:47:ARG:HG3    | 2.12                     | 0.49              |
| 9:SD:71:ILE:HD12    | 10:SE:249:ILE:CD1  | 2.37                     | 0.49              |
| 22:SQ:36:HIS:O      | 22:SQ:36:HIS:ND1   | 2.42                     | 0.49              |
| 22:SQ:90:ARG:HB2    | 22:SQ:90:ARG:NH2   | 2.27                     | 0.49              |
| 29:SX:75:VAL:O      | 29:SX:79:ARG:HG3   | 2.12                     | 0.49              |
| 40:LA:32:C:OP2      | 100:LA:201:HOH:O   | 2.20                     | 0.49              |
| 40:LA:35:A:OP1      | 40:LA:36:G:O2'     | 2.26                     | 0.49              |
| 47:LH:2634:C:H5''   | 55:LP:203:ALA:HB1  | 1.94                     | 0.49              |
| 47:LH:2895:C:H2'    | 47:LH:2896:U:C6    | 2.48                     | 0.49              |
| 48:LI:3289:U:H4'    | 48:LI:3290:G:OP2   | 2.13                     | 0.49              |
| 48:LI:3381:U:OP2    | 96:L4:63:LYS:HG2   | 2.13                     | 0.49              |
| 48:LI:3533:A2M:H5'' | 48:LI:3534:G:H5'   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:LL:3821:U:H2'   | 51:LL:3822:U:C6    | 2.47                     | 0.49              |
| 54:LO:4:U:H2'      | 54:LO:5:A:H8       | 1.77                     | 0.49              |
| 59:LT:107:ASP:OD1  | 59:LT:108:ASP:N    | 2.38                     | 0.49              |
| 64:LY:33:GLY:HA3   | 64:LY:69:LYS:HD2   | 1.95                     | 0.49              |
| 69:Ld:78:TYR:O     | 69:Ld:81:GLU:HG2   | 2.12                     | 0.49              |
| 1:S1:299:A:H2'     | 1:S1:300:A:C8      | 2.47                     | 0.49              |
| 1:S1:773:U:N3      | 1:S1:774:G:O6      | 2.46                     | 0.49              |
| 1:S1:1147:C:H2'    | 14:SI:73:ARG:HD3   | 1.93                     | 0.49              |
| 1:S1:1336:A:H2'    | 1:S1:1337:A:C8     | 2.47                     | 0.49              |
| 1:S1:1571:C:H2'    | 1:S1:1572:A:H8     | 1.78                     | 0.49              |
| 1:S1:1611:G:N2     | 1:S1:2103:A:H5'    | 2.27                     | 0.49              |
| 1:S1:2261:A:N6     | 21:SP:64:SER:OG    | 2.46                     | 0.49              |
| 7:SB:83:GLY:HA2    | 7:SB:171:ILE:HG21  | 1.94                     | 0.49              |
| 9:SD:34:TYR:HD2    | 9:SD:111:THR:HG21  | 1.77                     | 0.49              |
| 26:SU:62:LYS:HB3   | 26:SU:136:LEU:HD13 | 1.95                     | 0.49              |
| 30:SY:12:TYR:CG    | 30:SY:12:TYR:O     | 2.66                     | 0.49              |
| 42:LC:383:G:H2'    | 42:LC:384:U:O4'    | 2.13                     | 0.49              |
| 43:LD:697:U:O4     | 43:LD:698:C:N4     | 2.46                     | 0.49              |
| 44:LE:838:U:H2'    | 44:LE:839:G:H8     | 1.77                     | 0.49              |
| 44:LE:1198:PSU:H2' | 44:LE:1199:G:C8    | 2.46                     | 0.49              |
| 44:LE:1379:A:H5''  | 54:LO:98:G:O2'     | 2.12                     | 0.49              |
| 45:LF:1466:G:N7    | 73:Lh:123:LYS:NZ   | 2.47                     | 0.49              |
| 47:LH:2831:U:H2'   | 47:LH:2832:OMC:C6  | 2.47                     | 0.49              |
| 48:LI:3190:G:O2'   | 48:LI:3451:PSU:OP1 | 2.25                     | 0.49              |
| 50:LK:3760:G:N2    | 72:Lg:177:TYR:OH   | 2.37                     | 0.49              |
| 56:LQ:292:LEU:CD1  | 56:LQ:322:ARG:HB2  | 2.43                     | 0.49              |
| 59:LT:23:ARG:HD2   | 59:LT:45:MET:HE3   | 1.95                     | 0.49              |
| 59:LT:91:LYS:HG2   | 59:LT:147:VAL:HG12 | 1.94                     | 0.49              |
| 62:LW:43:CYS:SG    | 62:LW:109:VAL:HG13 | 2.52                     | 0.49              |
| 63:LX:134:PHE:HZ   | 63:LX:154:PRO:HB3  | 1.77                     | 0.49              |
| 65:LZ:15:ILE:HG22  | 65:LZ:61:LEU:HD23  | 1.95                     | 0.49              |
| 80:Lo:70:ALA:O     | 80:Lo:72:GLU:N     | 2.43                     | 0.49              |
| 1:S1:301:G:H2'     | 1:S1:302:G:H8      | 1.76                     | 0.49              |
| 1:S1:332:G:H21     | 16:SK:75:ALA:HB2   | 1.78                     | 0.49              |
| 1:S1:1864:U:H5''   | 18:SM:60:THR:HG23  | 1.93                     | 0.49              |
| 4:S4:14:A:H2'      | 4:S4:15:G:O4'      | 2.12                     | 0.49              |
| 7:SB:155:VAL:HA    | 30:SY:62:ALA:HB2   | 1.94                     | 0.49              |
| 14:SI:26:ASP:O     | 14:SI:30:GLN:HG3   | 2.13                     | 0.49              |
| 21:SP:131:MET:O    | 21:SP:135:ARG:HG2  | 2.12                     | 0.49              |
| 22:SQ:39:LEU:HD11  | 22:SQ:97:VAL:HG12  | 1.95                     | 0.49              |
| 23:SR:13:ILE:HB    | 58:LS:127:ASP:HB3  | 1.94                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 44:LE:913:U:H2'     | 44:LE:914:G:C8     | 2.48                     | 0.49              |
| 44:LE:1165:OMC:HM22 | 44:LE:1166:G:H5'   | 1.95                     | 0.49              |
| 45:LF:1580:U:H2'    | 93:L2:107:ASN:ND2  | 2.27                     | 0.49              |
| 50:LK:3809:U:O2     | 51:LL:3894:G:N2    | 2.36                     | 0.49              |
| 98:L7:53:ALA:O      | 98:L7:56:LYS:HG3   | 2.13                     | 0.49              |
| 1:S1:190:C:H2'      | 1:S1:191:G:H8      | 1.76                     | 0.49              |
| 1:S1:509:U:H2'      | 1:S1:510:A:H8      | 1.78                     | 0.49              |
| 1:S1:664:U:H2'      | 1:S1:665:G:H8      | 1.78                     | 0.49              |
| 1:S1:940:G:H4'      | 1:S1:941:C:OP1     | 2.13                     | 0.49              |
| 1:S1:1607:C:OP1     | 17:SL:146:ARG:NH1  | 2.45                     | 0.49              |
| 1:S1:1644:A:N3      | 37:Sf:141:TYR:OH   | 2.37                     | 0.49              |
| 1:S1:1754:A:O2'     | 1:S1:1757:A:N6     | 2.45                     | 0.49              |
| 13:SH:122:ARG:HG3   | 13:SH:189:ASN:ND2  | 2.28                     | 0.49              |
| 19:SN:88:SER:HA     | 19:SN:91:LYS:HG2   | 1.94                     | 0.49              |
| 43:LD:677:C:H2'     | 43:LD:678:U:C6     | 2.47                     | 0.49              |
| 46:LG:2173:G:H5''   | 46:LG:2175:G:O4'   | 2.13                     | 0.49              |
| 47:LH:2347:G:H2'    | 47:LH:2348:OMC:C6  | 2.47                     | 0.49              |
| 48:LI:3343:U:H2'    | 48:LI:3344:G:H8    | 1.78                     | 0.49              |
| 59:LT:63:LYS:O      | 59:LT:66:ASP:N     | 2.46                     | 0.49              |
| 59:LT:103:VAL:HA    | 59:LT:113:GLU:O    | 2.13                     | 0.49              |
| 63:LX:70:GLN:HE21   | 66:La:131:ARG:HH11 | 1.59                     | 0.49              |
| 67:Lb:159:ARG:HB3   | 67:Lb:164:VAL:HB   | 1.93                     | 0.49              |
| 88:Lw:13:HIS:NE2    | 92:L1:4:ILE:HD11   | 2.28                     | 0.49              |
| 1:S1:716:U:OP2      | 21:SP:3:LYS:NZ     | 2.38                     | 0.49              |
| 1:S1:828:G:H2'      | 1:S1:829:G:O4'     | 2.13                     | 0.49              |
| 1:S1:982:G:C6       | 1:S1:983:G:O6      | 2.65                     | 0.49              |
| 1:S1:1289:A:H2'     | 1:S1:1290:G:H8     | 1.77                     | 0.49              |
| 1:S1:1977:A:H5'     | 24:SS:21:ARG:NH2   | 2.28                     | 0.49              |
| 4:S4:8:U:H3         | 4:S4:14:A:N6       | 1.99                     | 0.49              |
| 6:SA:177:SER:OG     | 6:SA:181:SER:OG    | 2.30                     | 0.49              |
| 39:Sh:167:PRO:HB2   | 39:Sh:183:LEU:HD21 | 1.94                     | 0.49              |
| 42:LC:536:A:H2'     | 42:LC:537:OMC:H6   | 1.78                     | 0.49              |
| 44:LE:802:G:H1      | 44:LE:841:U:H3     | 1.61                     | 0.49              |
| 45:LF:1976:OMC:H5'  | 45:LF:1977:C:H5    | 1.77                     | 0.49              |
| 48:LI:3181:A:H2'    | 48:LI:3182:G:C8    | 2.47                     | 0.49              |
| 55:LP:122:ASP:OD2   | 55:LP:125:ARG:HD3  | 2.13                     | 0.49              |
| 64:LY:30:ASP:HB3    | 64:LY:32:THR:HG23  | 1.94                     | 0.49              |
| 1:S1:85:U:H2'       | 1:S1:86:C:H6       | 1.75                     | 0.48              |
| 1:S1:290:A:H3'      | 1:S1:291:G:H8      | 1.78                     | 0.48              |
| 1:S1:552:C:O2       | 31:SZ:89:ARG:NE    | 2.32                     | 0.48              |
| 1:S1:1300:U:O2'     | 1:S1:1302:A:N7     | 2.29                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:SE:166:THR:HG23 | 10:SE:168:LYS:H    | 1.78                     | 0.48              |
| 13:SH:36:PRO:HG3   | 13:SH:79:LEU:HD23  | 1.95                     | 0.48              |
| 14:SI:82:HIS:CD2   | 14:SI:86:THR:HB    | 2.48                     | 0.48              |
| 24:SS:21:ARG:NH1   | 24:SS:35:LEU:O     | 2.42                     | 0.48              |
| 44:LE:1172:C:H4'   | 47:LH:2366:A:H5'   | 1.95                     | 0.48              |
| 47:LH:2328:G:OP1   | 100:LH:3009:HOH:O  | 2.19                     | 0.48              |
| 48:LI:3146:C:H2'   | 48:LI:3147:C:C6    | 2.48                     | 0.48              |
| 53:LN:3995:G:H5'   | 56:LQ:172:ARG:HH22 | 1.77                     | 0.48              |
| 81:Lp:103:LYS:O    | 81:Lp:108:LYS:NZ   | 2.46                     | 0.48              |
| 1:S1:190:C:H2'     | 1:S1:191:G:C8      | 2.48                     | 0.48              |
| 1:S1:456:A:N6      | 21:SP:32:LEU:O     | 2.47                     | 0.48              |
| 1:S1:825:A:H2'     | 1:S1:826:A:C8      | 2.48                     | 0.48              |
| 1:S1:1014:A:O3'    | 10:SE:200:ARG:NH2  | 2.46                     | 0.48              |
| 1:S1:1876:U:OP2    | 39:Sh:285:ALA:HB2  | 2.13                     | 0.48              |
| 1:S1:1972:U:OP1    | 24:SS:33:TYR:OH    | 2.27                     | 0.48              |
| 4:S4:1:G:H2'       | 4:S4:2:C:C6        | 2.47                     | 0.48              |
| 25:ST:57:SER:HB3   | 34:Sc:56:VAL:HG22  | 1.94                     | 0.48              |
| 35:Sd:19:VAL:HG12  | 35:Sd:37:VAL:HG12  | 1.96                     | 0.48              |
| 39:Sh:111:ASP:HB3  | 39:Sh:129:ARG:HB2  | 1.94                     | 0.48              |
| 40:LA:19:C:OP1     | 57:LR:189:LYS:NZ   | 2.45                     | 0.48              |
| 42:LC:637:A:OP1    | 87:Lv:73:ARG:NH2   | 2.46                     | 0.48              |
| 44:LE:851:G:OP1    | 100:LE:1514:HOH:O  | 2.20                     | 0.48              |
| 44:LE:1330:G:H5''  | 68:Lc:40:LYS:HG2   | 1.95                     | 0.48              |
| 45:LF:1814:G:OP2   | 57:LR:103:ARG:NH2  | 2.38                     | 0.48              |
| 45:LF:1892:C:OP2   | 100:LH:3009:HOH:O  | 2.20                     | 0.48              |
| 45:LF:1901:A:H4'   | 88:Lw:9:ARG:HD2    | 1.95                     | 0.48              |
| 46:LG:2028:U:H2'   | 46:LG:2029:A:C8    | 2.48                     | 0.48              |
| 48:LI:3534:G:C2    | 56:LQ:252:ALA:HB1  | 2.48                     | 0.48              |
| 49:LJ:3593:A:H2'   | 49:LJ:3594:C:H6    | 1.78                     | 0.48              |
| 1:S1:29:U:H2'      | 1:S1:30:G:H8       | 1.78                     | 0.48              |
| 1:S1:205:G:N7      | 16:SK:235:ASN:ND2  | 2.58                     | 0.48              |
| 1:S1:2025:C:H3'    | 1:S1:2026:A:H5''   | 1.94                     | 0.48              |
| 1:S1:2094:U:H2'    | 1:S1:2095:G:C8     | 2.48                     | 0.48              |
| 8:SC:98:LEU:HD11   | 8:SC:200:MET:HG2   | 1.94                     | 0.48              |
| 14:SI:82:HIS:HD2   | 14:SI:86:THR:HB    | 1.78                     | 0.48              |
| 17:SL:67:ARG:HD2   | 17:SL:101:TYR:HE2  | 1.78                     | 0.48              |
| 29:SX:70:ASN:O     | 29:SX:73:THR:OG1   | 2.31                     | 0.48              |
| 40:LA:21:U:OP2     | 77:Ll:15:ARG:HD2   | 2.13                     | 0.48              |
| 44:LE:810:G:N2     | 44:LE:834:C:O2     | 2.46                     | 0.48              |
| 44:LE:1413:A:H4'   | 44:LE:1414:C:O5'   | 2.14                     | 0.48              |
| 45:LF:1739:G:C6    | 66:La:4:ARG:HG2    | 2.47                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:LF:1861:G:H5''  | 45:LF:1862:C:H5    | 1.77                     | 0.48              |
| 46:LG:2091:C:OP1   | 88:Lw:53:HIS:NE2   | 2.44                     | 0.48              |
| 46:LG:2208:U:H3'   | 46:LG:2209:C:C5    | 2.48                     | 0.48              |
| 47:LH:2916:U:H2'   | 47:LH:2917:G:C8    | 2.48                     | 0.48              |
| 48:LI:3290:G:C4    | 48:LI:3314:A:N6    | 2.82                     | 0.48              |
| 56:LQ:177:LYS:HG2  | 56:LQ:178:ALA:H    | 1.78                     | 0.48              |
| 63:LX:167:SER:O    | 63:LX:171:ASN:ND2  | 2.46                     | 0.48              |
| 71:Lf:164:LYS:HE2  | 71:Lf:164:LYS:HA   | 1.95                     | 0.48              |
| 1:S1:146:C:H2'     | 1:S1:147:A:C8      | 2.48                     | 0.48              |
| 1:S1:2095:G:H2'    | 1:S1:2096:G:H8     | 1.78                     | 0.48              |
| 1:S1:2193:G:H3'    | 1:S1:2194:G:H5''   | 1.93                     | 0.48              |
| 2:S2:57:G:N1       | 2:S2:60:U:O4       | 2.46                     | 0.48              |
| 13:SH:177:LYS:HE3  | 13:SH:177:LYS:HB2  | 1.61                     | 0.48              |
| 14:SI:79:HIS:HB3   | 14:SI:136:TYR:CZ   | 2.49                     | 0.48              |
| 27:SV:101:GLU:HA   | 27:SV:122:LYS:HB2  | 1.95                     | 0.48              |
| 40:LA:150:G:H2'    | 40:LA:151:U:H6     | 1.77                     | 0.48              |
| 45:LF:1517:G:OP1   | 87:Lv:22:ARG:NH2   | 2.47                     | 0.48              |
| 48:LI:3469:U:H2'   | 48:LI:3470:C:C6    | 2.47                     | 0.48              |
| 50:LK:3810:G:H2'   | 50:LK:3811:G:C8    | 2.48                     | 0.48              |
| 55:LP:112:ILE:HD12 | 95:L5:79:VAL:HG22  | 1.94                     | 0.48              |
| 60:LU:25:PHE:HD1   | 60:LU:28:ARG:NH1   | 2.10                     | 0.48              |
| 86:Lu:6:VAL:O      | 86:Lu:98:LYS:HE2   | 2.13                     | 0.48              |
| 94:L3:18:ARG:HG3   | 100:L3:105:HOH:O   | 2.13                     | 0.48              |
| 1:S1:7:G:O6        | 11:SF:206:ARG:NH2  | 2.46                     | 0.48              |
| 1:S1:1266:C:H2'    | 1:S1:1267:U:C6     | 2.48                     | 0.48              |
| 1:S1:1496:A:H5'    | 1:S1:1708:U:C5     | 2.48                     | 0.48              |
| 1:S1:1556:G:H2'    | 1:S1:1557:A:C8     | 2.48                     | 0.48              |
| 1:S1:2223:G:H2'    | 1:S1:2224:C:C6     | 2.49                     | 0.48              |
| 7:SB:176:TRP:CD1   | 7:SB:199:VAL:HG12  | 2.48                     | 0.48              |
| 11:SF:67:VAL:HG21  | 11:SF:134:LYS:HB3  | 1.95                     | 0.48              |
| 39:Sh:98:THR:O     | 39:Sh:100:THR:HG23 | 2.14                     | 0.48              |
| 47:LH:2691:U:H2'   | 47:LH:2692:C:C6    | 2.49                     | 0.48              |
| 48:LI:3009:U:H2'   | 48:LI:3010:U:H6    | 1.78                     | 0.48              |
| 49:LJ:3647:C:H5'   | 49:LJ:3676:A:H61   | 1.78                     | 0.48              |
| 54:LO:88:C:H2'     | 54:LO:89:G:O4'     | 2.14                     | 0.48              |
| 56:LQ:44:THR:HG21  | 56:LQ:186:ASN:OD1  | 2.13                     | 0.48              |
| 57:LR:302:LEU:HA   | 83:Lr:166:ASN:OD1  | 2.14                     | 0.48              |
| 59:LT:28:ARG:HD2   | 59:LT:33:THR:HG23  | 1.95                     | 0.48              |
| 60:LU:28:ARG:HE    | 60:LU:181:ILE:HD13 | 1.78                     | 0.48              |
| 62:LW:2:VAL:O      | 100:LW:301:HOH:O   | 2.20                     | 0.48              |
| 67:Lb:146:PRO:HA   | 67:Lb:149:ASN:HB2  | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 73:Lh:71:ALA:HA    | 73:Lh:92:ARG:HA    | 1.95                     | 0.48              |
| 95:L5:74:GLY:O     | 95:L5:78:THR:HG23  | 2.14                     | 0.48              |
| 1:S1:52:U:H2'      | 1:S1:53:G:C8       | 2.48                     | 0.48              |
| 1:S1:998:U:H2'     | 1:S1:999:C:C6      | 2.48                     | 0.48              |
| 1:S1:1310:A:H1'    | 47:LH:2694:G:N1    | 2.28                     | 0.48              |
| 11:SF:45:GLU:HG3   | 11:SF:247:PHE:HZ   | 1.78                     | 0.48              |
| 39:Sh:14:LYS:HA    | 39:Sh:310:THR:HG22 | 1.93                     | 0.48              |
| 47:LH:2947:A:H5''  | 48:LI:2987:A:N1    | 2.29                     | 0.48              |
| 48:LI:3144:G:N1    | 48:LI:3145:PSU:O2  | 2.46                     | 0.48              |
| 48:LI:3416:G:O6    | 100:LI:3607:HOH:O  | 2.19                     | 0.48              |
| 48:LI:3553:G:H5'   | 55:LP:220:GLY:HA3  | 1.95                     | 0.48              |
| 49:LJ:3595:A:P     | 49:LJ:3726:A:H61   | 2.35                     | 0.48              |
| 56:LQ:206:PRO:O    | 56:LQ:209:SER:OG   | 2.29                     | 0.48              |
| 58:LS:10:LYS:HE2   | 58:LS:14:LYS:HE3   | 1.94                     | 0.48              |
| 69:Ld:9:ARG:O      | 69:Ld:13:SER:OG    | 2.30                     | 0.48              |
| 91:Lz:57:GLN:HA    | 91:Lz:60:ILE:HD12  | 1.96                     | 0.48              |
| 1:S1:26:A:H2'      | 1:S1:27:PSU:C6     | 2.48                     | 0.48              |
| 1:S1:552:C:O2'     | 31:SZ:89:ARG:O     | 2.31                     | 0.48              |
| 1:S1:579:G:H22     | 1:S1:614:G:H22     | 1.62                     | 0.48              |
| 1:S1:741:C:O2      | 14:SI:119:ARG:NH2  | 2.45                     | 0.48              |
| 1:S1:1113:U:H2'    | 1:S1:1114:U:O4'    | 2.14                     | 0.48              |
| 1:S1:1293:C:OP1    | 6:SA:24:ARG:NH1    | 2.47                     | 0.48              |
| 1:S1:1475:G:H4'    | 33:Sb:13:LYS:HD3   | 1.95                     | 0.48              |
| 1:S1:1491:C:H2'    | 1:S1:1492:G:O4'    | 2.14                     | 0.48              |
| 1:S1:1718:G:H2'    | 1:S1:1719:G:C8     | 2.48                     | 0.48              |
| 1:S1:2038:U:O2'    | 32:Sa:43:ARG:NH2   | 2.46                     | 0.48              |
| 6:SA:170:ILE:O     | 6:SA:174:VAL:HG22  | 2.13                     | 0.48              |
| 10:SE:221:ARG:O    | 10:SE:225:VAL:HG13 | 2.14                     | 0.48              |
| 15:SJ:37:PHE:HD1   | 15:SJ:41:MET:HE2   | 1.78                     | 0.48              |
| 22:SQ:43:LEU:HD13  | 22:SQ:69:TYR:CE2   | 2.48                     | 0.48              |
| 25:ST:69:ARG:HB3   | 25:ST:73:ARG:HB3   | 1.94                     | 0.48              |
| 41:LB:172:G:H21    | 76:Lk:55:THR:HG21  | 1.78                     | 0.48              |
| 42:LC:581:G:H1'    | 42:LC:604:G:H21    | 1.78                     | 0.48              |
| 44:LE:1130:C:O2'   | 47:LH:2321:A:N3    | 2.41                     | 0.48              |
| 47:LH:2693:U:H2'   | 47:LH:2694:G:H2'   | 1.95                     | 0.48              |
| 52:LM:3947:U:H2'   | 52:LM:3948:G:O4'   | 2.14                     | 0.48              |
| 58:LS:182:THR:HG22 | 58:LS:183:ASP:OD1  | 2.14                     | 0.48              |
| 60:LU:78:ILE:HG23  | 60:LU:83:ILE:HD12  | 1.95                     | 0.48              |
| 61:LV:58:GLY:HA3   | 79:Ln:62:ILE:HD12  | 1.96                     | 0.48              |
| 72:Lg:5:SER:O      | 72:Lg:7:ILE:N      | 2.41                     | 0.48              |
| 73:Lh:12:ARG:O     | 73:Lh:16:SER:OG    | 2.26                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 83:Lr:183:ASP:O     | 83:Lr:187:GLN:HG2  | 2.13                     | 0.48              |
| 88:Lw:13:HIS:ND1    | 88:Lw:13:HIS:O     | 2.46                     | 0.48              |
| 1:S1:322:G:O2'      | 26:SU:44:GLY:O     | 2.18                     | 0.48              |
| 1:S1:581:A:H2'      | 1:S1:582:A:C8      | 2.48                     | 0.48              |
| 1:S1:599:U:H3'      | 1:S1:600:G:C8      | 2.49                     | 0.48              |
| 1:S1:983:G:N3       | 1:S1:983:G:H2'     | 2.29                     | 0.48              |
| 1:S1:1115:G:O2'     | 26:SU:33:SER:O     | 2.25                     | 0.48              |
| 1:S1:1409:U:H2'     | 1:S1:1410:A:C8     | 2.49                     | 0.48              |
| 1:S1:1958:U:H1'     | 13:SH:74:MET:HE3   | 1.96                     | 0.48              |
| 12:SG:243:LEU:HD12  | 38:Sg:234:ASN:HD22 | 1.78                     | 0.48              |
| 16:SK:44:ARG:CB     | 16:SK:60:LEU:O     | 2.62                     | 0.48              |
| 23:SR:87:ARG:NH1    | 23:SR:111:ASP:OD2  | 2.45                     | 0.48              |
| 38:Sg:217:LEU:O     | 38:Sg:221:THR:HG23 | 2.14                     | 0.48              |
| 40:LA:50:G:C2       | 92:L1:23:ILE:HG12  | 2.49                     | 0.48              |
| 40:LA:88:U:H2'      | 40:LA:89:C:C6      | 2.48                     | 0.48              |
| 43:LD:732:U:H2'     | 43:LD:742:G:H5''   | 1.96                     | 0.48              |
| 44:LE:1415:G:H2'    | 44:LE:1416:A:C8    | 2.48                     | 0.48              |
| 47:LH:2282:U:OP1    | 100:LH:3010:HOH:O  | 2.20                     | 0.48              |
| 47:LH:2839:U:H2'    | 47:LH:2840:G:C8    | 2.49                     | 0.48              |
| 47:LH:2849:A2M:HM'1 | 86:Lu:32:HIS:HE1   | 1.78                     | 0.48              |
| 47:LH:2938:G:O2'    | 47:LH:2939:G:O5'   | 2.30                     | 0.48              |
| 49:LJ:3679:C:H2'    | 49:LJ:3680:PSU:O4' | 2.14                     | 0.48              |
| 61:LV:125:LYS:O     | 61:LV:129:LYS:HG2  | 2.13                     | 0.48              |
| 62:LW:43:CYS:HA     | 62:LW:46:ILE:HG13  | 1.95                     | 0.48              |
| 88:Lw:23:ILE:HB     | 88:Lw:35:VAL:HB    | 1.95                     | 0.48              |
| 89:Lx:66:ARG:NH2    | 89:Lx:69:ARG:HG2   | 2.29                     | 0.48              |
| 1:S1:5:U:H2'        | 1:S1:6:G:C8        | 2.49                     | 0.48              |
| 1:S1:11:A:N3        | 1:S1:1710:A:O2'    | 2.35                     | 0.48              |
| 1:S1:341:U:H2'      | 1:S1:342:G:C8      | 2.49                     | 0.48              |
| 1:S1:420:A:OP2      | 16:SK:10:LYS:HD3   | 2.14                     | 0.48              |
| 1:S1:1096:A2M:H1'   | 1:S1:1098:C:C4     | 2.48                     | 0.48              |
| 11:SF:48:LEU:HD22   | 11:SF:53:GLU:HB3   | 1.95                     | 0.48              |
| 18:SM:50:LEU:HD13   | 18:SM:95:SER:HB2   | 1.95                     | 0.48              |
| 24:SS:29:ILE:HA     | 24:SS:38:THR:HA    | 1.96                     | 0.48              |
| 28:SW:62:LEU:HD22   | 28:SW:93:GLU:OE1   | 2.13                     | 0.48              |
| 29:SX:42:LEU:HD21   | 29:SX:55:TRP:CZ3   | 2.48                     | 0.48              |
| 33:Sb:41:VAL:HA     | 33:Sb:68:LEU:O     | 2.14                     | 0.48              |
| 38:Sg:99:ALA:O      | 38:Sg:103:LEU:HG   | 2.14                     | 0.48              |
| 42:LC:305:G:C2      | 90:Ly:77:ARG:HG3   | 2.49                     | 0.48              |
| 42:LC:550:G:OP2     | 100:LC:701:HOH:O   | 2.20                     | 0.48              |
| 42:LC:599:U:O2'     | 42:LC:601:A:N7     | 2.28                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:LE:954:G:H2'    | 44:LE:955:A:C8     | 2.49                     | 0.48              |
| 45:LF:1524:C:H1'   | 45:LF:1570:C:O2    | 2.14                     | 0.48              |
| 46:LG:1997:A:H2'   | 46:LG:1998:A:O4'   | 2.13                     | 0.48              |
| 47:LH:2328:G:C2    | 47:LH:2329:C:C5    | 3.02                     | 0.48              |
| 48:LI:3106:C:H2'   | 48:LI:3107:A:H8    | 1.79                     | 0.48              |
| 49:LJ:3643:G:H2'   | 49:LJ:3644:PSU:H6  | 1.78                     | 0.48              |
| 56:LQ:373:LYS:HG3  | 78:Lm:36:VAL:HG21  | 1.95                     | 0.48              |
| 66:La:108:LEU:HD12 | 66:La:130:ALA:HB2  | 1.94                     | 0.48              |
| 68:Lc:44:ASP:OD2   | 68:Lc:185:LYS:NZ   | 2.47                     | 0.48              |
| 68:Lc:47:PRO:HD2   | 68:Lc:141:LYS:HA   | 1.96                     | 0.48              |
| 69:Ld:102:LEU:HD11 | 69:Ld:246:ARG:NH2  | 2.29                     | 0.48              |
| 1:S1:1573:A:H2'    | 1:S1:1574:G:O4'    | 2.13                     | 0.48              |
| 9:SD:32:GLY:HA3    | 36:Se:40:TYR:CG    | 2.48                     | 0.48              |
| 9:SD:96:VAL:HA     | 9:SD:99:LEU:HD23   | 1.95                     | 0.48              |
| 11:SF:88:GLN:HE21  | 11:SF:97:THR:HG22  | 1.79                     | 0.48              |
| 13:SH:47:PHE:CZ    | 35:Sd:56:PRO:HB2   | 2.48                     | 0.48              |
| 14:SI:143:ARG:HG3  | 14:SI:157:ILE:HG13 | 1.95                     | 0.48              |
| 22:SQ:43:LEU:HD13  | 22:SQ:69:TYR:CD2   | 2.48                     | 0.48              |
| 28:SW:62:LEU:HG    | 28:SW:88:MET:HE1   | 1.96                     | 0.48              |
| 35:Sd:39:ILE:HD12  | 35:Sd:47:ARG:NH1   | 2.29                     | 0.48              |
| 42:LC:545:C:OP2    | 57:LR:191:ARG:NH1  | 2.31                     | 0.48              |
| 43:LD:666:U:O2'    | 60:LU:5:GLY:O      | 2.32                     | 0.48              |
| 44:LE:1211:U:H2'   | 44:LE:1212:G:C8    | 2.48                     | 0.48              |
| 45:LF:1498:A:H2'   | 45:LF:1499:A:C8    | 2.48                     | 0.48              |
| 45:LF:1856:OMG:H5' | 74:Li:51:ARG:HE    | 1.79                     | 0.48              |
| 47:LH:2249:A:H2'   | 47:LH:2250:C:C6    | 2.48                     | 0.48              |
| 47:LH:2254:C:H2'   | 47:LH:2255:U:C6    | 2.49                     | 0.48              |
| 47:LH:2877:C:H2'   | 47:LH:2878:A:C8    | 2.49                     | 0.48              |
| 50:LK:3788:C:O2    | 65:LZ:97:ARG:NH2   | 2.40                     | 0.48              |
| 51:LL:3852:C:H2'   | 51:LL:3853:G:O4'   | 2.14                     | 0.48              |
| 51:LL:3879:U:N3    | 65:LZ:171:LYS:HE3  | 2.29                     | 0.48              |
| 63:LX:73:ASN:HB2   | 66:La:131:ARG:HH22 | 1.78                     | 0.48              |
| 66:La:83:SER:HB3   | 66:La:120:GLY:HA3  | 1.96                     | 0.48              |
| 66:La:126:VAL:O    | 66:La:146:GLY:HA3  | 2.14                     | 0.48              |
| 68:Lc:17:TYR:HD2   | 68:Lc:96:VAL:HB    | 1.79                     | 0.48              |
| 96:L4:75:THR:O     | 96:L4:78:LYS:NZ    | 2.39                     | 0.48              |
| 1:S1:128:G:N1      | 1:S1:193:U:O4      | 2.45                     | 0.47              |
| 1:S1:736:U:H4'     | 21:SP:9:THR:HG22   | 1.96                     | 0.47              |
| 4:S4:18:G:H5'      | 4:S4:60:U:H3       | 1.79                     | 0.47              |
| 19:SN:67:LEU:HD13  | 19:SN:72:ILE:HG22  | 1.96                     | 0.47              |
| 40:LA:1:A:O3'      | 74:Li:63:ARG:HD3   | 2.14                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 41:LB:199:A:H5''    | 66:La:42:ALA:HB2   | 1.96                     | 0.47              |
| 43:LD:663:G:OP1     | 83:Lr:211:ARG:HD3  | 2.14                     | 0.47              |
| 44:LE:859:G:H2'     | 44:LE:860:C:C6     | 2.48                     | 0.47              |
| 44:LE:1104:OMG:H5'' | 57:LR:71:PRO:HD3   | 1.96                     | 0.47              |
| 46:LG:2209:C:H2'    | 46:LG:2210:U:C6    | 2.49                     | 0.47              |
| 48:LI:3123:G:H2'    | 48:LI:3124:A:C8    | 2.49                     | 0.47              |
| 48:LI:3302:A:C2     | 66:La:50:ILE:HG23  | 2.48                     | 0.47              |
| 61:LV:148:LYS:HA    | 61:LV:151:GLU:HG3  | 1.96                     | 0.47              |
| 62:LW:208:SER:OG    | 62:LW:209:LEU:N    | 2.47                     | 0.47              |
| 68:Lc:153:LYS:HE3   | 68:Lc:157:TYR:CE2  | 2.48                     | 0.47              |
| 85:Lt:123:GLU:HB3   | 85:Lt:125:SER:H    | 1.79                     | 0.47              |
| 1:S1:606:G:H2'      | 1:S1:607:G:H8      | 1.79                     | 0.47              |
| 1:S1:1347:C:H2'     | 1:S1:1348:A:C8     | 2.48                     | 0.47              |
| 1:S1:1549:A2M:H8    | 1:S1:1549:A2M:C5'  | 2.43                     | 0.47              |
| 1:S1:2068:C:OP1     | 23:SR:40:ARG:NH1   | 2.41                     | 0.47              |
| 1:S1:2099:C:H3'     | 24:SS:31:ARG:HH22  | 1.79                     | 0.47              |
| 7:SB:41:ARG:HG2     | 7:SB:47:HIS:CD2    | 2.49                     | 0.47              |
| 19:SN:70:GLU:OE1    | 19:SN:70:GLU:N     | 2.34                     | 0.47              |
| 26:SU:128:VAL:HG11  | 26:SU:144:VAL:HG22 | 1.96                     | 0.47              |
| 28:SW:89:VAL:HG22   | 28:SW:120:TYR:HE1  | 1.79                     | 0.47              |
| 38:Sg:53:ILE:O      | 38:Sg:94:LYS:NZ    | 2.27                     | 0.47              |
| 41:LB:178:A:OP2     | 76:Lk:64:TYR:OH    | 2.17                     | 0.47              |
| 42:LC:617:C:H2'     | 42:LC:618:A:C8     | 2.48                     | 0.47              |
| 47:LH:2877:C:O2'    | 52:LM:3925:A:N1    | 2.41                     | 0.47              |
| 48:LI:3343:U:H2'    | 48:LI:3344:G:C8    | 2.49                     | 0.47              |
| 56:LQ:47:LEU:HD12   | 56:LQ:84:MET:HE3   | 1.96                     | 0.47              |
| 88:Lw:103:GLN:HG3   | 88:Lw:107:LYS:HE2  | 1.96                     | 0.47              |
| 92:L1:24:PRO:HB2    | 92:L1:27:VAL:HG23  | 1.95                     | 0.47              |
| 1:S1:495:G:P        | 16:SK:49:ARG:HH12  | 2.37                     | 0.47              |
| 1:S1:977:A:H5'      | 1:S1:978:G:O4'     | 2.14                     | 0.47              |
| 8:SC:139:ILE:HG12   | 8:SC:153:LYS:HG3   | 1.96                     | 0.47              |
| 40:LA:36:G:C6       | 81:Lp:92:ARG:HD3   | 2.49                     | 0.47              |
| 45:LF:1856:OMG:H3'  | 74:Li:47:PHE:CD2   | 2.50                     | 0.47              |
| 47:LH:2238:G:H2'    | 47:LH:2239:G:O4'   | 2.14                     | 0.47              |
| 47:LH:2376:U:H2'    | 47:LH:2377:G:O4'   | 2.14                     | 0.47              |
| 47:LH:2598:G:O2'    | 47:LH:2601:G:N2    | 2.42                     | 0.47              |
| 50:LK:3761:C:O2'    | 72:Lg:176:THR:OG1  | 2.23                     | 0.47              |
| 50:LK:3779:G:H2'    | 50:LK:3780:G:C8    | 2.49                     | 0.47              |
| 50:LK:3795:A:C8     | 65:LZ:5:LYS:HG2    | 2.50                     | 0.47              |
| 66:La:35:HIS:CD2    | 66:La:39:ARG:HG2   | 2.49                     | 0.47              |
| 75:Lj:65:ILE:HD12   | 75:Lj:131:THR:HG21 | 1.94                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 96:L4:65:THR:HG22  | 96:L4:87:ARG:HD3   | 1.96                     | 0.47              |
| 1:S1:634:C:C2      | 1:S1:635:A:C8      | 3.01                     | 0.47              |
| 1:S1:736:U:O2'     | 1:S1:1513:U:OP1    | 2.31                     | 0.47              |
| 1:S1:1370:A:H2'    | 1:S1:1371:A2M:H8   | 1.97                     | 0.47              |
| 1:S1:1722:G:OP1    | 27:SV:2:GLY:N      | 2.47                     | 0.47              |
| 1:S1:1965:G:H4'    | 29:SX:14:PRO:HB2   | 1.96                     | 0.47              |
| 1:S1:1983:C:H2'    | 1:S1:1984:C:H6     | 1.79                     | 0.47              |
| 12:SG:31:ARG:O     | 12:SG:34:GLN:HG2   | 2.14                     | 0.47              |
| 13:SH:131:ARG:HD3  | 35:Sd:54:LYS:O     | 2.15                     | 0.47              |
| 16:SK:7:ASP:OD1    | 16:SK:7:ASP:N      | 2.39                     | 0.47              |
| 21:SP:90:CYS:HA    | 21:SP:93:PHE:CD2   | 2.49                     | 0.47              |
| 22:SQ:123:GLY:HA3  | 22:SQ:129:LEU:HD13 | 1.95                     | 0.47              |
| 25:ST:62:SER:O     | 25:ST:65:SER:OG    | 2.31                     | 0.47              |
| 34:Sc:58:CYS:HB2   | 34:Sc:62:ASN:H     | 1.78                     | 0.47              |
| 40:LA:138:C:H2'    | 40:LA:139:C:C6     | 2.49                     | 0.47              |
| 41:LB:232:C:H1'    | 63:LX:68:LYS:O     | 2.14                     | 0.47              |
| 43:LD:676:G:H2'    | 43:LD:677:C:C6     | 2.50                     | 0.47              |
| 44:LE:941:C:H5''   | 86:Lu:33:VAL:HB    | 1.95                     | 0.47              |
| 44:LE:1196:A:H5'   | 55:LP:183:GLY:CA   | 2.44                     | 0.47              |
| 45:LF:1935:G:H5'   | 76:Lk:90:THR:HG21  | 1.97                     | 0.47              |
| 46:LG:2019:G:H2'   | 46:LG:2020:C:H5''  | 1.96                     | 0.47              |
| 48:LI:3249:A:H5'   | 48:LI:3250:G:C8    | 2.50                     | 0.47              |
| 49:LJ:3654:G:H2'   | 49:LJ:3655:A:C8    | 2.48                     | 0.47              |
| 55:LP:126:LEU:HD23 | 55:LP:150:LEU:HD21 | 1.96                     | 0.47              |
| 62:LW:175:LYS:HG3  | 65:LZ:197:LEU:HD23 | 1.96                     | 0.47              |
| 66:La:82:ILE:HG23  | 66:La:122:LEU:HD13 | 1.95                     | 0.47              |
| 67:Lb:165:THR:HG22 | 67:Lb:166:SER:N    | 2.30                     | 0.47              |
| 68:Lc:53:ILE:HA    | 68:Lc:134:PRO:HA   | 1.97                     | 0.47              |
| 69:Ld:117:LYS:HE2  | 69:Ld:134:GLN:HB2  | 1.97                     | 0.47              |
| 72:Lg:65:ARG:HA    | 72:Lg:65:ARG:HD2   | 1.64                     | 0.47              |
| 83:Lr:97:PRO:HB2   | 83:Lr:100:PRO:HD2  | 1.96                     | 0.47              |
| 86:Lu:18:LYS:HE3   | 86:Lu:70:VAL:HG22  | 1.97                     | 0.47              |
| 1:S1:430:A:OP1     | 16:SK:31:ARG:NH2   | 2.47                     | 0.47              |
| 1:S1:483:G:OP1     | 16:SK:23:LYS:HG2   | 2.15                     | 0.47              |
| 1:S1:861:G:H2'     | 1:S1:862:C:C6      | 2.49                     | 0.47              |
| 13:SH:85:ILE:HB    | 32:Sa:110:LEU:HD11 | 1.97                     | 0.47              |
| 16:SK:255:LEU:HD11 | 16:SK:286:GLU:HG2  | 1.97                     | 0.47              |
| 33:Sb:18:VAL:HG21  | 33:Sb:33:ASP:OD2   | 2.14                     | 0.47              |
| 41:LB:263:A:H5''   | 63:LX:67:CYS:HB3   | 1.95                     | 0.47              |
| 44:LE:941:C:H2'    | 44:LE:942:A:H8     | 1.79                     | 0.47              |
| 44:LE:1166:G:H2'   | 44:LE:1167:C:C6    | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:LE:1362:C:H2'   | 44:LE:1363:PSU:C6  | 2.50                     | 0.47              |
| 45:LF:1510:U:O2'   | 45:LF:1522:C:O2    | 2.33                     | 0.47              |
| 47:LH:2681:U:H5''  | 47:LH:2682:G:H5'   | 1.97                     | 0.47              |
| 48:LI:3124:A:H2'   | 48:LI:3125:C:C6    | 2.49                     | 0.47              |
| 51:LL:3821:U:OP2   | 65:LZ:136:LYS:NZ   | 2.33                     | 0.47              |
| 53:LN:4010:G:H2'   | 53:LN:4011:G:C8    | 2.50                     | 0.47              |
| 63:LX:149:GLU:HA   | 63:LX:152:LYS:HG2  | 1.97                     | 0.47              |
| 66:La:12:HIS:O     | 66:La:16:ARG:HG2   | 2.14                     | 0.47              |
| 67:Lb:8:GLN:HB2    | 67:Lb:50:ARG:HH12  | 1.78                     | 0.47              |
| 68:Lc:206:LEU:HD11 | 97:L6:52:ARG:HG2   | 1.97                     | 0.47              |
| 72:Lg:39:VAL:O     | 72:Lg:43:ARG:HG2   | 2.14                     | 0.47              |
| 1:S1:579:G:N2      | 1:S1:614:G:H1      | 2.06                     | 0.47              |
| 1:S1:1568:C:H42    | 1:S1:1573:A:H62    | 1.62                     | 0.47              |
| 1:S1:1614:U:OP2    | 1:S1:1615:G:N2     | 2.47                     | 0.47              |
| 3:S3:26:A:C4       | 3:S3:27:G:C8       | 3.02                     | 0.47              |
| 6:SA:27:TRP:CD2    | 20:SO:20:PRO:HB3   | 2.49                     | 0.47              |
| 22:SQ:28:GLU:HB3   | 22:SQ:32:ARG:NH2   | 2.30                     | 0.47              |
| 34:Sc:57:VAL:HB    | 34:Sc:62:ASN:HA    | 1.96                     | 0.47              |
| 38:Sg:147:LYS:HD3  | 38:Sg:163:VAL:HG23 | 1.96                     | 0.47              |
| 41:LB:202:C:OP1    | 100:LH:3004:HOH:O  | 2.20                     | 0.47              |
| 42:LC:551:U:O2'    | 57:LR:55:LYS:NZ    | 2.46                     | 0.47              |
| 44:LE:951:A:H2'    | 44:LE:952:A:C8     | 2.49                     | 0.47              |
| 44:LE:1162:G:H2'   | 44:LE:1163:G:O4'   | 2.14                     | 0.47              |
| 44:LE:1186:G:H3'   | 44:LE:1187:U:H5''  | 1.97                     | 0.47              |
| 62:LW:135:ALA:HB3  | 62:LW:138:ARG:HG2  | 1.97                     | 0.47              |
| 67:Lb:64:VAL:CG1   | 67:Lb:102:ALA:HB1  | 2.45                     | 0.47              |
| 68:Lc:57:ARG:HG3   | 68:Lc:130:ARG:HE   | 1.80                     | 0.47              |
| 85:Lt:141:PHE:HA   | 85:Lt:144:LEU:HD12 | 1.96                     | 0.47              |
| 92:L1:34:LYS:HG3   | 92:L1:35:GLN:N     | 2.27                     | 0.47              |
| 97:L6:11:LEU:HD21  | 97:L6:16:LYS:HA    | 1.96                     | 0.47              |
| 98:L7:32:GLN:HB3   | 98:L7:36:ARG:HH21  | 1.80                     | 0.47              |
| 1:S1:57:OMG:OP2    | 31:SZ:120:LYS:NZ   | 2.40                     | 0.47              |
| 1:S1:72:G:H2'      | 1:S1:73:A:O4'      | 2.15                     | 0.47              |
| 1:S1:578:A:O3'     | 36:Se:33:ARG:NH2   | 2.47                     | 0.47              |
| 1:S1:824:C:H2'     | 1:S1:825:A:H8      | 1.79                     | 0.47              |
| 1:S1:993:U:H4'     | 38:Sg:87:LYS:HE2   | 1.95                     | 0.47              |
| 1:S1:1245:C:O2'    | 1:S1:1246:A:OP1    | 2.30                     | 0.47              |
| 1:S1:1549:A2M:HM'2 | 1:S1:1550:G:H5'    | 1.97                     | 0.47              |
| 1:S1:1580:G:C2     | 1:S1:1581:A:C8     | 3.03                     | 0.47              |
| 1:S1:1629:A:H5'    | 19:SN:1:MET:HE2    | 1.96                     | 0.47              |
| 1:S1:1646:A:H2'    | 1:S1:1647:G:H8     | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:1714:G:OP2    | 1:S1:1715:PSU:O2'  | 2.29                     | 0.47              |
| 1:S1:1896:U:OP1    | 17:SL:122:ARG:NH2  | 2.39                     | 0.47              |
| 1:S1:2095:G:H2'    | 1:S1:2096:G:C8     | 2.50                     | 0.47              |
| 1:S1:2104:G:C5     | 29:SX:91:ARG:HG2   | 2.49                     | 0.47              |
| 3:S3:43:C:H2'      | 3:S3:44:G:C8       | 2.49                     | 0.47              |
| 6:SA:193:LYS:HA    | 6:SA:196:GLU:HG2   | 1.96                     | 0.47              |
| 10:SE:11:ARG:NH1   | 10:SE:21:ASP:OD1   | 2.47                     | 0.47              |
| 10:SE:44:LEU:HG    | 10:SE:82:PHE:HB3   | 1.96                     | 0.47              |
| 12:SG:7:SER:OG     | 12:SG:10:CYS:HB2   | 2.14                     | 0.47              |
| 22:SQ:61:ALA:HA    | 22:SQ:87:VAL:O     | 2.15                     | 0.47              |
| 27:SV:51:ALA:O     | 27:SV:55:THR:HG23  | 2.15                     | 0.47              |
| 29:SX:80:LYS:HG3   | 29:SX:97:LYS:HE2   | 1.96                     | 0.47              |
| 38:Sg:50:ILE:HD12  | 38:Sg:58:LEU:HA    | 1.95                     | 0.47              |
| 38:Sg:142:PRO:HB3  | 38:Sg:207:LYS:HE2  | 1.95                     | 0.47              |
| 39:Sh:234:LEU:HD21 | 39:Sh:263:TRP:CH2  | 2.50                     | 0.47              |
| 41:LB:196:C:H4'    | 44:LE:1107:A:H2    | 1.80                     | 0.47              |
| 42:LC:353:G:O6     | 42:LC:455:U:C4     | 2.68                     | 0.47              |
| 43:LD:679:G:H2'    | 43:LD:713:U:O2'    | 2.13                     | 0.47              |
| 44:LE:792:G:H2'    | 44:LE:793:U:H6     | 1.80                     | 0.47              |
| 44:LE:826:C:H2'    | 44:LE:827:G:C8     | 2.49                     | 0.47              |
| 44:LE:869:A:H2'    | 44:LE:870:G:C8     | 2.50                     | 0.47              |
| 44:LE:871:U:H2'    | 44:LE:872:G:C8     | 2.50                     | 0.47              |
| 44:LE:1180:C:H2'   | 44:LE:1181:A:H8    | 1.80                     | 0.47              |
| 44:LE:1209:G:OP2   | 100:LE:1515:HOH:O  | 2.20                     | 0.47              |
| 45:LF:1585:C:H2'   | 45:LF:1586:PSU:C6  | 2.50                     | 0.47              |
| 45:LF:1887:G:H5''  | 71:Lf:24:TRP:CD1   | 2.49                     | 0.47              |
| 47:LH:2629:U:H2'   | 100:LH:3019:HOH:O  | 2.14                     | 0.47              |
| 47:LH:2713:OMU:O5' | 47:LH:2713:OMU:H6  | 2.15                     | 0.47              |
| 47:LH:2771:G:H1'   | 47:LH:2773:C:H42   | 1.79                     | 0.47              |
| 47:LH:2964:G:H4'   | 47:LH:2965:C:O5'   | 2.15                     | 0.47              |
| 54:LO:4:U:H2'      | 54:LO:5:A:C8       | 2.50                     | 0.47              |
| 62:LW:70:GLN:HG3   | 62:LW:72:LYS:HG2   | 1.97                     | 0.47              |
| 75:Lj:79:ASP:HB3   | 75:Lj:82:LYS:HG2   | 1.96                     | 0.47              |
| 75:Lj:84:PHE:CZ    | 75:Lj:131:THR:HG22 | 2.50                     | 0.47              |
| 83:Lr:111:GLN:HB3  | 83:Lr:114:ASN:CG   | 2.40                     | 0.47              |
| 83:Lr:149:MET:HG3  | 83:Lr:185:ILE:HG12 | 1.95                     | 0.47              |
| 88:Lw:3:ILE:HD12   | 88:Lw:31:SER:HB2   | 1.97                     | 0.47              |
| 89:Lx:80:THR:HB    | 89:Lx:83:GLN:HG3   | 1.96                     | 0.47              |
| 93:L2:92:MET:HG3   | 93:L2:101:LEU:HB2  | 1.96                     | 0.47              |
| 98:L7:16:TRP:CZ2   | 98:L7:20:LEU:HD11  | 2.50                     | 0.47              |
| 1:S1:556:C:O2'     | 1:S1:557:U:H5''    | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:1114:U:H4'    | 1:S1:1115:G:OP2    | 2.15                     | 0.47              |
| 1:S1:2151:G:H2'    | 1:S1:2152:C:C6     | 2.50                     | 0.47              |
| 9:SD:113:VAL:HG12  | 9:SD:156:ILE:HG21  | 1.97                     | 0.47              |
| 10:SE:139:VAL:HG13 | 10:SE:150:PRO:HG3  | 1.96                     | 0.47              |
| 10:SE:252:ASP:OD2  | 10:SE:256:LYS:NZ   | 2.34                     | 0.47              |
| 13:SH:181:GLU:O    | 13:SH:185:VAL:HG13 | 2.15                     | 0.47              |
| 22:SQ:101:SER:N    | 22:SQ:109:LYS:HE3  | 2.30                     | 0.47              |
| 23:SR:2:SER:O      | 32:Sa:57:ARG:NH2   | 2.48                     | 0.47              |
| 46:LG:2158:U:H4'   | 46:LG:2159:C:H3'   | 1.95                     | 0.47              |
| 48:LI:3118:U:H2'   | 48:LI:3119:U:C6    | 2.50                     | 0.47              |
| 48:LI:3317:C:H2'   | 48:LI:3318:G:H8    | 1.80                     | 0.47              |
| 68:Lc:86:HIS:HB3   | 68:Lc:139:ARG:HE   | 1.80                     | 0.47              |
| 77:LI:53:ASP:HB2   | 77:LI:107:LYS:O    | 2.13                     | 0.47              |
| 88:Lw:10:TYR:CD2   | 88:Lw:15:THR:HA    | 2.50                     | 0.47              |
| 90:Ly:2:THR:O      | 90:Ly:7:SER:OG     | 2.32                     | 0.47              |
| 1:S1:100:U:O2      | 16:SK:21:HIS:HB2   | 2.15                     | 0.47              |
| 1:S1:883:A:H61     | 1:S1:1012:C:H42    | 1.63                     | 0.47              |
| 1:S1:1129:C:H2'    | 1:S1:1130:U:O4'    | 2.15                     | 0.47              |
| 1:S1:2274:G:OP1    | 100:S1:2423:HOH:O  | 2.20                     | 0.47              |
| 3:S3:76:A:N6       | 48:LI:3405:A:O2'   | 2.46                     | 0.47              |
| 22:SQ:27:LYS:HG3   | 22:SQ:96:TRP:CD1   | 2.48                     | 0.47              |
| 38:Sg:192:LEU:HD22 | 38:Sg:206:PRO:HB3  | 1.97                     | 0.47              |
| 42:LC:585:U:H2'    | 42:LC:586:C:C6     | 2.50                     | 0.47              |
| 44:LE:780:U:H2'    | 44:LE:781:G:H8     | 1.79                     | 0.47              |
| 44:LE:845:U:H2'    | 44:LE:846:G:O4'    | 2.15                     | 0.47              |
| 44:LE:994:G:H2'    | 44:LE:995:G:C8     | 2.49                     | 0.47              |
| 45:LF:1846:A:H2'   | 45:LF:1847:C:C6    | 2.50                     | 0.47              |
| 47:LH:2341:C:O2    | 100:LH:3011:HOH:O  | 2.20                     | 0.47              |
| 47:LH:2911:U:H2'   | 47:LH:2912:A:H8    | 1.80                     | 0.47              |
| 50:LK:3764:A:H2'   | 50:LK:3765:G:C8    | 2.49                     | 0.47              |
| 54:LO:37:G:H2'     | 54:LO:38:U:O4'     | 2.14                     | 0.47              |
| 58:LS:64:ILE:HG22  | 58:LS:66:SER:H     | 1.79                     | 0.47              |
| 58:LS:89:LEU:HG    | 58:LS:137:PHE:CE2  | 2.49                     | 0.47              |
| 61:LV:119:VAL:HG13 | 61:LV:215:ILE:O    | 2.14                     | 0.47              |
| 61:LV:279:LYS:HA   | 61:LV:282:MET:HE2  | 1.97                     | 0.47              |
| 64:LY:88:TRP:HH2   | 64:LY:98:PHE:CE1   | 2.32                     | 0.47              |
| 66:La:104:PRO:HG2  | 66:La:126:VAL:HG12 | 1.96                     | 0.47              |
| 68:Lc:48:LEU:O     | 68:Lc:139:ARG:HA   | 2.14                     | 0.47              |
| 69:Ld:189:ASP:HB3  | 69:Ld:192:THR:HG22 | 1.97                     | 0.47              |
| 95:L5:7:LYS:O      | 95:L5:27:LYS:NZ    | 2.47                     | 0.47              |
| 1:S1:133:C:N3      | 1:S1:145:G:N1      | 2.45                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:262:G:H2'     | 1:S1:263:G:N7      | 2.30                     | 0.47              |
| 1:S1:772:U:N3      | 1:S1:830:C:O2      | 2.48                     | 0.47              |
| 1:S1:1281:G:H5''   | 6:SA:134:ARG:CZ    | 2.45                     | 0.47              |
| 14:SI:90:GLU:HG2   | 14:SI:96:LYS:O     | 2.14                     | 0.47              |
| 14:SI:127:ARG:HG2  | 14:SI:182:THR:HB   | 1.97                     | 0.47              |
| 17:SL:106:ASP:HB3  | 17:SL:109:GLN:HG3  | 1.97                     | 0.47              |
| 30:SY:30:ALA:O     | 30:SY:59:ARG:HD3   | 2.14                     | 0.47              |
| 30:SY:52:ILE:HD11  | 30:SY:72:MET:HE3   | 1.97                     | 0.47              |
| 37:Sf:119:ARG:HB2  | 37:Sf:132:PHE:HD2  | 1.80                     | 0.47              |
| 40:LA:123:A:H2'    | 40:LA:124:G:C8     | 2.50                     | 0.47              |
| 42:LC:323:C:H4'    | 42:LC:324:A:H5'    | 1.97                     | 0.47              |
| 42:LC:438:C:H2'    | 42:LC:439:U:C6     | 2.50                     | 0.47              |
| 42:LC:481:G:H8     | 67:Lb:93:MET:HE1   | 1.80                     | 0.47              |
| 42:LC:564:U:H4'    | 44:LE:1116:A:N6    | 2.30                     | 0.47              |
| 43:LD:651:C:H2'    | 43:LD:652:C:C6     | 2.49                     | 0.47              |
| 43:LD:674:G:H2'    | 43:LD:675:G:O4'    | 2.15                     | 0.47              |
| 44:LE:1057:A:H2'   | 48:LI:3357:A:N6    | 2.29                     | 0.47              |
| 48:LI:3531:PSU:H1' | 56:LQ:253:CYS:SG   | 2.55                     | 0.47              |
| 49:LJ:3630:U:H2'   | 49:LJ:3631:G:H8    | 1.78                     | 0.47              |
| 49:LJ:3693:A:OP2   | 100:LJ:3802:HOH:O  | 2.20                     | 0.47              |
| 55:LP:180:LEU:HD22 | 95:L5:18:TYR:HB3   | 1.97                     | 0.47              |
| 57:LR:203:VAL:HB   | 57:LR:223:ILE:HD13 | 1.97                     | 0.47              |
| 65:LZ:13:ARG:HD2   | 65:LZ:65:LYS:HG3   | 1.97                     | 0.47              |
| 75:Lj:65:ILE:HD13  | 75:Lj:154:TYR:HB2  | 1.97                     | 0.47              |
| 83:Lr:31:LYS:HD3   | 83:Lr:35:LYS:HE2   | 1.96                     | 0.47              |
| 1:S1:72:G:N7       | 12:SG:173:ARG:NH1  | 2.41                     | 0.46              |
| 1:S1:545:G:OP1     | 10:SE:49:ARG:NH2   | 2.42                     | 0.46              |
| 1:S1:1070:A:C4     | 10:SE:19:MET:HG2   | 2.50                     | 0.46              |
| 1:S1:1113:U:O2     | 1:S1:1134:G:C6     | 2.68                     | 0.46              |
| 1:S1:1133:G:H2'    | 1:S1:1134:G:O4'    | 2.15                     | 0.46              |
| 1:S1:2189:U:H2'    | 1:S1:2190:G:C4     | 2.50                     | 0.46              |
| 11:SF:164:GLY:HA3  | 11:SF:210:ASN:HD22 | 1.79                     | 0.46              |
| 11:SF:189:LEU:HD22 | 11:SF:194:VAL:HG21 | 1.97                     | 0.46              |
| 12:SG:239:ARG:HG3  | 38:Sg:235:ARG:NH2  | 2.30                     | 0.46              |
| 13:SH:40:GLN:HB2   | 13:SH:42:TRP:CH2   | 2.50                     | 0.46              |
| 30:SY:14:PRO:HG2   | 30:SY:23:LEU:HD22  | 1.96                     | 0.46              |
| 38:Sg:169:LYS:HB2  | 38:Sg:171:MET:HG2  | 1.97                     | 0.46              |
| 41:LB:172:G:H2'    | 41:LB:173:C:C6     | 2.51                     | 0.46              |
| 44:LE:834:C:H2'    | 44:LE:835:C:H6     | 1.79                     | 0.46              |
| 44:LE:942:A:H2'    | 44:LE:943:A:H8     | 1.79                     | 0.46              |
| 45:LF:1912:A:H2'   | 45:LF:1913:C:C6    | 2.49                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 48:LI:3207:A:H5'   | 48:LI:3208:OMC:C2   | 2.49                     | 0.46              |
| 56:LQ:5:LYS:HD2    | 56:LQ:5:LYS:N       | 2.30                     | 0.46              |
| 56:LQ:133:TYR:CE1  | 56:LQ:137:LEU:HD22  | 2.50                     | 0.46              |
| 61:LV:244:LYS:O    | 61:LV:248:GLU:HG2   | 2.15                     | 0.46              |
| 62:LW:55:ASN:HB3   | 62:LW:146:LEU:HD11  | 1.97                     | 0.46              |
| 69:Ld:88:VAL:HG12  | 69:Ld:227:LYS:HE3   | 1.96                     | 0.46              |
| 69:Ld:158:PHE:HA   | 69:Ld:161:LEU:HB3   | 1.96                     | 0.46              |
| 69:Ld:206:GLN:HB2  | 69:Ld:231:PRO:HB3   | 1.98                     | 0.46              |
| 72:Lg:142:ILE:O    | 72:Lg:146:LEU:HG    | 2.15                     | 0.46              |
| 77:LI:90:ASN:OD1   | 77:LI:90:ASN:N      | 2.44                     | 0.46              |
| 90:Ly:13:GLY:O     | 90:Ly:14:ARG:NH1    | 2.39                     | 0.46              |
| 94:L3:10:MET:HE3   | 94:L3:15:ARG:CB     | 2.45                     | 0.46              |
| 1:S1:601:C:H2'     | 1:S1:602:C:C6       | 2.51                     | 0.46              |
| 1:S1:608:G:P       | 36:Se:41:ASN:HD22   | 2.37                     | 0.46              |
| 1:S1:649:A2M:N7    | 36:Se:31:VAL:HG11   | 2.30                     | 0.46              |
| 1:S1:714:G:H21     | 21:SP:17:ARG:HH22   | 1.63                     | 0.46              |
| 1:S1:1750:U:H2'    | 1:S1:1751:C:H6      | 1.80                     | 0.46              |
| 1:S1:2083:C:H2'    | 1:S1:2084:C:O4'     | 2.16                     | 0.46              |
| 1:S1:2114:A:N3     | 13:SH:64:TYR:OH     | 2.36                     | 0.46              |
| 1:S1:2131:PSU:H2'  | 1:S1:2132:G:C8      | 2.50                     | 0.46              |
| 1:S1:2231:U:H2'    | 1:S1:2232:G:O4'     | 2.15                     | 0.46              |
| 6:SA:119:VAL:HG13  | 6:SA:159:VAL:HG13   | 1.97                     | 0.46              |
| 8:SC:44:THR:OG1    | 8:SC:47:ARG:O       | 2.21                     | 0.46              |
| 8:SC:163:GLY:O     | 8:SC:166:ALA:N      | 2.49                     | 0.46              |
| 12:SG:167:LYS:HD3  | 12:SG:167:LYS:HA    | 1.72                     | 0.46              |
| 15:SJ:90:ILE:HD11  | 15:SJ:113:HIS:CD2   | 2.50                     | 0.46              |
| 39:Sh:110:LYS:O    | 39:Sh:128:SER:OG    | 2.33                     | 0.46              |
| 39:Sh:153:ASP:OD1  | 39:Sh:154:TRP:N     | 2.36                     | 0.46              |
| 42:LC:363:G:H2'    | 42:LC:364:C:H5      | 1.81                     | 0.46              |
| 42:LC:517:G:H2'    | 42:LC:518:U:C6      | 2.51                     | 0.46              |
| 44:LE:834:C:H2'    | 44:LE:835:C:C6      | 2.50                     | 0.46              |
| 44:LE:916:U:H2'    | 44:LE:917:C:H6      | 1.80                     | 0.46              |
| 44:LE:1315:OMU:H4' | 48:LI:3208:OMC:H5'' | 1.97                     | 0.46              |
| 51:LL:3821:U:H2'   | 51:LL:3822:U:H6     | 1.78                     | 0.46              |
| 59:LT:77:VAL:O     | 59:LT:81:ILE:HG12   | 2.15                     | 0.46              |
| 65:LZ:98:ARG:NH2   | 65:LZ:213:SER:OG    | 2.48                     | 0.46              |
| 71:Lf:8:GLN:HG2    | 71:Lf:33:ILE:O      | 2.14                     | 0.46              |
| 1:S1:128:G:N1      | 1:S1:193:U:C5       | 2.83                     | 0.46              |
| 1:S1:933:G:H22     | 38:Sg:87:LYS:HD2    | 1.80                     | 0.46              |
| 1:S1:1625:OMC:H1'  | 1:S1:1625:OMC:HM23  | 1.65                     | 0.46              |
| 1:S1:1716:C:O2'    | 100:S1:2424:HOH:O   | 2.20                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:S1:2055:U:O2'   | 1:S1:2100:A:N3     | 2.43                     | 0.46              |
| 11:SF:49:ARG:HD3  | 11:SF:49:ARG:HA    | 1.75                     | 0.46              |
| 13:SH:19:VAL:HG22 | 13:SH:99:VAL:HG11  | 1.97                     | 0.46              |
| 13:SH:40:GLN:NE2  | 17:SL:123:THR:OG1  | 2.29                     | 0.46              |
| 39:Sh:23:LEU:O    | 39:Sh:294:GLN:NE2  | 2.48                     | 0.46              |
| 39:Sh:306:TYR:OH  | 39:Sh:312:ARG:NH1  | 2.48                     | 0.46              |
| 40:LA:43:C:P      | 92:L1:15:LYS:HD3   | 2.56                     | 0.46              |
| 42:LC:475:U:H2'   | 42:LC:476:A:C8     | 2.51                     | 0.46              |
| 44:LE:1398:G:O2'  | 98:L7:40:GLU:HG2   | 2.15                     | 0.46              |
| 45:LF:1963:G:H2'  | 45:LF:1964:U:O4'   | 2.16                     | 0.46              |
| 46:LG:2096:A:H2'  | 46:LG:2097:A:C8    | 2.50                     | 0.46              |
| 47:LH:2684:C:H2'  | 47:LH:2730:A:H61   | 1.79                     | 0.46              |
| 48:LI:3006:U:H2'  | 48:LI:3007:G:H8    | 1.81                     | 0.46              |
| 48:LI:3403:A:HO2' | 82:Lq:2:ALA:N      | 2.13                     | 0.46              |
| 50:LK:3756:C:OP1  | 62:LW:176:LYS:NZ   | 2.47                     | 0.46              |
| 54:LO:74:A:N1     | 54:LO:100:A:H5''   | 2.29                     | 0.46              |
| 59:LT:43:TYR:OH   | 59:LT:66:ASP:OD1   | 2.32                     | 0.46              |
| 64:LY:9:GLY:HA3   | 64:LY:128:ILE:CG2  | 2.46                     | 0.46              |
| 67:Lb:80:CYS:HB2  | 67:Lb:87:ALA:HA    | 1.97                     | 0.46              |
| 68:Lc:65:LEU:HD22 | 68:Lc:93:PRO:HG3   | 1.97                     | 0.46              |
| 91:Lz:10:GLN:HA   | 91:Lz:13:VAL:HG22  | 1.98                     | 0.46              |
| 91:Lz:49:ASP:OD1  | 91:Lz:50:HIS:N     | 2.49                     | 0.46              |
| 1:S1:209:U:H2'    | 1:S1:210:G:H8      | 1.81                     | 0.46              |
| 1:S1:472:U:HO2'   | 1:S1:706:C:HO2'    | 1.61                     | 0.46              |
| 1:S1:494:A:H2'    | 1:S1:495:G:C8      | 2.51                     | 0.46              |
| 1:S1:714:G:H21    | 21:SP:17:ARG:NH2   | 2.12                     | 0.46              |
| 1:S1:773:U:H3     | 1:S1:829:G:N2      | 2.09                     | 0.46              |
| 1:S1:1439:G:H5''  | 7:SB:32:LYS:HD3    | 1.97                     | 0.46              |
| 1:S1:1587:C:H41   | 23:SR:138:LYS:HE3  | 1.81                     | 0.46              |
| 1:S1:1780:G:H2'   | 1:S1:1781:G:C8     | 2.50                     | 0.46              |
| 1:S1:1914:G:H2'   | 1:S1:1915:U:C6     | 2.50                     | 0.46              |
| 14:SI:68:ILE:HB   | 14:SI:100:VAL:HG12 | 1.98                     | 0.46              |
| 30:SY:19:ALA:HB2  | 30:SY:67:ALA:HB1   | 1.98                     | 0.46              |
| 38:Sg:161:LYS:HE2 | 38:Sg:177:LYS:HE2  | 1.98                     | 0.46              |
| 40:LA:23:G:N7     | 77:LI:12:ARG:NH1   | 2.63                     | 0.46              |
| 44:LE:931:1MA:O2' | 44:LE:933:A:OP2    | 2.34                     | 0.46              |
| 45:LF:1782:U:H2'  | 45:LF:1783:U:C6    | 2.49                     | 0.46              |
| 47:LH:2928:A:H2'  | 47:LH:2929:C:C6    | 2.51                     | 0.46              |
| 48:LI:3009:U:H2'  | 48:LI:3010:U:C6    | 2.50                     | 0.46              |
| 48:LI:3287:G:H4'  | 48:LI:3288:A:H5''  | 1.97                     | 0.46              |
| 52:LM:3910:C:H2'  | 52:LM:3911:A:O4'   | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:LR:10:GLN:O     | 57:LR:149:PRO:HD3  | 2.15                     | 0.46              |
| 77:Ll:49:ILE:HD11  | 77:Ll:55:VAL:HG11  | 1.97                     | 0.46              |
| 79:Ln:68:LEU:HD21  | 79:Ln:116:PHE:HB3  | 1.98                     | 0.46              |
| 90:Ly:102:ARG:HG3  | 90:Ly:106:LEU:HD23 | 1.96                     | 0.46              |
| 95:L5:78:THR:O     | 95:L5:82:THR:HG23  | 2.14                     | 0.46              |
| 1:S1:977:A:N6      | 38:Sg:220:ARG:HH12 | 2.12                     | 0.46              |
| 1:S1:2001:G:H2'    | 1:S1:2002:C:H6     | 1.80                     | 0.46              |
| 4:S4:36:A:H2'      | 4:S4:36:A:N3       | 2.31                     | 0.46              |
| 6:SA:136:PHE:HB3   | 6:SA:211:ARG:HH11  | 1.79                     | 0.46              |
| 13:SH:74:MET:HG2   | 13:SH:78:HIS:CE1   | 2.51                     | 0.46              |
| 24:SS:30:ILE:HD11  | 24:SS:39:ARG:HA    | 1.96                     | 0.46              |
| 25:ST:115:LEU:HA   | 25:ST:118:VAL:HG12 | 1.97                     | 0.46              |
| 29:SX:111:GLU:HB3  | 29:SX:116:VAL:HG23 | 1.98                     | 0.46              |
| 40:LA:149:U:H4'    | 67:Lb:110:CYS:SG   | 2.55                     | 0.46              |
| 41:LB:293:G:H2'    | 41:LB:294:C:H6     | 1.81                     | 0.46              |
| 42:LC:427:U:P      | 42:LC:430:A:H61    | 2.38                     | 0.46              |
| 42:LC:577:OMC:H1'  | 42:LC:577:OMC:HM23 | 1.57                     | 0.46              |
| 42:LC:581:G:OP2    | 77:Ll:88:LYS:HG2   | 2.16                     | 0.46              |
| 43:LD:698:C:P      | 59:LT:51:LYS:H     | 2.39                     | 0.46              |
| 44:LE:846:G:H2'    | 44:LE:847:C:C6     | 2.50                     | 0.46              |
| 44:LE:1088:A:H2'   | 44:LE:1089:A:C8    | 2.50                     | 0.46              |
| 44:LE:1132:G:OP1   | 71:Lf:87:ASN:HB3   | 2.16                     | 0.46              |
| 44:LE:1141:U:H2'   | 44:LE:1142:G:H8    | 1.80                     | 0.46              |
| 44:LE:1165:OMC:H2' | 44:LE:1166:G:O4'   | 2.15                     | 0.46              |
| 45:LF:1799:U:OP2   | 100:LF:2007:HOH:O  | 2.20                     | 0.46              |
| 47:LH:2230:C:H2'   | 47:LH:2231:A:C8    | 2.50                     | 0.46              |
| 48:LI:3105:G:H2'   | 48:LI:3106:C:C6    | 2.51                     | 0.46              |
| 56:LQ:296:ALA:HB2  | 56:LQ:306:ASP:HB3  | 1.97                     | 0.46              |
| 57:LR:178:ALA:HB2  | 57:LR:219:PRO:HG2  | 1.97                     | 0.46              |
| 72:Lg:127:ILE:HG22 | 72:Lg:128:GLY:H    | 1.80                     | 0.46              |
| 78:Lm:7:LEU:HD11   | 78:Lm:30:ARG:NH1   | 2.25                     | 0.46              |
| 98:L7:5:ASN:HB2    | 98:L7:10:ARG:HG3   | 1.98                     | 0.46              |
| 1:S1:640:PSU:H3'   | 1:S1:641:OMG:H8    | 1.80                     | 0.46              |
| 1:S1:1258:U:H2'    | 1:S1:1259:G:O4'    | 2.16                     | 0.46              |
| 1:S1:1693:U:OP1    | 100:S1:2422:HOH:O  | 2.20                     | 0.46              |
| 1:S1:1887:G:OP1    | 27:SV:10:LYS:NZ    | 2.49                     | 0.46              |
| 1:S1:1949:G:H2'    | 1:S1:1950:C:O4'    | 2.15                     | 0.46              |
| 1:S1:2179:C:H2'    | 1:S1:2180:A2M:O4'  | 2.15                     | 0.46              |
| 1:S1:2295:G:N7     | 20:SO:147:ARG:NH1  | 2.63                     | 0.46              |
| 7:SB:79:ALA:HB3    | 7:SB:129:THR:HG22  | 1.96                     | 0.46              |
| 10:SE:115:LYS:O    | 10:SE:119:VAL:HG13 | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:SJ:19:LYS:HB2   | 15:SJ:19:LYS:HE3   | 1.58                     | 0.46              |
| 22:SQ:122:TYR:CE2  | 22:SQ:129:LEU:HD21 | 2.51                     | 0.46              |
| 24:SS:4:LYS:C      | 24:SS:6:ILE:H      | 2.23                     | 0.46              |
| 39:Sh:17:ASN:O     | 39:Sh:37:SER:OG    | 2.34                     | 0.46              |
| 40:LA:151:U:H2'    | 40:LA:152:G:C8     | 2.51                     | 0.46              |
| 42:LC:558:G:O2'    | 42:LC:569:G:O6     | 2.28                     | 0.46              |
| 45:LF:1710:A:H2'   | 45:LF:1711:G:H8    | 1.79                     | 0.46              |
| 45:LF:1984:G:H2'   | 45:LF:1985:C:C6    | 2.51                     | 0.46              |
| 47:LH:2835:OMU:H2' | 47:LH:2836:G:O4'   | 2.16                     | 0.46              |
| 48:LI:2994:U:O2'   | 48:LI:2995:A:O5'   | 2.32                     | 0.46              |
| 48:LI:3015:C:O2'   | 48:LI:3164:A:N6    | 2.48                     | 0.46              |
| 48:LI:3156:G:H3'   | 48:LI:3157:U:H5''  | 1.97                     | 0.46              |
| 48:LI:3556:A:N7    | 55:LP:215:ASN:ND2  | 2.64                     | 0.46              |
| 50:LK:3809:U:H3    | 51:LL:3894:G:H1    | 1.63                     | 0.46              |
| 52:LM:3938:U:OP1   | 85:Lt:58:ARG:NH1   | 2.48                     | 0.46              |
| 54:LO:40:C:O2      | 58:LS:82:ARG:NE    | 2.31                     | 0.46              |
| 55:LP:145:LYS:C    | 55:LP:146:SER:HG   | 2.24                     | 0.46              |
| 58:LS:90:LEU:HD13  | 58:LS:139:VAL:HG21 | 1.97                     | 0.46              |
| 69:Ld:68:ILE:HB    | 98:L7:23:GLU:OE1   | 2.16                     | 0.46              |
| 79:Ln:88:ASP:C     | 79:Ln:89:LEU:HD22  | 2.41                     | 0.46              |
| 91:Lz:54:GLU:OE2   | 91:Lz:54:GLU:N     | 2.48                     | 0.46              |
| 1:S1:30:G:H2'      | 1:S1:31:C:C6       | 2.51                     | 0.46              |
| 1:S1:824:C:H2'     | 1:S1:825:A:C8      | 2.51                     | 0.46              |
| 1:S1:1495:A:H2'    | 1:S1:1496:A:C8     | 2.51                     | 0.46              |
| 1:S1:1876:U:H2'    | 1:S1:1877:C:H6     | 1.80                     | 0.46              |
| 1:S1:2133:U:O2'    | 1:S1:2270:C:O2'    | 2.23                     | 0.46              |
| 1:S1:2246:C:H2'    | 1:S1:2247:A:H8     | 1.81                     | 0.46              |
| 6:SA:156:HIS:O     | 6:SA:160:LEU:HG    | 2.16                     | 0.46              |
| 8:SC:181:GLN:HE21  | 36:Se:67:GLY:HA2   | 1.80                     | 0.46              |
| 11:SF:41:ARG:NH2   | 11:SF:248:LEU:O    | 2.48                     | 0.46              |
| 11:SF:89:LYS:HD3   | 11:SF:96:ARG:HH11  | 1.81                     | 0.46              |
| 11:SF:242:GLN:OE1  | 30:SY:35:ASN:ND2   | 2.48                     | 0.46              |
| 18:SM:100:VAL:HA   | 18:SM:103:ILE:HG12 | 1.98                     | 0.46              |
| 27:SV:103:ASP:HA   | 27:SV:124:VAL:O    | 2.15                     | 0.46              |
| 40:LA:140:C:H2'    | 40:LA:141:G:O4'    | 2.15                     | 0.46              |
| 41:LB:215:OMG:HM23 | 41:LB:215:OMG:H1'  | 1.57                     | 0.46              |
| 41:LB:245:A:H5'    | 41:LB:247:OMU:C1'  | 2.43                     | 0.46              |
| 41:LB:278:U:H2'    | 41:LB:279:C:C6     | 2.49                     | 0.46              |
| 43:LD:694:G:H2'    | 43:LD:695:U:C6     | 2.51                     | 0.46              |
| 46:LG:2126:U:H5''  | 71:Lf:62:ALA:HB2   | 1.97                     | 0.46              |
| 48:LI:3233:A:OP1   | 48:LI:3325:C:O2'   | 2.33                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:LI:3576:U:O2'   | 56:LQ:269:ALA:O    | 2.25                     | 0.46              |
| 50:LK:3751:A:N6    | 87:Lv:34:LYS:HD2   | 2.30                     | 0.46              |
| 56:LQ:211:PHE:HD1  | 56:LQ:215:GLU:OE2  | 1.97                     | 0.46              |
| 56:LQ:288:GLY:HA3  | 56:LQ:325:TYR:CE2  | 2.50                     | 0.46              |
| 62:LW:199:TYR:HB3  | 65:LZ:104:ASN:HB3  | 1.98                     | 0.46              |
| 75:Lj:81:LEU:HD21  | 75:Lj:109:ILE:HG21 | 1.98                     | 0.46              |
| 76:Lk:70:ARG:HB2   | 76:Lk:74:ILE:HG13  | 1.98                     | 0.46              |
| 78:Lm:61:LYS:HB2   | 78:Lm:61:LYS:HE3   | 1.71                     | 0.46              |
| 85:Lt:62:GLY:O     | 100:Lt:201:HOH:O   | 2.21                     | 0.46              |
| 94:L3:33:SER:OG    | 94:L3:34:LYS:N     | 2.49                     | 0.46              |
| 1:S1:167:A:C2      | 1:S1:180:OMG:C5    | 3.03                     | 0.46              |
| 1:S1:900:A:H2'     | 1:S1:901:A:O4'     | 2.14                     | 0.46              |
| 1:S1:940:G:OP1     | 38:Sg:214:LYS:HG3  | 2.16                     | 0.46              |
| 1:S1:1313:U:O4     | 20:SO:56:ARG:NH2   | 2.49                     | 0.46              |
| 1:S1:2083:C:H4'    | 17:SL:145:ARG:HB2  | 1.98                     | 0.46              |
| 1:S1:2086:A:C6     | 13:SH:43:THR:HG21  | 2.51                     | 0.46              |
| 1:S1:2113:G:OP1    | 13:SH:37:HIS:NE2   | 2.48                     | 0.46              |
| 4:S4:37:A:H2'      | 4:S4:38:A:C8       | 2.51                     | 0.46              |
| 7:SB:65:LEU:HD11   | 7:SB:74:VAL:HG11   | 1.97                     | 0.46              |
| 10:SE:126:VAL:HB   | 10:SE:156:LYS:O    | 2.16                     | 0.46              |
| 13:SH:28:ILE:HD13  | 13:SH:99:VAL:HG13  | 1.97                     | 0.46              |
| 34:Sc:8:ASN:HD21   | 34:Sc:11:PHE:HD2   | 1.63                     | 0.46              |
| 41:LB:193:G:H21    | 41:LB:211:C:H5     | 1.63                     | 0.46              |
| 42:LC:402:A:H4'    | 42:LC:404:A:C8     | 2.50                     | 0.46              |
| 47:LH:2821:C:H2'   | 47:LH:2822:U:O4'   | 2.16                     | 0.46              |
| 48:LI:3123:G:H2'   | 48:LI:3124:A:H8    | 1.81                     | 0.46              |
| 48:LI:3225:C:O2'   | 48:LI:3230:A:N1    | 2.42                     | 0.46              |
| 49:LJ:3596:A:H2'   | 49:LJ:3597:U:O4'   | 2.16                     | 0.46              |
| 53:LN:4000:U:H2'   | 53:LN:4001:G:C8    | 2.51                     | 0.46              |
| 55:LP:83:TYR:CE1   | 55:LP:86:GLN:HG3   | 2.51                     | 0.46              |
| 60:LU:12:PRO:HB3   | 60:LU:18:LEU:HD21  | 1.98                     | 0.46              |
| 60:LU:154:GLN:O    | 60:LU:157:LYS:HG3  | 2.16                     | 0.46              |
| 62:LW:193:ILE:HG22 | 62:LW:194:ILE:HG13 | 1.98                     | 0.46              |
| 72:Lg:5:SER:HB2    | 72:Lg:107:HIS:HB3  | 1.97                     | 0.46              |
| 81:Lp:67:ASN:O     | 81:Lp:71:LYS:HG2   | 2.15                     | 0.46              |
| 88:Lw:42:PRO:HG3   | 88:Lw:63:ARG:HA    | 1.96                     | 0.46              |
| 1:S1:492:U:H2'     | 1:S1:493:G:O4'     | 2.16                     | 0.46              |
| 1:S1:504:A:H2'     | 1:S1:505:C:C6      | 2.51                     | 0.46              |
| 1:S1:999:C:H2'     | 1:S1:1000:C:C6     | 2.50                     | 0.46              |
| 1:S1:1726:C:OP1    | 27:SV:7:LYS:N      | 2.44                     | 0.46              |
| 1:S1:2114:A:H2'    | 13:SH:64:TYR:OH    | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:S4:8:U:H5''      | 4:S4:9:A:OP1       | 2.15                     | 0.46              |
| 13:SH:74:MET:HG3   | 13:SH:77:ARG:HH21  | 1.81                     | 0.46              |
| 38:Sg:249:ALA:O    | 38:Sg:253:ALA:N    | 2.48                     | 0.46              |
| 44:LE:780:U:H5'    | 73:Lh:136:LEU:HD23 | 1.97                     | 0.46              |
| 44:LE:1200:C:H2'   | 44:LE:1201:OMG:C8  | 2.51                     | 0.46              |
| 44:LE:1248:U:H2'   | 44:LE:1249:C:H6    | 1.81                     | 0.46              |
| 47:LH:2755:C:H2'   | 47:LH:2756:U:O4'   | 2.16                     | 0.46              |
| 48:LI:3295:G:H2'   | 48:LI:3296:A:H8    | 1.81                     | 0.46              |
| 53:LN:3973:A:H2'   | 53:LN:3974:U:O4'   | 2.15                     | 0.46              |
| 55:LP:58:LEU:HD23  | 55:LP:75:LEU:HD21  | 1.98                     | 0.46              |
| 57:LR:165:LEU:HD13 | 57:LR:174:VAL:HG21 | 1.98                     | 0.46              |
| 58:LS:53:GLN:HE22  | 58:LS:81:VAL:HG12  | 1.81                     | 0.46              |
| 67:Lb:47:LYS:HD2   | 67:Lb:50:ARG:HH21  | 1.81                     | 0.46              |
| 73:Lh:150:LYS:HE3  | 73:Lh:150:LYS:HB2  | 1.70                     | 0.46              |
| 85:Lt:142:LYS:HB2  | 85:Lt:142:LYS:HE2  | 1.84                     | 0.46              |
| 1:S1:1356:G:O6     | 25:ST:19:ARG:NH2   | 2.49                     | 0.46              |
| 1:S1:1704:G:C6     | 1:S1:1705:OMG:N7   | 2.84                     | 0.46              |
| 1:S1:1974:U:H1'    | 1:S1:1997:C:C4     | 2.50                     | 0.46              |
| 1:S1:2120:U:H2'    | 1:S1:2121:C:C6     | 2.51                     | 0.46              |
| 1:S1:2175:U:H2'    | 1:S1:2176:C:C6     | 2.50                     | 0.46              |
| 3:S3:4:C:H2'       | 3:S3:5:G:H8        | 1.80                     | 0.46              |
| 13:SH:83:PHE:HZ    | 13:SH:98:LEU:HD22  | 1.81                     | 0.46              |
| 14:SI:118:PRO:HG2  | 14:SI:121:ARG:HD2  | 1.98                     | 0.46              |
| 17:SL:24:ALA:HB2   | 17:SL:80:GLY:HA3   | 1.97                     | 0.46              |
| 20:SO:98:MET:HE2   | 20:SO:98:MET:HB3   | 1.90                     | 0.46              |
| 22:SQ:102:TYR:HB3  | 22:SQ:107:ASN:HA   | 1.97                     | 0.46              |
| 26:SU:98:TYR:HB2   | 26:SU:105:TYR:CE2  | 2.51                     | 0.46              |
| 27:SV:31:ASN:ND2   | 27:SV:55:THR:HG22  | 2.31                     | 0.46              |
| 40:LA:146:G:H2'    | 40:LA:147:C:C6     | 2.51                     | 0.46              |
| 40:LA:151:U:H2'    | 40:LA:152:G:H8     | 1.81                     | 0.46              |
| 41:LB:183:A2M:HM'3 | 41:LB:183:A2M:H1'  | 1.77                     | 0.46              |
| 41:LB:242:U:H2'    | 41:LB:243:G:O4'    | 2.16                     | 0.46              |
| 41:LB:272:C:C5     | 42:LC:528:G:H1'    | 2.51                     | 0.46              |
| 41:LB:291:G:C8     | 61:LV:143:ARG:NH2  | 2.84                     | 0.46              |
| 42:LC:350:G:N1     | 42:LC:459:U:C2     | 2.84                     | 0.46              |
| 43:LD:703:C:H2'    | 43:LD:704:A:H8     | 1.81                     | 0.46              |
| 46:LG:2197:A:H62   | 91:Lz:35:LYS:HE2   | 1.81                     | 0.46              |
| 47:LH:2911:U:H2'   | 47:LH:2912:A:C8    | 2.51                     | 0.46              |
| 47:LH:2955:G:H2'   | 47:LH:2956:A:N7    | 2.30                     | 0.46              |
| 48:LI:2975:G:H2'   | 48:LI:2976:C:O4'   | 2.17                     | 0.46              |
| 48:LI:3296:A:H2'   | 48:LI:3297:C:O4'   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:LI:3297:C:O2'  | 73:Lh:88:LYS:O     | 2.29                     | 0.46              |
| 50:LK:3766:C:H2'  | 50:LK:3767:A:H8    | 1.81                     | 0.46              |
| 57:LR:208:ARG:HA  | 57:LR:212:GLN:NE2  | 2.31                     | 0.46              |
| 60:LU:18:LEU:HD11 | 60:LU:32:CYS:HB2   | 1.98                     | 0.46              |
| 63:LX:191:PHE:CD2 | 66:La:135:GLN:HB3  | 2.50                     | 0.46              |
| 71:Lf:58:VAL:HG12 | 71:Lf:60:SER:H     | 1.81                     | 0.46              |
| 76:Lk:114:ASN:O   | 76:Lk:118:THR:HG23 | 2.16                     | 0.46              |
| 1:S1:71:G:H1      | 12:SG:175:LYS:NZ   | 2.14                     | 0.45              |
| 1:S1:85:U:O3'     | 31:SZ:123:ARG:NH1  | 2.41                     | 0.45              |
| 1:S1:154:C:N3     | 1:S1:193:U:O4      | 2.49                     | 0.45              |
| 1:S1:616:A:H2'    | 1:S1:617:U:C6      | 2.51                     | 0.45              |
| 1:S1:706:C:H5''   | 21:SP:30:ARG:HD3   | 1.98                     | 0.45              |
| 1:S1:1591:PSU:O4  | 1:S1:1595:U:H5     | 1.99                     | 0.45              |
| 1:S1:1595:U:O2    | 1:S1:1940:G:O2'    | 2.22                     | 0.45              |
| 1:S1:1968:A:OP2   | 100:S1:2426:HOH:O  | 2.21                     | 0.45              |
| 4:S4:73:A:H2'     | 4:S4:74:C:C6       | 2.51                     | 0.45              |
| 7:SB:51:LEU:HA    | 7:SB:54:THR:HB     | 1.98                     | 0.45              |
| 13:SH:95:ILE:O    | 13:SH:99:VAL:HG23  | 2.16                     | 0.45              |
| 15:SJ:55:ASN:OD1  | 15:SJ:60:LYS:NZ    | 2.41                     | 0.45              |
| 21:SP:35:THR:O    | 21:SP:39:SER:OG    | 2.20                     | 0.45              |
| 30:SY:32:VAL:HG22 | 30:SY:59:ARG:HD2   | 1.96                     | 0.45              |
| 43:LD:653:A:H2'   | 43:LD:654:A:H8     | 1.81                     | 0.45              |
| 43:LD:751:G:H1'   | 57:LR:317:TYR:CE2  | 2.52                     | 0.45              |
| 45:LF:1507:U:H2'  | 45:LF:1508:G:C8    | 2.51                     | 0.45              |
| 46:LG:2037:G:H2'  | 46:LG:2038:G:C8    | 2.51                     | 0.45              |
| 47:LH:2287:C:H2'  | 47:LH:2288:C:H6    | 1.82                     | 0.45              |
| 53:LN:3980:G:C6   | 56:LQ:384:MET:HG2  | 2.51                     | 0.45              |
| 56:LQ:45:ALA:HB3  | 56:LQ:183:ILE:HG23 | 1.98                     | 0.45              |
| 69:Ld:97:ALA:HB1  | 69:Ld:160:VAL:HG23 | 1.98                     | 0.45              |
| 69:Ld:216:LYS:O   | 69:Ld:220:VAL:HG12 | 2.16                     | 0.45              |
| 71:Lf:171:ARG:HG3 | 71:Lf:172:GLU:N    | 2.31                     | 0.45              |
| 79:Ln:3:LYS:HE2   | 79:Ln:3:LYS:HB2    | 1.66                     | 0.45              |
| 84:Ls:28:LEU:HD23 | 84:Ls:93:LEU:HD13  | 1.98                     | 0.45              |
| 1:S1:681:G:H1'    | 2:S2:35:A:O2'      | 2.16                     | 0.45              |
| 1:S1:899:A:H3'    | 1:S1:900:A:C8      | 2.51                     | 0.45              |
| 1:S1:2115:U:O4'   | 13:SH:64:TYR:OH    | 2.33                     | 0.45              |
| 1:S1:2118:U:H2'   | 13:SH:46:ARG:HG3   | 1.97                     | 0.45              |
| 1:S1:2232:G:H2'   | 1:S1:2233:G:C8     | 2.51                     | 0.45              |
| 13:SH:164:ILE:O   | 13:SH:168:LYS:HG2  | 2.17                     | 0.45              |
| 22:SQ:63:ASP:O    | 22:SQ:90:ARG:NE    | 2.47                     | 0.45              |
| 29:SX:88:ARG:HD3  | 29:SX:92:PRO:O     | 2.17                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 37:Sf:108:LYS:N     | 37:Sf:116:THR:O     | 2.48                     | 0.45              |
| 38:Sg:236:ARG:HG3   | 38:Sg:240:GLU:HG2   | 1.99                     | 0.45              |
| 40:LA:92:G:O6       | 90:Ly:73:LYS:NZ     | 2.29                     | 0.45              |
| 41:LB:172:G:N2      | 76:Lk:55:THR:HG21   | 2.30                     | 0.45              |
| 41:LB:275:G:N2      | 81:Lp:114:TYR:O     | 2.46                     | 0.45              |
| 42:LC:643:G:H2'     | 42:LC:644:U:O4'     | 2.16                     | 0.45              |
| 44:LE:1247:U:H2'    | 44:LE:1248:U:C6     | 2.51                     | 0.45              |
| 44:LE:1341:U:H2'    | 44:LE:1342:G:C8     | 2.51                     | 0.45              |
| 44:LE:1409:U:O2'    | 69:Ld:137:ARG:HB3   | 2.17                     | 0.45              |
| 47:LH:2685:OMC:O2   | 47:LH:2685:OMC:H2'  | 2.16                     | 0.45              |
| 47:LH:2848:A:O2'    | 47:LH:2850:C:OP2    | 2.27                     | 0.45              |
| 47:LH:2849:A2M:HM'2 | 47:LH:2849:A2M:H1'  | 1.71                     | 0.45              |
| 48:LI:3033:C:H2'    | 48:LI:3034:G:C8     | 2.51                     | 0.45              |
| 48:LI:3191:OMG:H1'  | 48:LI:3191:OMG:HM23 | 1.51                     | 0.45              |
| 48:LI:3394:A:H61    | 48:LI:3541:U:H5'    | 1.81                     | 0.45              |
| 56:LQ:90:VAL:CG2    | 56:LQ:161:ARG:HB2   | 2.47                     | 0.45              |
| 67:Lb:168:GLY:HA2   | 67:Lb:171:HIS:ND1   | 2.30                     | 0.45              |
| 72:Lg:16:ALA:HA     | 72:Lg:59:GLY:HA2    | 1.98                     | 0.45              |
| 75:Lj:85:GLU:HG3    | 75:Lj:109:ILE:HD11  | 1.97                     | 0.45              |
| 83:Lr:226:ASP:HB3   | 83:Lr:230:ARG:HH21  | 1.80                     | 0.45              |
| 96:L4:9:LYS:HD2     | 96:L4:22:THR:HA     | 1.98                     | 0.45              |
| 97:L6:17:GLU:CD     | 97:L6:17:GLU:H      | 2.24                     | 0.45              |
| 1:S1:661:G:N3       | 36:Se:61:GLN:NE2    | 2.64                     | 0.45              |
| 1:S1:704:OMU:H1'    | 1:S1:704:OMU:HM23   | 1.54                     | 0.45              |
| 1:S1:726:A:O2'      | 1:S1:1431:G:H5'     | 2.16                     | 0.45              |
| 4:S4:19:G:C5        | 47:LH:2940:G:H5'    | 2.51                     | 0.45              |
| 11:SF:114:LEU:HD12  | 11:SF:212:VAL:HG22  | 1.98                     | 0.45              |
| 12:SG:57:ASP:HA     | 12:SG:109:ALA:H     | 1.81                     | 0.45              |
| 25:ST:72:LEU:HG     | 25:ST:76:LYS:HE2    | 1.98                     | 0.45              |
| 37:Sf:101:LEU:HB3   | 37:Sf:104:LEU:HG    | 1.99                     | 0.45              |
| 38:Sg:151:ARG:HG2   | 38:Sg:160:VAL:HG21  | 1.98                     | 0.45              |
| 39:Sh:55:VAL:HG11   | 39:Sh:313:VAL:HG11  | 1.98                     | 0.45              |
| 39:Sh:185:ASN:O     | 39:Sh:187:LYS:HG3   | 2.16                     | 0.45              |
| 40:LA:92:G:C6       | 90:Ly:73:LYS:HD2    | 2.51                     | 0.45              |
| 42:LC:341:G:H2'     | 42:LC:342:A:H8      | 1.81                     | 0.45              |
| 42:LC:436:U:H2'     | 42:LC:437:G:C8      | 2.51                     | 0.45              |
| 44:LE:835:C:H1'     | 97:L6:54:GLN:NE2    | 2.32                     | 0.45              |
| 44:LE:1259:C:O2'    | 47:LH:2898:U:C2     | 2.69                     | 0.45              |
| 47:LH:2845:A:H2'    | 47:LH:2846:C:H6     | 1.82                     | 0.45              |
| 47:LH:2897:OMG:HM21 | 47:LH:2899:PSU:H5'  | 1.98                     | 0.45              |
| 48:LI:3477:U:O2'    | 49:LJ:3604:A:OP1    | 2.23                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:LK:3788:C:H3'   | 50:LK:3792:A:H61   | 1.81                     | 0.45              |
| 54:LO:11:A:N1      | 54:LO:66:G:O2'     | 2.38                     | 0.45              |
| 54:LO:22:A:H2'     | 54:LO:23:A:C8      | 2.50                     | 0.45              |
| 64:LY:112:MET:C    | 64:LY:114:GLY:H    | 2.25                     | 0.45              |
| 79:Ln:89:LEU:HA    | 79:Ln:89:LEU:HD13  | 1.80                     | 0.45              |
| 81:Lp:48:LYS:O     | 81:Lp:52:ARG:HG2   | 2.16                     | 0.45              |
| 85:Lt:65:PHE:CD1   | 85:Lt:105:LYS:HB2  | 2.51                     | 0.45              |
| 1:S1:52:U:H2'      | 1:S1:53:G:H8       | 1.82                     | 0.45              |
| 1:S1:209:U:H2'     | 1:S1:210:G:C8      | 2.51                     | 0.45              |
| 1:S1:427:U:H2'     | 1:S1:428:G:C8      | 2.52                     | 0.45              |
| 1:S1:604:A:H2'     | 1:S1:605:U:C6      | 2.51                     | 0.45              |
| 1:S1:1059:C:N4     | 31:SZ:12:SER:OG    | 2.45                     | 0.45              |
| 1:S1:1095:C:H6     | 25:ST:73:ARG:HH21  | 1.62                     | 0.45              |
| 1:S1:1345:U:H2'    | 1:S1:1346:G:H8     | 1.80                     | 0.45              |
| 13:SH:85:ILE:HD12  | 32:Sa:110:LEU:HD21 | 1.99                     | 0.45              |
| 17:SL:87:TYR:O     | 17:SL:90:ARG:HG2   | 2.17                     | 0.45              |
| 27:SV:96:MET:HE3   | 27:SV:96:MET:HB3   | 1.91                     | 0.45              |
| 39:Sh:42:LEU:HB2   | 39:Sh:63:LEU:HB2   | 1.98                     | 0.45              |
| 39:Sh:97:SER:O     | 39:Sh:98:THR:HG22  | 2.16                     | 0.45              |
| 39:Sh:291:ILE:HB   | 39:Sh:306:TYR:HA   | 1.98                     | 0.45              |
| 41:LB:186:A:H4'    | 42:LC:534:A:H2'    | 1.97                     | 0.45              |
| 44:LE:1067:G:H3'   | 48:LI:3356:G:N2    | 2.31                     | 0.45              |
| 44:LE:1159:G:C2    | 47:LH:2621:PSU:H1' | 2.51                     | 0.45              |
| 44:LE:1306:U:H2'   | 44:LE:1307:G:H8    | 1.82                     | 0.45              |
| 47:LH:2662:G:H5''  | 55:LP:18:THR:HG21  | 1.97                     | 0.45              |
| 47:LH:2757:U:O2'   | 47:LH:2759:A:N7    | 2.41                     | 0.45              |
| 48:LI:3028:G:H2'   | 48:LI:3029:A:H8    | 1.81                     | 0.45              |
| 61:LV:94:LYS:HE2   | 61:LV:94:LYS:HB2   | 1.79                     | 0.45              |
| 61:LV:148:LYS:O    | 61:LV:151:GLU:HG3  | 2.16                     | 0.45              |
| 63:LX:92:LEU:HD11  | 63:LX:128:LEU:HD11 | 1.98                     | 0.45              |
| 83:Lr:178:ILE:HG12 | 83:Lr:183:ASP:HB3  | 1.97                     | 0.45              |
| 88:Lw:73:ARG:O     | 100:Lw:201:HOH:O   | 2.20                     | 0.45              |
| 93:L2:92:MET:HG2   | 93:L2:102:PRO:O    | 2.17                     | 0.45              |
| 1:S1:1400:A:O2'    | 1:S1:1402:A:N7     | 2.45                     | 0.45              |
| 1:S1:1731:A:H4'    | 1:S1:1732:A:O5'    | 2.16                     | 0.45              |
| 1:S1:1895:A:H5''   | 17:SL:126:VAL:HG13 | 1.98                     | 0.45              |
| 1:S1:2058:A:OP1    | 28:SW:52:ARG:HG2   | 2.17                     | 0.45              |
| 7:SB:122:LEU:HD11  | 7:SB:144:VAL:HG22  | 1.99                     | 0.45              |
| 8:SC:111:LEU:HD12  | 8:SC:186:ILE:HD11  | 1.97                     | 0.45              |
| 13:SH:96:GLN:NE2   | 13:SH:96:GLN:O     | 2.46                     | 0.45              |
| 18:SM:88:LYS:C     | 18:SM:89:ARG:HD2   | 2.41                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:SZ:93:LYS:HE2    | 31:SZ:102:ARG:HH12 | 1.80                     | 0.45              |
| 38:Sg:233:TYR:CD2   | 38:Sg:236:ARG:HB2  | 2.52                     | 0.45              |
| 45:LF:1488:C:H2'    | 45:LF:1489:A:H8    | 1.79                     | 0.45              |
| 46:LG:2086:C:H2'    | 46:LG:2087:C:H6    | 1.81                     | 0.45              |
| 46:LG:2127:C:H2'    | 46:LG:2128:C:C6    | 2.52                     | 0.45              |
| 47:LH:2408:C:H2'    | 47:LH:2409:C:C6    | 2.51                     | 0.45              |
| 50:LK:3781:U:H5'    | 59:LT:19:PHE:HB3   | 1.98                     | 0.45              |
| 61:LV:181:GLN:HE21  | 61:LV:183:ARG:HD2  | 1.80                     | 0.45              |
| 67:Lb:117:ASN:HD21  | 67:Lb:166:SER:HB2  | 1.81                     | 0.45              |
| 67:Lb:165:THR:O     | 67:Lb:169:ARG:HG3  | 2.16                     | 0.45              |
| 84:Ls:77:ASN:HB2    | 84:Ls:89:THR:HB    | 1.99                     | 0.45              |
| 84:Ls:104:ILE:H     | 84:Ls:104:ILE:HD12 | 1.82                     | 0.45              |
| 92:L1:21:ARG:O      | 92:L1:38:ASN:ND2   | 2.50                     | 0.45              |
| 1:S1:1025:C:H2'     | 1:S1:1026:A:H8     | 1.81                     | 0.45              |
| 1:S1:1085:A:H2'     | 15:SJ:107:SER:O    | 2.15                     | 0.45              |
| 1:S1:1379:U:H2'     | 1:S1:1380:C:C6     | 2.51                     | 0.45              |
| 1:S1:2287:MA6:O5'   | 1:S1:2287:MA6:H8   | 2.17                     | 0.45              |
| 7:SB:134:ILE:CG2    | 7:SB:156:TYR:HB2   | 2.44                     | 0.45              |
| 8:SC:71:LEU:HA      | 8:SC:74:VAL:HG12   | 1.98                     | 0.45              |
| 23:SR:121:HIS:N     | 28:SW:123:GLU:O    | 2.47                     | 0.45              |
| 34:Sc:48:VAL:HG12   | 34:Sc:56:VAL:HG11  | 1.98                     | 0.45              |
| 42:LC:409:G:H2'     | 42:LC:410:A:O4'    | 2.17                     | 0.45              |
| 44:LE:1002:G:N2     | 44:LE:1005:G:OP2   | 2.42                     | 0.45              |
| 44:LE:1311:C:H5''   | 98:L7:11:VAL:HG13  | 1.98                     | 0.45              |
| 44:LE:1316:A:H2'    | 44:LE:1317:A:O4'   | 2.15                     | 0.45              |
| 46:LG:2129:OMU:HM23 | 46:LG:2129:OMU:H1' | 1.52                     | 0.45              |
| 46:LG:2201:G:H2'    | 46:LG:2202:G:O4'   | 2.17                     | 0.45              |
| 47:LH:2870:OMG:OP2  | 62:LW:95:TYR:OH    | 2.26                     | 0.45              |
| 48:LI:3499:G:H2'    | 48:LI:3500:A2M:C8  | 2.46                     | 0.45              |
| 51:LL:3892:C:H2'    | 51:LL:3893:C:C6    | 2.51                     | 0.45              |
| 54:LO:90:A:C5       | 54:LO:91:C:H1'     | 2.51                     | 0.45              |
| 57:LR:30:VAL:HG11   | 57:LR:116:LEU:HD22 | 1.99                     | 0.45              |
| 60:LU:112:ALA:O     | 60:LU:116:ARG:HG2  | 2.17                     | 0.45              |
| 75:Lj:101:LEU:HD23  | 75:Lj:101:LEU:H    | 1.81                     | 0.45              |
| 76:Lk:121:ARG:O     | 76:Lk:125:ASP:HA   | 2.17                     | 0.45              |
| 77:Ll:43:LYS:HE3    | 77:Ll:124:ARG:HH21 | 1.81                     | 0.45              |
| 92:L1:23:ILE:HG13   | 92:L1:38:ASN:HB2   | 1.98                     | 0.45              |
| 1:S1:180:OMG:H2'    | 1:S1:181:G:H8      | 1.82                     | 0.45              |
| 1:S1:2045:G:N2      | 1:S1:2071:G:H1'    | 2.31                     | 0.45              |
| 1:S1:2225:C:H2'     | 1:S1:2226:G:O4'    | 2.16                     | 0.45              |
| 6:SA:57:ASP:OD1     | 6:SA:57:ASP:N      | 2.45                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:SA:229:GLU:OE1   | 48:LI:3039:C:N4     | 2.50                     | 0.45              |
| 8:SC:206:ILE:HB    | 8:SC:209:GLN:HG3    | 1.99                     | 0.45              |
| 8:SC:210:VAL:HG13  | 27:SV:41:VAL:HG12   | 1.99                     | 0.45              |
| 12:SG:42:ASP:OD1   | 12:SG:44:LYS:HG2    | 2.17                     | 0.45              |
| 12:SG:161:ARG:HD3  | 12:SG:174:SER:OG    | 2.17                     | 0.45              |
| 18:SM:55:PRO:HA    | 18:SM:90:LEU:O      | 2.16                     | 0.45              |
| 23:SR:138:LYS:HG2  | 23:SR:139:THR:HG23  | 1.98                     | 0.45              |
| 27:SV:7:LYS:HZ3    | 27:SV:11:ARG:HH21   | 1.64                     | 0.45              |
| 33:Sb:39:PHE:CZ    | 33:Sb:69:TYR:HB3    | 2.52                     | 0.45              |
| 38:Sg:137:TRP:HB2  | 38:Sg:214:LYS:HE2   | 1.99                     | 0.45              |
| 39:Sh:290:CYS:HA   | 39:Sh:306:TYR:CD2   | 2.52                     | 0.45              |
| 39:Sh:306:TYR:OH   | 39:Sh:312:ARG:HD2   | 2.16                     | 0.45              |
| 41:LB:228:G:O6     | 42:LC:519:C:O2'     | 2.32                     | 0.45              |
| 41:LB:245:A:H61    | 41:LB:259:A:H3'     | 1.82                     | 0.45              |
| 42:LC:404:A:OP2    | 57:LR:217:ASN:HB2   | 2.16                     | 0.45              |
| 44:LE:941:C:H2'    | 44:LE:942:A:C8      | 2.51                     | 0.45              |
| 45:LF:1727:G:OP1   | 45:LF:1738:A2M:N6   | 2.41                     | 0.45              |
| 47:LH:2780:A:N7    | 100:LH:3036:HOH:O   | 2.36                     | 0.45              |
| 48:LI:3402:G:O4'   | 48:LI:3456:5MC:HM53 | 2.16                     | 0.45              |
| 52:LM:3912:A:OP1   | 56:LQ:126:LYS:HE3   | 2.16                     | 0.45              |
| 56:LQ:137:LEU:HD12 | 56:LQ:137:LEU:HA    | 1.75                     | 0.45              |
| 57:LR:32:ARG:NH2   | 80:Lo:28:PHE:O      | 2.42                     | 0.45              |
| 61:LV:127:LEU:HD13 | 61:LV:188:LEU:HD21  | 1.99                     | 0.45              |
| 61:LV:140:PHE:HA   | 61:LV:143:ARG:NE    | 2.27                     | 0.45              |
| 63:LX:134:PHE:O    | 81:Lp:117:ARG:NH2   | 2.50                     | 0.45              |
| 78:Lm:49:ASN:HB3   | 78:Lm:52:VAL:HG22   | 1.98                     | 0.45              |
| 81:Lp:28:LEU:HA    | 81:Lp:31:LEU:HD12   | 1.98                     | 0.45              |
| 84:Ls:59:VAL:HG21  | 84:Ls:92:MET:SD     | 2.57                     | 0.45              |
| 96:L4:70:LEU:HD21  | 96:L4:91:PHE:CZ     | 2.51                     | 0.45              |
| 1:S1:256:G:O2'     | 1:S1:257:G:H5'      | 2.17                     | 0.45              |
| 1:S1:602:C:H2'     | 1:S1:603:G:C8       | 2.52                     | 0.45              |
| 1:S1:1114:U:O2'    | 1:S1:1117:A:OP1     | 2.26                     | 0.45              |
| 1:S1:1261:U:O2     | 34:Sc:24:LYS:NZ     | 2.48                     | 0.45              |
| 1:S1:1637:G:O2'    | 22:SQ:41:ILE:HG22   | 2.17                     | 0.45              |
| 1:S1:1833:A:H2'    | 1:S1:1834:U:C6      | 2.52                     | 0.45              |
| 1:S1:1965:G:H4'    | 29:SX:14:PRO:CB     | 2.47                     | 0.45              |
| 3:S3:75:C:C5       | 3:S3:76:A:H3'       | 2.52                     | 0.45              |
| 4:S4:2:C:H2'       | 4:S4:3:G:H8         | 1.81                     | 0.45              |
| 12:SG:21:GLU:O     | 12:SG:25:VAL:HG13   | 2.17                     | 0.45              |
| 20:SO:47:ASP:OD1   | 20:SO:48:ILE:N      | 2.50                     | 0.45              |
| 23:SR:124:LEU:O    | 23:SR:127:MET:HG2   | 2.17                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 28:SW:22:TYR:HB3    | 28:SW:30:LEU:HD11   | 1.98                     | 0.45              |
| 41:LB:229:C:H2'     | 41:LB:230:A:O4'     | 2.16                     | 0.45              |
| 42:LC:387:U:H2'     | 42:LC:388:G:O4'     | 2.17                     | 0.45              |
| 44:LE:979:C:OP2     | 44:LE:980:A:O2'     | 2.31                     | 0.45              |
| 44:LE:1010:C:H2'    | 44:LE:1011:U:O4'    | 2.17                     | 0.45              |
| 44:LE:1419:G:OP2    | 82:Lq:70:ARG:NH2    | 2.50                     | 0.45              |
| 46:LG:2067:C:OP1    | 88:Lw:57:PRO:HB2    | 2.17                     | 0.45              |
| 47:LH:2346:OMU:H1'  | 47:LH:2346:OMU:HM23 | 1.75                     | 0.45              |
| 49:LJ:3628:U:H5''   | 56:LQ:62:ARG:HG2    | 1.99                     | 0.45              |
| 49:LJ:3663:G:H2'    | 49:LJ:3664:A:O4'    | 2.17                     | 0.45              |
| 56:LQ:189:SER:OG    | 56:LQ:190:ILE:N     | 2.50                     | 0.45              |
| 62:LW:63:MET:HE1    | 62:LW:79:ARG:CZ     | 2.47                     | 0.45              |
| 65:LZ:134:LEU:HD22  | 65:LZ:187:ILE:HD11  | 1.99                     | 0.45              |
| 68:Lc:55:MET:HE2    | 68:Lc:164:VAL:HG11  | 1.98                     | 0.45              |
| 76:Lk:158:ASN:OD1   | 76:Lk:159:LYS:HD2   | 2.16                     | 0.45              |
| 83:Lr:210:PRO:HB3   | 83:Lr:241:MET:HG2   | 1.98                     | 0.45              |
| 85:Lt:145:THR:HG22  | 85:Lt:146:HIS:H     | 1.82                     | 0.45              |
| 87:Lv:19:ARG:HA     | 87:Lv:24:GLN:HA     | 1.98                     | 0.45              |
| 1:S1:1713:U:O2'     | 1:S1:1732:A:OP2     | 2.32                     | 0.45              |
| 1:S1:2153:U:H2'     | 1:S1:2154:A:C8      | 2.51                     | 0.45              |
| 1:S1:2223:G:H2'     | 1:S1:2224:C:H6      | 1.80                     | 0.45              |
| 9:SD:106:GLU:HG2    | 9:SD:115:LYS:NZ     | 2.32                     | 0.45              |
| 18:SM:42:ILE:HD11   | 18:SM:55:PRO:HD3    | 1.98                     | 0.45              |
| 25:ST:113:PHE:O     | 25:ST:117:LEU:HD13  | 2.17                     | 0.45              |
| 27:SV:7:LYS:NZ      | 27:SV:11:ARG:HH21   | 2.14                     | 0.45              |
| 40:LA:65:C:H5'      | 81:Lp:10:ARG:NH2    | 2.31                     | 0.45              |
| 41:LB:235:C:H5''    | 63:LX:65:VAL:HB     | 1.98                     | 0.45              |
| 42:LC:535:G:H2'     | 42:LC:536:A:C8      | 2.52                     | 0.45              |
| 44:LE:940:C:H2'     | 44:LE:941:C:C6      | 2.52                     | 0.45              |
| 44:LE:1204:A2M:HM'3 | 44:LE:1204:A2M:H1'  | 1.81                     | 0.45              |
| 44:LE:1273:G:H2'    | 44:LE:1274:A:O4'    | 2.16                     | 0.45              |
| 44:LE:1330:G:N2     | 68:Lc:193:ASP:OD2   | 2.50                     | 0.45              |
| 44:LE:1436:A:H2'    | 44:LE:1437:G:C8     | 2.51                     | 0.45              |
| 45:LF:1663:C:H2'    | 45:LF:1664:G:O4'    | 2.16                     | 0.45              |
| 46:LG:2064:C:P      | 79:Ln:36:ARG:HH22   | 2.40                     | 0.45              |
| 48:LI:3426:C:H2'    | 48:LI:3427:G:O4'    | 2.17                     | 0.45              |
| 51:LL:3904:A:H2'    | 51:LL:3907:G:O6     | 2.17                     | 0.45              |
| 54:LO:90:A:N6       | 54:LO:91:C:O2       | 2.50                     | 0.45              |
| 54:LO:92:C:H2'      | 54:LO:93:A:C8       | 2.52                     | 0.45              |
| 54:LO:118:C:H2'     | 54:LO:119:U:O4'     | 2.17                     | 0.45              |
| 57:LR:104:LYS:HB3   | 57:LR:104:LYS:HE2   | 1.69                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:LW:179:LEU:HD22 | 65:LZ:135:LYS:HG3  | 1.99                     | 0.45              |
| 70:Le:38:VAL:HG12  | 70:Le:40:THR:HG23  | 1.99                     | 0.45              |
| 79:Ln:36:ARG:NH1   | 79:Ln:38:TYR:OH    | 2.48                     | 0.45              |
| 1:S1:306:G:N2      | 100:S1:2459:HOH:O  | 2.35                     | 0.45              |
| 1:S1:469:G:O2'     | 26:SU:103:LYS:NZ   | 2.49                     | 0.45              |
| 1:S1:1558:C:H2'    | 1:S1:1559:G:C8     | 2.53                     | 0.45              |
| 1:S1:1672:U:H2'    | 1:S1:1673:G:C8     | 2.52                     | 0.45              |
| 1:S1:1681:OMG:HM23 | 1:S1:1681:OMG:H1'  | 1.66                     | 0.45              |
| 1:S1:1855:C:H4'    | 18:SM:51:ARG:HH11  | 1.82                     | 0.45              |
| 1:S1:1944:C:OP2    | 23:SR:137:THR:HB   | 2.17                     | 0.45              |
| 1:S1:2149:U:H2'    | 1:S1:2150:U:C6     | 2.52                     | 0.45              |
| 4:S4:75:A:H1'      | 96:L4:55:LYS:CB    | 2.47                     | 0.45              |
| 7:SB:158:ASP:CB    | 30:SY:34:PHE:HZ    | 2.30                     | 0.45              |
| 22:SQ:72:LEU:HD21  | 37:Sf:103:VAL:HG12 | 1.99                     | 0.45              |
| 42:LC:299:C:H2'    | 42:LC:300:G:H8     | 1.82                     | 0.45              |
| 42:LC:494:A:H2'    | 42:LC:495:G:H8     | 1.80                     | 0.45              |
| 43:LD:669:G:O2'    | 57:LR:320:ARG:NH1  | 2.49                     | 0.45              |
| 45:LF:1689:A:H5''  | 62:LW:133:ARG:NH1  | 2.31                     | 0.45              |
| 45:LF:1711:G:H5''  | 83:Lr:111:GLN:OE1  | 2.17                     | 0.45              |
| 47:LH:2664:U:OP1   | 55:LP:54:ARG:NH2   | 2.35                     | 0.45              |
| 48:LI:3032:G:H2'   | 48:LI:3033:C:C6    | 2.51                     | 0.45              |
| 50:LK:3762:A:C4    | 72:Lg:155:LEU:HD13 | 2.52                     | 0.45              |
| 51:LL:3865:PSU:H2' | 51:LL:3866:U:O4'   | 2.17                     | 0.45              |
| 61:LV:200:LEU:HD21 | 67:Lb:18:VAL:HG11  | 1.99                     | 0.45              |
| 63:LX:67:CYS:HB2   | 63:LX:72:PHE:O     | 2.16                     | 0.45              |
| 72:Lg:109:MET:HE3  | 72:Lg:109:MET:HB3  | 1.76                     | 0.45              |
| 74:Li:18:LYS:O     | 74:Li:103:ASN:ND2  | 2.50                     | 0.45              |
| 85:Lt:81:ARG:HG2   | 85:Lt:86:THR:O     | 2.16                     | 0.45              |
| 1:S1:303:C:OP1     | 38:Sg:251:ARG:HD2  | 2.17                     | 0.44              |
| 1:S1:1152:U:O2'    | 1:S1:1153:G:O5'    | 2.30                     | 0.44              |
| 1:S1:1243:C:HO2'   | 1:S1:1244:C:P      | 2.41                     | 0.44              |
| 1:S1:1494:G:N2     | 1:S1:1497:A:OP2    | 2.37                     | 0.44              |
| 3:S3:7:A:O2'       | 3:S3:49:C:O4'      | 2.35                     | 0.44              |
| 3:S3:25:C:C4       | 3:S3:26:A:C8       | 3.04                     | 0.44              |
| 14:SI:51:VAL:HG12  | 14:SI:52:ASN:O     | 2.17                     | 0.44              |
| 16:SK:292:PHE:O    | 16:SK:296:LYS:HG2  | 2.17                     | 0.44              |
| 22:SQ:109:LYS:HG3  | 22:SQ:111:MET:H    | 1.82                     | 0.44              |
| 35:Sd:36:ARG:NH2   | 35:Sd:50:ILE:HD11  | 2.31                     | 0.44              |
| 42:LC:517:G:H2'    | 42:LC:518:U:H6     | 1.82                     | 0.44              |
| 43:LD:722:A:H2'    | 43:LD:723:G:C8     | 2.52                     | 0.44              |
| 46:LG:1992:G:H2'   | 46:LG:1993:C:C6    | 2.52                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:LH:2710:A:H2'   | 47:LH:2711:G:C8    | 2.52                     | 0.44              |
| 48:LI:3139:U:O2'   | 48:LI:3141:A:N7    | 2.50                     | 0.44              |
| 48:LI:3373:G:H2'   | 48:LI:3374:OMC:C6  | 2.52                     | 0.44              |
| 49:LJ:3694:OMU:O4  | 49:LJ:3719:G:O2'   | 2.32                     | 0.44              |
| 50:LK:3771:C:H2'   | 50:LK:3772:C:C6    | 2.51                     | 0.44              |
| 53:LN:4024:C:H2'   | 53:LN:4025:U:C6    | 2.52                     | 0.44              |
| 56:LQ:50:LYS:HB3   | 56:LQ:336:ILE:HA   | 1.97                     | 0.44              |
| 56:LQ:181:MET:HE2  | 56:LQ:183:ILE:HG12 | 1.99                     | 0.44              |
| 57:LR:102:PHE:HB3  | 63:LX:30:CYS:SG    | 2.57                     | 0.44              |
| 57:LR:187:LYS:HA   | 57:LR:190:ARG:HG3  | 1.99                     | 0.44              |
| 79:Ln:11:VAL:HG12  | 79:Ln:82:PRO:HA    | 1.99                     | 0.44              |
| 97:L6:66:LEU:HD23  | 97:L6:66:LEU:HA    | 1.79                     | 0.44              |
| 1:S1:156:A:N1      | 12:SG:185:PRO:HD3  | 2.32                     | 0.44              |
| 1:S1:736:U:OP1     | 26:SU:107:LYS:HD2  | 2.17                     | 0.44              |
| 1:S1:1646:A:H2'    | 1:S1:1647:G:C8     | 2.51                     | 0.44              |
| 1:S1:1958:U:H1'    | 13:SH:74:MET:CE    | 2.47                     | 0.44              |
| 1:S1:2000:G:O6     | 1:S1:2013:U:C2     | 2.70                     | 0.44              |
| 3:S3:25:C:O2'      | 47:LH:2753:C:H4'   | 2.17                     | 0.44              |
| 3:S3:53:G:H3'      | 3:S3:54:U:C5'      | 2.47                     | 0.44              |
| 7:SB:49:LEU:HD12   | 7:SB:162:PRO:CB    | 2.47                     | 0.44              |
| 15:SJ:32:LYS:O     | 15:SJ:36:ARG:HG3   | 2.16                     | 0.44              |
| 28:SW:21:THR:OG1   | 28:SW:26:GLU:OE2   | 2.35                     | 0.44              |
| 39:Sh:83:LEU:HD13  | 39:Sh:93:LEU:HG    | 1.98                     | 0.44              |
| 39:Sh:149:ASP:HB3  | 39:Sh:188:LEU:HD22 | 1.99                     | 0.44              |
| 39:Sh:175:ASP:OD1  | 39:Sh:175:ASP:N    | 2.49                     | 0.44              |
| 40:LA:35:A:N6      | 41:LB:181:G:O2'    | 2.48                     | 0.44              |
| 44:LE:962:C:C2     | 70:Le:86:ILE:HG21  | 2.53                     | 0.44              |
| 44:LE:1247:U:H2'   | 44:LE:1248:U:H6    | 1.82                     | 0.44              |
| 44:LE:1426:G:H2'   | 44:LE:1427:U:C6    | 2.51                     | 0.44              |
| 45:LF:1856:OMG:H5' | 74:Li:51:ARG:HH21  | 1.83                     | 0.44              |
| 46:LG:2166:A:H61   | 71:Lf:129:LYS:HD2  | 1.81                     | 0.44              |
| 47:LH:2250:C:H2'   | 47:LH:2251:A:H8    | 1.78                     | 0.44              |
| 47:LH:2321:A:H2'   | 47:LH:2322:G:C8    | 2.52                     | 0.44              |
| 47:LH:2788:U:H2'   | 47:LH:2789:U:H6    | 1.82                     | 0.44              |
| 48:LI:3094:G:OP2   | 55:LP:87:TYR:OH    | 2.32                     | 0.44              |
| 48:LI:3381:U:OP1   | 96:L4:62:ALA:N     | 2.50                     | 0.44              |
| 54:LO:111:C:H2'    | 54:LO:112:U:O4'    | 2.17                     | 0.44              |
| 56:LQ:232:ILE:HD12 | 56:LQ:239:ARG:HB3  | 1.99                     | 0.44              |
| 65:LZ:197:LEU:HD23 | 65:LZ:197:LEU:HA   | 1.84                     | 0.44              |
| 66:La:42:ALA:O     | 66:La:48:HIS:ND1   | 2.51                     | 0.44              |
| 69:Ld:54:MET:HE2   | 69:Ld:54:MET:HB3   | 1.80                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 70:Le:148:TYR:HA   | 70:Le:151:PHE:CD2   | 2.52                     | 0.44              |
| 76:Lk:39:LYS:HG2   | 76:Lk:41:TYR:CE1    | 2.52                     | 0.44              |
| 83:Lr:63:LEU:HD22  | 83:Lr:77:PHE:HZ     | 1.82                     | 0.44              |
| 91:Lz:39:LYS:O     | 91:Lz:40:THR:OG1    | 2.25                     | 0.44              |
| 1:S1:378:C:N4      | 1:S1:379:A:N6       | 2.65                     | 0.44              |
| 1:S1:1536:OMG:H5'  | 94:L3:20:LYS:HE3    | 1.99                     | 0.44              |
| 1:S1:2062:G:O5'    | 23:SR:134:GLY:HA3   | 2.17                     | 0.44              |
| 3:S3:29:G:H5''     | 28:SW:141:THR:HG21  | 2.00                     | 0.44              |
| 7:SB:5:ARG:NE      | 30:SY:39:ILE:O      | 2.50                     | 0.44              |
| 9:SD:41:GLU:HG2    | 9:SD:44:ARG:NH2     | 2.33                     | 0.44              |
| 9:SD:135:ARG:HD3   | 9:SD:160:PRO:HD2    | 1.98                     | 0.44              |
| 12:SG:50:PHE:CE1   | 12:SG:115:ILE:HG22  | 2.52                     | 0.44              |
| 22:SQ:69:TYR:O     | 22:SQ:73:VAL:HG23   | 2.16                     | 0.44              |
| 29:SX:27:LYS:O     | 29:SX:27:LYS:HG2    | 2.18                     | 0.44              |
| 29:SX:109:GLN:O    | 29:SX:112:LYS:HG3   | 2.17                     | 0.44              |
| 40:LA:41:OMG:H1'   | 40:LA:41:OMG:HM23   | 1.74                     | 0.44              |
| 44:LE:946:A:N1     | 44:LE:1241:G:O2'    | 2.42                     | 0.44              |
| 44:LE:970:U:H2'    | 44:LE:971:G:H8      | 1.82                     | 0.44              |
| 46:LG:2109:C:H2'   | 46:LG:2110:C:H6     | 1.81                     | 0.44              |
| 48:LI:3566:U:H5'   | 48:LI:3567:U:H5'    | 1.99                     | 0.44              |
| 49:LJ:3636:OMU:H1' | 49:LJ:3636:OMU:HM23 | 1.41                     | 0.44              |
| 54:LO:102:C:H2'    | 54:LO:103:A:O4'     | 2.17                     | 0.44              |
| 63:LX:137:LYS:HE3  | 63:LX:140:LYS:HD3   | 1.99                     | 0.44              |
| 66:La:58:GLY:C     | 70:Le:178:GLU:HA    | 2.42                     | 0.44              |
| 69:Ld:89:VAL:HG22  | 69:Ld:90:GLY:H      | 1.82                     | 0.44              |
| 77:Ll:11:ARG:NH1   | 77:Ll:15:ARG:HH21   | 2.14                     | 0.44              |
| 77:Ll:30:MET:SD    | 77:Ll:74:ARG:HA     | 2.57                     | 0.44              |
| 77:Ll:58:LYS:HB3   | 77:Ll:58:LYS:HE3    | 1.73                     | 0.44              |
| 85:Lt:68:ARG:HD2   | 85:Lt:105:LYS:HA    | 1.99                     | 0.44              |
| 93:L2:92:MET:SD    | 93:L2:119:LEU:HD23  | 2.56                     | 0.44              |
| 1:S1:96:C:O2       | 1:S1:522:A:O2'      | 2.32                     | 0.44              |
| 1:S1:285:A:O3'     | 38:Sg:243:ARG:NH2   | 2.47                     | 0.44              |
| 1:S1:288:C:H2'     | 1:S1:289:C:C6       | 2.52                     | 0.44              |
| 1:S1:919:C:H2'     | 1:S1:920:C:O4'      | 2.16                     | 0.44              |
| 1:S1:1035:A:H2'    | 1:S1:1036:A:C8      | 2.52                     | 0.44              |
| 1:S1:1100:A:OP1    | 1:S1:1101:C:H4'     | 2.18                     | 0.44              |
| 1:S1:1353:C:H2'    | 1:S1:1354:A:H8      | 1.81                     | 0.44              |
| 1:S1:1556:G:H2'    | 1:S1:1557:A:H8      | 1.82                     | 0.44              |
| 1:S1:1617:U:H4'    | 1:S1:1618:A:O4'     | 2.18                     | 0.44              |
| 1:S1:1641:OMU:C4   | 1:S1:1664:U:H3      | 2.27                     | 0.44              |
| 1:S1:1678:G:O2'    | 1:S1:1680:G:OP1     | 2.32                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:S1:1962:A:H2'     | 1:S1:1963:C:C6     | 2.53                     | 0.44              |
| 2:S2:33:U:O2'       | 2:S2:35:A:N7       | 2.49                     | 0.44              |
| 6:SA:95:LEU:HD12    | 6:SA:231:HIS:CE1   | 2.53                     | 0.44              |
| 12:SG:187:VAL:O     | 12:SG:191:ARG:HG2  | 2.17                     | 0.44              |
| 13:SH:85:ILE:HB     | 32:Sa:110:LEU:HD21 | 1.99                     | 0.44              |
| 16:SK:115:TYR:HB3   | 16:SK:123:LEU:HD11 | 1.99                     | 0.44              |
| 18:SM:69:LYS:HE2    | 18:SM:80:ASP:OD1   | 2.17                     | 0.44              |
| 20:SO:117:LEU:HB3   | 33:Sb:53:ILE:HD11  | 1.99                     | 0.44              |
| 30:SY:1:MET:HG2     | 30:SY:10:ASP:HB2   | 1.98                     | 0.44              |
| 33:Sb:61:THR:HG23   | 33:Sb:62:GLY:O     | 2.17                     | 0.44              |
| 40:LA:26:C:H2'      | 40:LA:27:A:H8      | 1.83                     | 0.44              |
| 40:LA:157:A:H5'     | 76:Lk:53:PRO:HG3   | 1.99                     | 0.44              |
| 42:LC:397:C:H2'     | 42:LC:398:C:O4'    | 2.17                     | 0.44              |
| 44:LE:1259:C:O2'    | 47:LH:2898:U:N3    | 2.40                     | 0.44              |
| 44:LE:1268:G:N3     | 82:Lq:15:LYS:NZ    | 2.66                     | 0.44              |
| 46:LG:2000:G:H2'    | 46:LG:2001:G:O4'   | 2.18                     | 0.44              |
| 46:LG:2015:G:H1     | 46:LG:2028:U:H5    | 1.66                     | 0.44              |
| 47:LH:2666:C:OP1    | 55:LP:128:LYS:N    | 2.47                     | 0.44              |
| 47:LH:2840:G:H5''   | 74:Li:85:TRP:O     | 2.18                     | 0.44              |
| 48:LI:3374:OMC:HM23 | 48:LI:3374:OMC:H1' | 1.72                     | 0.44              |
| 50:LK:3757:G:H2'    | 50:LK:3758:A:C8    | 2.53                     | 0.44              |
| 51:LL:3857:U:H2'    | 51:LL:3858:G:C8    | 2.52                     | 0.44              |
| 55:LP:44:VAL:HG22   | 55:LP:87:TYR:CE1   | 2.53                     | 0.44              |
| 56:LQ:258:HIS:HA    | 56:LQ:259:PRO:C    | 2.42                     | 0.44              |
| 57:LR:229:LEU:HD22  | 57:LR:234:LEU:HD21 | 1.98                     | 0.44              |
| 60:LU:103:ARG:O     | 60:LU:108:LYS:HG3  | 2.17                     | 0.44              |
| 64:LY:8:LYS:HG3     | 64:LY:9:GLY:H      | 1.82                     | 0.44              |
| 64:LY:84:GLN:NE2    | 64:LY:86:LYS:O     | 2.32                     | 0.44              |
| 65:LZ:55:ASN:O      | 65:LZ:59:ILE:HG23  | 2.18                     | 0.44              |
| 65:LZ:179:LEU:HD22  | 65:LZ:183:GLU:HB3  | 2.00                     | 0.44              |
| 70:Le:49:ARG:NH1    | 70:Le:139:ARG:HG2  | 2.32                     | 0.44              |
| 83:Lr:37:LYS:O      | 83:Lr:41:LYS:HG2   | 2.17                     | 0.44              |
| 1:S1:179:OMU:H1'    | 1:S1:179:OMU:HM23  | 1.68                     | 0.44              |
| 1:S1:428:G:H4'      | 16:SK:31:ARG:O     | 2.18                     | 0.44              |
| 1:S1:821:C:H2'      | 1:S1:822:U:C6      | 2.53                     | 0.44              |
| 1:S1:1434:G:O2'     | 15:SJ:3:ARG:HD2    | 2.18                     | 0.44              |
| 1:S1:1750:U:H2'     | 1:S1:1751:C:C6     | 2.52                     | 0.44              |
| 4:S4:25:C:N3        | 4:S4:26:A:C8       | 2.85                     | 0.44              |
| 4:S4:32:U:H2'       | 4:S4:33:U:C2       | 2.52                     | 0.44              |
| 7:SB:207:PRO:HA     | 27:SV:78:ARG:HD3   | 1.98                     | 0.44              |
| 8:SC:96:ARG:HD3     | 8:SC:127:PHE:HZ    | 1.82                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:SH:187:LYS:HA    | 13:SH:190:ARG:HG3   | 2.00                     | 0.44              |
| 15:SJ:54:ASP:HA     | 15:SJ:59:ASN:ND2    | 2.33                     | 0.44              |
| 16:SK:78:CYS:SG     | 16:SK:106:ILE:HD12  | 2.58                     | 0.44              |
| 26:SU:102:TYR:O     | 26:SU:104:ARG:N     | 2.48                     | 0.44              |
| 29:SX:41:LYS:HD2    | 29:SX:46:LYS:HB2    | 1.99                     | 0.44              |
| 41:LB:277:C:OP1     | 63:LX:107:ARG:NH2   | 2.50                     | 0.44              |
| 44:LE:1164:U:H4'    | 47:LH:2324:C:H4'    | 1.99                     | 0.44              |
| 44:LE:1246:C:H5''   | 86:Lu:60:VAL:HG12   | 1.99                     | 0.44              |
| 47:LH:2909:OMU:H1'  | 47:LH:2909:OMU:HM23 | 1.72                     | 0.44              |
| 48:LI:3270:A:H2'    | 48:LI:3271:G:H8     | 1.81                     | 0.44              |
| 48:LI:3518:5MC:H5'' | 64:LY:43:LYS:CD     | 2.48                     | 0.44              |
| 48:LI:3519:C:O2     | 48:LI:3521:A2M:H8   | 2.17                     | 0.44              |
| 49:LJ:3743:U:H2'    | 49:LJ:3744:G:C8     | 2.52                     | 0.44              |
| 53:LN:3995:G:H5'    | 56:LQ:172:ARG:HH12  | 1.81                     | 0.44              |
| 54:LO:5:A:O2'       | 69:Ld:62:GLN:OE1    | 2.28                     | 0.44              |
| 56:LQ:106:TRP:HB2   | 56:LQ:133:TYR:CE1   | 2.52                     | 0.44              |
| 59:LT:22:ASN:HB3    | 59:LT:39:ARG:NH1    | 2.33                     | 0.44              |
| 59:LT:36:ARG:HH11   | 59:LT:38:MET:HE3    | 1.82                     | 0.44              |
| 62:LW:148:THR:HA    | 62:LW:151:GLY:O     | 2.17                     | 0.44              |
| 68:Lc:145:GLU:O     | 68:Lc:149:VAL:HG23  | 2.18                     | 0.44              |
| 74:Li:86:PRO:HB2    | 74:Li:89:SER:OG     | 2.17                     | 0.44              |
| 77:LI:51:LYS:HG2    | 77:LI:52:GLU:HG2    | 1.99                     | 0.44              |
| 82:Lq:35:LEU:HD23   | 82:Lq:40:LYS:HG2    | 1.99                     | 0.44              |
| 89:Lx:44:LEU:O      | 89:Lx:48:VAL:HG23   | 2.18                     | 0.44              |
| 1:S1:483:G:P        | 16:SK:25:ARG:HH12   | 2.40                     | 0.44              |
| 1:S1:485:OMG:HM23   | 1:S1:485:OMG:H1'    | 1.77                     | 0.44              |
| 1:S1:502:C:H5''     | 12:SG:95:ARG:NH1    | 2.32                     | 0.44              |
| 1:S1:1037:OMC:HM22  | 1:S1:1038:U:H5'     | 2.00                     | 0.44              |
| 1:S1:2060:C:O2'     | 1:S1:2061:U:H2'     | 2.18                     | 0.44              |
| 1:S1:2300:A:OP2     | 33:Sb:4:LYS:NZ      | 2.50                     | 0.44              |
| 8:SC:14:VAL:O       | 8:SC:18:VAL:HG23    | 2.18                     | 0.44              |
| 19:SN:29:SER:OG     | 19:SN:30:LYS:N      | 2.49                     | 0.44              |
| 21:SP:5:HIS:HA      | 26:SU:104:ARG:HH21  | 1.83                     | 0.44              |
| 44:LE:965:U:H2'     | 44:LE:966:C:C6      | 2.53                     | 0.44              |
| 44:LE:1159:G:C5     | 55:LP:181:LYS:HB3   | 2.52                     | 0.44              |
| 47:LH:2356:G:H2'    | 47:LH:2357:G:O4'    | 2.17                     | 0.44              |
| 47:LH:2367:A:H2'    | 47:LH:2368:A:C8     | 2.53                     | 0.44              |
| 47:LH:2801:A:OP2    | 100:LH:3012:HOH:O   | 2.21                     | 0.44              |
| 47:LH:2855:A:H2'    | 47:LH:2856:A:C8     | 2.53                     | 0.44              |
| 48:LI:3304:U:H2'    | 48:LI:3305:A:H8     | 1.82                     | 0.44              |
| 50:LK:3753:C:H4'    | 50:LK:3754:A:OP2    | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:Ld:40:LYS:HD2   | 73:Lh:93:THR:HG21  | 1.99                     | 0.44              |
| 90:Ly:33:ARG:HD3   | 90:Ly:40:PRO:HD2   | 2.00                     | 0.44              |
| 1:S1:28:A2M:HM'2   | 1:S1:29:U:O4'      | 2.17                     | 0.44              |
| 1:S1:121:PSU:H2'   | 1:S1:122:G:C8      | 2.53                     | 0.44              |
| 1:S1:588:U:H2'     | 1:S1:589:C:C6      | 2.53                     | 0.44              |
| 1:S1:670:C:O2      | 36:Se:13:LYS:HE3   | 2.18                     | 0.44              |
| 1:S1:964:G:H5''    | 38:Sg:129:ARG:NH2  | 2.27                     | 0.44              |
| 1:S1:1425:A:N3     | 1:S1:2296:C:O2'    | 2.43                     | 0.44              |
| 1:S1:1744:OMU:HM22 | 1:S1:1745:C:O4'    | 2.18                     | 0.44              |
| 1:S1:1759:C:H2'    | 1:S1:1760:C:C6     | 2.52                     | 0.44              |
| 1:S1:2277:G:H2'    | 1:S1:2278:C:O4'    | 2.18                     | 0.44              |
| 39:Sh:133:MET:HE1  | 39:Sh:181:TRP:CD1  | 2.52                     | 0.44              |
| 42:LC:526:U:H2'    | 42:LC:527:G:O4'    | 2.18                     | 0.44              |
| 43:LD:749:A:C6     | 83:Lr:53:ARG:HG3   | 2.52                     | 0.44              |
| 45:LF:1575:A:H2'   | 45:LF:1576:A:H8    | 1.79                     | 0.44              |
| 45:LF:1719:U:H2'   | 45:LF:1720:C:C6    | 2.53                     | 0.44              |
| 45:LF:1871:C:H2'   | 45:LF:1872:C:O4'   | 2.17                     | 0.44              |
| 47:LH:2828:U:OP2   | 56:LQ:239:ARG:HG2  | 2.17                     | 0.44              |
| 56:LQ:94:LYS:HE2   | 56:LQ:94:LYS:HB3   | 1.78                     | 0.44              |
| 59:LT:5:TYR:OH     | 59:LT:58:GLU:OE2   | 2.36                     | 0.44              |
| 63:LX:119:LEU:O    | 63:LX:122:GLU:HG3  | 2.17                     | 0.44              |
| 69:Ld:120:GLY:HA2  | 69:Ld:129:TYR:CE2  | 2.51                     | 0.44              |
| 1:S1:354:G:H2'     | 1:S1:354:G:N3      | 2.32                     | 0.44              |
| 1:S1:552:C:H2'     | 1:S1:553:A:C8      | 2.53                     | 0.44              |
| 1:S1:709:A:OP2     | 1:S1:710:C:O2'     | 2.26                     | 0.44              |
| 1:S1:1095:C:H2'    | 25:ST:73:ARG:HH21  | 1.83                     | 0.44              |
| 1:S1:1301:G:P      | 20:SO:150:ARG:HH12 | 2.41                     | 0.44              |
| 1:S1:1763:A:H2'    | 1:S1:1764:G:C8     | 2.52                     | 0.44              |
| 1:S1:2189:U:H2'    | 1:S1:2190:G:C8     | 2.53                     | 0.44              |
| 3:S3:48:C:H5'      | 3:S3:49:C:C5'      | 2.44                     | 0.44              |
| 4:S4:8:U:H2'       | 4:S4:13:C:H41      | 1.83                     | 0.44              |
| 6:SA:134:ARG:O     | 6:SA:213:VAL:HA    | 2.18                     | 0.44              |
| 6:SA:161:ARG:HD3   | 6:SA:202:TYR:CE1   | 2.53                     | 0.44              |
| 7:SB:155:VAL:HG13  | 7:SB:156:TYR:N     | 2.33                     | 0.44              |
| 11:SF:83:LYS:HB2   | 11:SF:208:LEU:HD13 | 1.99                     | 0.44              |
| 14:SI:138:VAL:HG11 | 14:SI:167:VAL:HG21 | 2.00                     | 0.44              |
| 16:SK:110:PRO:C    | 16:SK:112:ARG:H    | 2.26                     | 0.44              |
| 18:SM:26:LEU:HG    | 18:SM:114:VAL:HG22 | 2.00                     | 0.44              |
| 18:SM:37:VAL:O     | 18:SM:41:LEU:HG    | 2.18                     | 0.44              |
| 22:SQ:102:TYR:CB   | 22:SQ:107:ASN:HA   | 2.47                     | 0.44              |
| 34:Sc:3:THR:O      | 34:Sc:4:PHE:HB2    | 2.17                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 38:Sg:193:PHE:HB3  | 38:Sg:207:LYS:HB2   | 2.00                     | 0.44              |
| 40:LA:109:G:OP2    | 40:LA:111:A:O2'     | 2.19                     | 0.44              |
| 42:LC:503:A:C4     | 89:Lx:34:PRO:HB3    | 2.53                     | 0.44              |
| 44:LE:1136:A:OP2   | 95:L5:4:ARG:NE      | 2.51                     | 0.44              |
| 45:LF:1839:G:OP2   | 100:LF:2011:HOH:O   | 2.21                     | 0.44              |
| 47:LH:2312:U:O2'   | 88:Lw:15:THR:O      | 2.28                     | 0.44              |
| 47:LH:2916:U:H2'   | 47:LH:2917:G:H8     | 1.83                     | 0.44              |
| 47:LH:2925:OMG:H1' | 47:LH:2925:OMG:HM23 | 1.63                     | 0.44              |
| 48:LI:3256:U:H2'   | 48:LI:3257:C:H6     | 1.81                     | 0.44              |
| 48:LI:3548:G:H2'   | 48:LI:3549:U:C6     | 2.52                     | 0.44              |
| 49:LJ:3617:A:H2'   | 49:LJ:3618:G:O4'    | 2.17                     | 0.44              |
| 57:LR:165:LEU:HD22 | 57:LR:170:ALA:HB3   | 1.99                     | 0.44              |
| 69:Ld:54:MET:HE1   | 69:Ld:156:ARG:NE    | 2.33                     | 0.44              |
| 78:Lm:35:PHE:CD2   | 78:Lm:41:ARG:HG3    | 2.52                     | 0.44              |
| 79:Ln:47:GLU:HG2   | 79:Ln:48:GLN:HG3    | 1.99                     | 0.44              |
| 86:Lu:105:HIS:O    | 86:Lu:132:ARG:NH2   | 2.50                     | 0.44              |
| 98:L7:16:TRP:CH2   | 98:L7:20:LEU:HD11   | 2.53                     | 0.44              |
| 1:S1:434:G:O2'     | 16:SK:10:LYS:NZ     | 2.49                     | 0.44              |
| 1:S1:1517:G:O2'    | 1:S1:1518:G:H5'     | 2.18                     | 0.44              |
| 1:S1:1767:U:H2'    | 1:S1:1768:C:H6      | 1.82                     | 0.44              |
| 11:SF:159:VAL:HG11 | 11:SF:218:ALA:O     | 2.18                     | 0.44              |
| 21:SP:81:ILE:HD11  | 21:SP:102:VAL:HG21  | 2.00                     | 0.44              |
| 40:LA:2:C:H5'      | 74:Li:63:ARG:HB3    | 1.98                     | 0.44              |
| 40:LA:97:A2M:OP2   | 90:Ly:89:ARG:NH2    | 2.50                     | 0.44              |
| 41:LB:225:C:N3     | 63:LX:80:ARG:NH2    | 2.66                     | 0.44              |
| 42:LC:522:A:OP2    | 100:LC:702:HOH:O    | 2.21                     | 0.44              |
| 44:LE:936:OMC:HM22 | 44:LE:937:G:O4'     | 2.18                     | 0.44              |
| 44:LE:1139:C:H2'   | 44:LE:1140:A:C8     | 2.53                     | 0.44              |
| 44:LE:1401:U:H2'   | 44:LE:1402:G:H8     | 1.82                     | 0.44              |
| 47:LH:2232:G:H2'   | 47:LH:2233:U:H6     | 1.83                     | 0.44              |
| 47:LH:2256:G:H2'   | 47:LH:2257:A:C8     | 2.53                     | 0.44              |
| 47:LH:2707:A:H2'   | 47:LH:2708:A2M:C8   | 2.46                     | 0.44              |
| 47:LH:2850:C:H2'   | 47:LH:2851:A:O4'    | 2.18                     | 0.44              |
| 48:LI:3444:PSU:O4  | 48:LI:3446:PSU:N1   | 2.51                     | 0.44              |
| 53:LN:3979:U:C2    | 53:LN:3981:A:H1'    | 2.52                     | 0.44              |
| 57:LR:124:ALA:HB3  | 57:LR:240:ILE:HG12  | 2.00                     | 0.44              |
| 57:LR:158:THR:O    | 57:LR:162:VAL:HG12  | 2.18                     | 0.44              |
| 59:LT:9:LYS:HG2    | 59:LT:56:ARG:HB3    | 2.00                     | 0.44              |
| 61:LV:115:PHE:HE1  | 61:LV:189:ILE:HG21  | 1.83                     | 0.44              |
| 61:LV:261:LYS:O    | 61:LV:265:LEU:HG    | 2.16                     | 0.44              |
| 65:LZ:66:LEU:HD21  | 65:LZ:86:VAL:HG11   | 2.00                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 69:Ld:181:TYR:HA    | 69:Ld:188:MET:HA   | 2.00                     | 0.44              |
| 80:Lo:19:LYS:HG2    | 80:Lo:23:TRP:HD1   | 1.83                     | 0.44              |
| 84:Ls:25:LYS:HE3    | 84:Ls:25:LYS:HB3   | 1.73                     | 0.44              |
| 90:Ly:31:LYS:O      | 90:Ly:33:ARG:N     | 2.50                     | 0.44              |
| 1:S1:438:A:O2'      | 16:SK:89:ASN:HB3   | 2.18                     | 0.43              |
| 1:S1:1248:C:H2'     | 1:S1:1249:G:C8     | 2.53                     | 0.43              |
| 1:S1:1302:A:H5''    | 20:SO:67:ARG:HG2   | 2.00                     | 0.43              |
| 1:S1:1365:U:H2'     | 1:S1:1366:C:O4'    | 2.18                     | 0.43              |
| 1:S1:1830:U:H3'     | 1:S1:1831:G:H8     | 1.82                     | 0.43              |
| 2:S2:1:G:H1         | 2:S2:72:C:N4       | 2.16                     | 0.43              |
| 7:SB:31:VAL:HG12    | 7:SB:33:GLN:H      | 1.81                     | 0.43              |
| 30:SY:56:GLY:O      | 30:SY:60:ARG:HG3   | 2.18                     | 0.43              |
| 37:Sf:128:GLY:O     | 37:Sf:131:VAL:HG12 | 2.18                     | 0.43              |
| 39:Sh:211:CYS:CB    | 39:Sh:225:LEU:HD21 | 2.48                     | 0.43              |
| 44:LE:869:A:H2'     | 44:LE:870:G:H8     | 1.82                     | 0.43              |
| 45:LF:1773:C:OP1    | 86:Lu:85:ASN:ND2   | 2.51                     | 0.43              |
| 46:LG:2122:C:P      | 75:Lj:91:ARG:HH12  | 2.41                     | 0.43              |
| 47:LH:2959:U:H5''   | 48:LI:2968:G:H5'   | 1.99                     | 0.43              |
| 48:LI:3250:G:H2'    | 48:LI:3250:G:N3    | 2.33                     | 0.43              |
| 53:LN:4043:A:H2'    | 53:LN:4044:G:C8    | 2.53                     | 0.43              |
| 56:LQ:216:VAL:CG1   | 56:LQ:281:ASN:HA   | 2.48                     | 0.43              |
| 61:LV:170:SER:HB3   | 61:LV:226:VAL:HG11 | 2.00                     | 0.43              |
| 64:LY:39:ILE:HG23   | 64:LY:61:VAL:HB    | 2.00                     | 0.43              |
| 65:LZ:152:ILE:H     | 65:LZ:152:ILE:HD12 | 1.83                     | 0.43              |
| 69:Ld:146:THR:HG22  | 69:Ld:157:ILE:HG21 | 2.00                     | 0.43              |
| 79:Ln:100:THR:OG1   | 79:Ln:104:LYS:HG3  | 2.18                     | 0.43              |
| 1:S1:703:A:H2'      | 1:S1:704:OMU:H6    | 1.99                     | 0.43              |
| 1:S1:935:C:H42      | 1:S1:947:C:H42     | 1.67                     | 0.43              |
| 1:S1:1740:G:H21     | 27:SV:8:THR:HG21   | 1.83                     | 0.43              |
| 1:S1:1834:U:H2'     | 1:S1:1835:G:C8     | 2.54                     | 0.43              |
| 3:S3:18:G:H21       | 3:S3:58:A:H61      | 1.66                     | 0.43              |
| 22:SQ:89:GLU:O      | 22:SQ:92:LYS:N     | 2.50                     | 0.43              |
| 41:LB:192:C:H2'     | 41:LB:193:G:O4'    | 2.18                     | 0.43              |
| 42:LC:430:A:H8      | 42:LC:432:C:N4     | 2.16                     | 0.43              |
| 44:LE:1098:G:OP2    | 66:La:39:ARG:HD3   | 2.18                     | 0.43              |
| 45:LF:1768:A:N3     | 57:LR:239:HIS:HE1  | 2.15                     | 0.43              |
| 46:LG:2146:OMG:HM23 | 46:LG:2146:OMG:HI' | 1.80                     | 0.43              |
| 47:LH:2695:A:H2'    | 47:LH:2695:A:N3    | 2.32                     | 0.43              |
| 57:LR:344:TRP:CZ2   | 57:LR:348:VAL:HG11 | 2.54                     | 0.43              |
| 59:LT:114:ILE:HB    | 59:LT:124:ARG:HB2  | 1.99                     | 0.43              |
| 62:LW:187:GLU:OE1   | 65:LZ:209:ILE:HD12 | 2.18                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 75:Lj:69:ILE:HG22   | 75:Lj:158:TYR:CE2  | 2.53                     | 0.43              |
| 83:Lr:100:PRO:HA    | 83:Lr:131:VAL:HG12 | 1.99                     | 0.43              |
| 1:S1:592:C:H2'      | 1:S1:593:C:O4'     | 2.17                     | 0.43              |
| 1:S1:903:U:H3       | 1:S1:919:C:H42     | 1.66                     | 0.43              |
| 1:S1:1284:A:H5''    | 20:SO:135:PRO:HB3  | 2.00                     | 0.43              |
| 1:S1:2037:G:H2'     | 32:Sa:82:ASN:OD1   | 2.18                     | 0.43              |
| 2:S2:56:C:H2'       | 2:S2:57:G:C8       | 2.52                     | 0.43              |
| 8:SC:28:LYS:HB3     | 8:SC:28:LYS:HE2    | 1.66                     | 0.43              |
| 8:SC:159:MET:HE3    | 8:SC:191:MET:HG2   | 1.99                     | 0.43              |
| 31:SZ:60:ILE:HG12   | 31:SZ:80:ILE:HG12  | 2.00                     | 0.43              |
| 39:Sh:278:LEU:HD22  | 39:Sh:288:PRO:CD   | 2.38                     | 0.43              |
| 42:LC:579:A:H4'     | 42:LC:580:A:OP1    | 2.18                     | 0.43              |
| 44:LE:1092:U:H2'    | 44:LE:1093:C:C6    | 2.53                     | 0.43              |
| 45:LF:1768:A:H5'    | 57:LR:199:LYS:HG3  | 1.99                     | 0.43              |
| 46:LG:2208:U:H3'    | 46:LG:2209:C:C6    | 2.53                     | 0.43              |
| 47:LH:2691:U:H2'    | 47:LH:2692:C:H6    | 1.84                     | 0.43              |
| 47:LH:2879:OMG:HM23 | 47:LH:2879:OMG:H1' | 1.59                     | 0.43              |
| 48:LI:3116:U:H2'    | 48:LI:3117:G:H8    | 1.83                     | 0.43              |
| 48:LI:3142:C:H2'    | 48:LI:3143:A:O4'   | 2.19                     | 0.43              |
| 48:LI:3298:U:H2'    | 48:LI:3299:C:H6    | 1.84                     | 0.43              |
| 48:LI:3402:G:C8     | 48:LI:3455:U:H3'   | 2.52                     | 0.43              |
| 49:LJ:3658:C:OP2    | 71:Lf:63:ARG:NH1   | 2.46                     | 0.43              |
| 56:LQ:150:ILE:HG22  | 56:LQ:154:LYS:HE2  | 2.00                     | 0.43              |
| 56:LQ:262:VAL:HG11  | 56:LQ:268:ARG:HH11 | 1.83                     | 0.43              |
| 59:LT:88:PHE:CE2    | 59:LT:153:ILE:HB   | 2.54                     | 0.43              |
| 61:LV:100:ARG:HD2   | 61:LV:100:ARG:HA   | 1.84                     | 0.43              |
| 61:LV:105:ARG:HD3   | 61:LV:273:ARG:O    | 2.19                     | 0.43              |
| 61:LV:208:LYS:HD3   | 89:Lx:44:LEU:HD13  | 2.00                     | 0.43              |
| 64:LY:21:PRO:HA     | 64:LY:54:ALA:HA    | 1.99                     | 0.43              |
| 64:LY:43:LYS:HD3    | 64:LY:62:LEU:CD1   | 2.49                     | 0.43              |
| 73:Lh:155:GLU:HA    | 73:Lh:158:ASN:HD21 | 1.83                     | 0.43              |
| 77:Ll:59:ARG:HB2    | 77:Ll:102:ASN:HB3  | 2.00                     | 0.43              |
| 86:Lu:47:SER:O      | 86:Lu:51:ARG:HG3   | 2.19                     | 0.43              |
| 88:Lw:45:PRO:CG     | 88:Lw:59:VAL:HG21  | 2.47                     | 0.43              |
| 1:S1:74:G:H22       | 12:SG:171:LYS:NZ   | 2.16                     | 0.43              |
| 1:S1:197:C:H2'      | 1:S1:198:C:O4'     | 2.18                     | 0.43              |
| 1:S1:636:G:P        | 9:SD:132:ARG:HH22  | 2.41                     | 0.43              |
| 1:S1:773:U:H2'      | 1:S1:774:G:C8      | 2.53                     | 0.43              |
| 1:S1:891:U:H2'      | 1:S1:892:C:H6      | 1.84                     | 0.43              |
| 1:S1:1414:C:H2'     | 1:S1:1415:G:C8     | 2.53                     | 0.43              |
| 1:S1:1455:G:H1      | 1:S1:1461:U:H3     | 1.66                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:SA:210:VAL:HG23  | 6:SA:210:VAL:O     | 2.18                     | 0.43              |
| 14:SI:72:LEU:HD11  | 14:SI:104:ARG:HG2  | 2.00                     | 0.43              |
| 20:SO:99:ARG:HD3   | 100:SO:201:HOH:O   | 2.19                     | 0.43              |
| 27:SV:78:ARG:O     | 27:SV:81:ARG:HG2   | 2.18                     | 0.43              |
| 28:SW:20:PHE:CE2   | 28:SW:22:TYR:HB2   | 2.53                     | 0.43              |
| 31:SZ:17:MET:HE3   | 31:SZ:17:MET:HB2   | 1.86                     | 0.43              |
| 43:LD:726:C:O2'    | 43:LD:727:C:OP1    | 2.30                     | 0.43              |
| 44:LE:1121:A2M:H1' | 55:LP:15:ILE:HB    | 2.00                     | 0.43              |
| 44:LE:1252:A:H5''  | 82:Lq:15:LYS:HD3   | 2.01                     | 0.43              |
| 45:LF:1527:A:OP1   | 83:Lr:92:GLY:N     | 2.52                     | 0.43              |
| 46:LG:2200:C:OP1   | 71:Lf:17:LYS:NZ    | 2.36                     | 0.43              |
| 47:LH:2384:U:H5''  | 95:L5:8:VAL:HG23   | 1.99                     | 0.43              |
| 47:LH:2646:A:OP2   | 55:LP:156:LYS:NZ   | 2.47                     | 0.43              |
| 47:LH:2761:G:O2'   | 47:LH:2799:G:O6    | 2.29                     | 0.43              |
| 47:LH:2769:A2M:H8  | 47:LH:2769:A2M:H2' | 1.87                     | 0.43              |
| 47:LH:2785:U:O2    | 47:LH:2785:U:H2'   | 2.18                     | 0.43              |
| 47:LH:2849:A2M:H2' | 47:LH:2850:C:H6    | 1.82                     | 0.43              |
| 48:LI:3234:U:O2'   | 48:LI:3320:G:H4'   | 2.18                     | 0.43              |
| 48:LI:3422:C:H2'   | 48:LI:3423:A:O4'   | 2.17                     | 0.43              |
| 49:LJ:3735:C:N4    | 62:LW:105:GLU:O    | 2.46                     | 0.43              |
| 52:LM:3933:G:H5'   | 52:LM:3935:A:H1'   | 2.00                     | 0.43              |
| 56:LQ:231:VAL:HG21 | 56:LQ:251:VAL:HG23 | 2.00                     | 0.43              |
| 57:LR:343:LEU:HG   | 57:LR:347:LYS:HE2  | 2.01                     | 0.43              |
| 65:LZ:133:LYS:O    | 65:LZ:137:LYS:HG2  | 2.18                     | 0.43              |
| 66:La:7:LYS:C      | 66:La:9:LYS:HG3    | 2.43                     | 0.43              |
| 73:Lh:3:HIS:HA     | 73:Lh:5:TRP:CH2    | 2.53                     | 0.43              |
| 1:S1:29:U:H2'      | 1:S1:30:G:C8       | 2.53                     | 0.43              |
| 1:S1:617:U:H4'     | 9:SD:131:GLN:HB3   | 1.99                     | 0.43              |
| 1:S1:1864:U:O2'    | 1:S1:1865:G:N7     | 2.31                     | 0.43              |
| 5:S5:10:C:H5'      | 21:SP:61:GLN:NE2   | 2.33                     | 0.43              |
| 10:SE:136:THR:HG21 | 10:SE:148:ARG:HG2  | 2.00                     | 0.43              |
| 28:SW:98:MET:HE3   | 28:SW:98:MET:HB3   | 1.81                     | 0.43              |
| 34:Sc:64:VAL:HG23  | 34:Sc:76:THR:HG21  | 1.99                     | 0.43              |
| 40:LA:22:G:H1'     | 42:LC:554:A:C4     | 2.53                     | 0.43              |
| 42:LC:396:C:N3     | 42:LC:397:C:N4     | 2.66                     | 0.43              |
| 44:LE:1399:C:H2'   | 44:LE:1400:A:H8    | 1.82                     | 0.43              |
| 46:LG:2184:C:H2'   | 46:LG:2185:C:C6    | 2.53                     | 0.43              |
| 47:LH:2689:G:H2'   | 47:LH:2690:C:C6    | 2.53                     | 0.43              |
| 47:LH:2709:G:N2    | 47:LH:2712:A:OP2   | 2.47                     | 0.43              |
| 47:LH:2788:U:H2'   | 47:LH:2789:U:C6    | 2.53                     | 0.43              |
| 48:LI:3003:C:H3'   | 48:LI:3004:G:C8    | 2.47                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:LI:3203:U:H2'   | 48:LI:3204:PSU:C6  | 2.53                     | 0.43              |
| 48:LI:3553:G:C5'   | 55:LP:220:GLY:HA3  | 2.49                     | 0.43              |
| 56:LQ:160:VAL:HG12 | 56:LQ:193:LYS:HD3  | 2.00                     | 0.43              |
| 63:LX:122:GLU:O    | 63:LX:126:THR:HG23 | 2.17                     | 0.43              |
| 65:LZ:135:LYS:HE2  | 65:LZ:135:LYS:HB3  | 1.75                     | 0.43              |
| 66:La:82:ILE:HD11  | 66:La:137:ALA:HA   | 2.01                     | 0.43              |
| 66:La:131:ARG:NE   | 66:La:152:ALA:O    | 2.47                     | 0.43              |
| 69:Ld:120:GLY:HA3  | 69:Ld:166:ASP:O    | 2.17                     | 0.43              |
| 70:Le:179:ASN:HA   | 70:Le:183:ARG:HG3  | 2.00                     | 0.43              |
| 73:Lh:92:ARG:HB3   | 73:Lh:94:GLU:OE1   | 2.19                     | 0.43              |
| 79:Ln:51:LYS:HB2   | 79:Ln:65:ARG:HB3   | 2.00                     | 0.43              |
| 91:Lz:3:LYS:HE3    | 91:Lz:41:TYR:CZ    | 2.54                     | 0.43              |
| 94:L3:19:MET:HE3   | 94:L3:19:MET:HB2   | 1.90                     | 0.43              |
| 1:S1:357:G:H2'     | 1:S1:358:G:C8      | 2.53                     | 0.43              |
| 1:S1:893:C:H2'     | 1:S1:894:U:O4'     | 2.18                     | 0.43              |
| 1:S1:1007:G:H2'    | 1:S1:1008:G:C8     | 2.50                     | 0.43              |
| 1:S1:1299:G:H2'    | 1:S1:1300:U:C6     | 2.53                     | 0.43              |
| 1:S1:1299:G:O2'    | 1:S1:1405:G:H4'    | 2.18                     | 0.43              |
| 1:S1:1733:C:H2'    | 1:S1:1734:G:O4'    | 2.19                     | 0.43              |
| 1:S1:1779:G:H2'    | 1:S1:1780:G:C8     | 2.53                     | 0.43              |
| 1:S1:2271:A:OP1    | 94:L3:2:GLY:HA3    | 2.17                     | 0.43              |
| 3:S3:75:C:H3'      | 3:S3:76:A:H5''     | 2.00                     | 0.43              |
| 6:SA:29:ASP:N      | 6:SA:92:ARG:O      | 2.44                     | 0.43              |
| 6:SA:218:LEU:HD23  | 6:SA:218:LEU:H     | 1.83                     | 0.43              |
| 8:SC:134:LYS:HE3   | 8:SC:193:PRO:HA    | 1.99                     | 0.43              |
| 38:Sg:104:GLU:O    | 38:Sg:105:PHE:C    | 2.60                     | 0.43              |
| 42:LC:594:A2M:HM'3 | 42:LC:594:A2M:H1'  | 1.88                     | 0.43              |
| 44:LE:1161:C:OP2   | 100:LE:1516:HOH:O  | 2.21                     | 0.43              |
| 44:LE:1248:U:H2'   | 44:LE:1249:C:C6    | 2.52                     | 0.43              |
| 44:LE:1362:C:H2'   | 44:LE:1363:PSU:H6  | 1.84                     | 0.43              |
| 44:LE:1432:C:H5'   | 44:LE:1433:A:C8    | 2.53                     | 0.43              |
| 45:LF:1587:U:H2'   | 45:LF:1588:A:C8    | 2.53                     | 0.43              |
| 45:LF:1833:U:H5''  | 74:Li:68:GLY:HA3   | 2.00                     | 0.43              |
| 47:LH:2255:U:H5''  | 88:Lw:76:THR:HG22  | 2.00                     | 0.43              |
| 47:LH:2677:C:O3'   | 95:L5:21:ASN:HB2   | 2.19                     | 0.43              |
| 47:LH:2706:G:H2'   | 47:LH:2707:A:H8    | 1.84                     | 0.43              |
| 47:LH:2861:A:C6    | 48:LI:3453:C:H1'   | 2.54                     | 0.43              |
| 48:LI:2996:C:N4    | 48:LI:2997:C:O2    | 2.51                     | 0.43              |
| 48:LI:3247:A:H5''  | 58:LS:115:GLY:HA3  | 1.99                     | 0.43              |
| 48:LI:3356:G:O2'   | 48:LI:3357:A:O4'   | 2.33                     | 0.43              |
| 50:LK:3799:G:C4    | 72:Lg:171:TYR:HB2  | 2.53                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 53:LN:3987:A:O2'    | 53:LN:3988:A:H2'   | 2.18                     | 0.43              |
| 56:LQ:21:ARG:O      | 56:LQ:23:ARG:NH2   | 2.51                     | 0.43              |
| 63:LX:69:SER:OG     | 63:LX:70:GLN:N     | 2.52                     | 0.43              |
| 63:LX:181:LEU:HD23  | 63:LX:181:LEU:HA   | 1.87                     | 0.43              |
| 66:La:80:THR:HG23   | 66:La:116:LEU:HD12 | 1.99                     | 0.43              |
| 77:Ll:27:ARG:O      | 77:Ll:48:PRO:HB3   | 2.19                     | 0.43              |
| 79:Ln:5:LEU:HD21    | 79:Ln:82:PRO:HG3   | 2.00                     | 0.43              |
| 79:Ln:102:PRO:O     | 79:Ln:106:THR:HG23 | 2.18                     | 0.43              |
| 83:Lr:191:CYS:O     | 83:Lr:195:PHE:HB2  | 2.18                     | 0.43              |
| 1:S1:15:U:H2'       | 1:S1:16:G:O4'      | 2.17                     | 0.43              |
| 1:S1:664:U:H2'      | 1:S1:665:G:C8      | 2.54                     | 0.43              |
| 1:S1:714:G:H2'      | 1:S1:718:C:C5      | 2.53                     | 0.43              |
| 1:S1:729:C:H2'      | 1:S1:730:U:H6      | 1.82                     | 0.43              |
| 1:S1:1662:C:H5'     | 37:Sf:106:PHE:CZ   | 2.54                     | 0.43              |
| 1:S1:1944:C:OP1     | 23:SR:125:ARG:NH2  | 2.52                     | 0.43              |
| 1:S1:2016:G:O2'     | 1:S1:2018:A:N3     | 2.41                     | 0.43              |
| 1:S1:2056:G:N7      | 28:SW:52:ARG:NH1   | 2.56                     | 0.43              |
| 3:S3:75:C:H3'       | 3:S3:76:A:C5'      | 2.48                     | 0.43              |
| 12:SG:1:MET:HE3     | 12:SG:108:ILE:HB   | 2.01                     | 0.43              |
| 17:SL:150:TYR:O     | 17:SL:151:ARG:HG2  | 2.19                     | 0.43              |
| 23:SR:37:ILE:HG12   | 23:SR:72:MET:HE3   | 2.00                     | 0.43              |
| 38:Sg:56:ARG:HH21   | 38:Sg:91:ILE:HD12  | 1.82                     | 0.43              |
| 39:Sh:177:VAL:HG12  | 39:Sh:193:LEU:HD23 | 2.01                     | 0.43              |
| 39:Sh:205:SER:HA    | 39:Sh:245:PHE:CD2  | 2.53                     | 0.43              |
| 41:LB:254:G:H2'     | 41:LB:255:A:C8     | 2.53                     | 0.43              |
| 41:LB:259:A:OP1     | 67:Lb:195:ARG:HD2  | 2.18                     | 0.43              |
| 42:LC:558:G:O6      | 90:Ly:55:ARG:NH1   | 2.52                     | 0.43              |
| 44:LE:1081:OMU:HM23 | 44:LE:1081:OMU:H1' | 1.45                     | 0.43              |
| 44:LE:1185:OMU:HM23 | 44:LE:1185:OMU:H1' | 1.63                     | 0.43              |
| 45:LF:1497:U:H2'    | 45:LF:1498:A:O4'   | 2.19                     | 0.43              |
| 46:LG:2127:C:H2'    | 46:LG:2128:C:H6    | 1.83                     | 0.43              |
| 48:LI:3486:C:OP2    | 100:LI:3609:HOH:O  | 2.21                     | 0.43              |
| 49:LJ:3710:C:O2'    | 49:LJ:3711:U:H2'   | 2.18                     | 0.43              |
| 55:LP:83:TYR:O      | 55:LP:86:GLN:HB2   | 2.19                     | 0.43              |
| 56:LQ:19:ARG:NH2    | 56:LQ:234:ARG:HG2  | 2.33                     | 0.43              |
| 60:LU:183:THR:HB    | 87:Lv:6:VAL:HG23   | 2.00                     | 0.43              |
| 61:LV:179:VAL:HG13  | 61:LV:211:ILE:HD12 | 2.01                     | 0.43              |
| 63:LX:119:LEU:HD11  | 63:LX:168:TYR:CD2  | 2.53                     | 0.43              |
| 63:LX:123:ARG:HG3   | 63:LX:162:PHE:CE1  | 2.53                     | 0.43              |
| 67:Lb:119:TYR:OH    | 67:Lb:131:GLU:OE1  | 2.29                     | 0.43              |
| 69:Ld:75:ALA:HB2    | 69:Ld:111:LYS:HD3  | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:L1:71:ALA:HB3   | 77:L1:80:HIS:HB2   | 2.00                     | 0.43              |
| 1:S1:88:G:H2'      | 1:S1:89:PSU:O4'    | 2.18                     | 0.43              |
| 1:S1:600:G:H2'     | 1:S1:601:C:C6      | 2.53                     | 0.43              |
| 1:S1:1282:A:H2'    | 1:S1:1283:U:C6     | 2.53                     | 0.43              |
| 1:S1:1718:G:H2'    | 1:S1:1719:G:H8     | 1.83                     | 0.43              |
| 1:S1:1918:G:H4'    | 24:SS:25:ASN:ND2   | 2.33                     | 0.43              |
| 1:S1:2279:U:H2'    | 1:S1:2280:G:C8     | 2.54                     | 0.43              |
| 6:SA:193:LYS:NZ    | 6:SA:197:THR:OG1   | 2.51                     | 0.43              |
| 8:SC:142:GLY:HA3   | 8:SC:184:LEU:HD23  | 2.00                     | 0.43              |
| 10:SE:56:LEU:HD23  | 31:SZ:24:ARG:NH2   | 2.34                     | 0.43              |
| 38:Sg:214:LYS:HE2  | 38:Sg:214:LYS:HB2  | 1.72                     | 0.43              |
| 39:Sh:146:ILE:HD13 | 39:Sh:146:ILE:HA   | 1.89                     | 0.43              |
| 39:Sh:253:CYS:HA   | 39:Sh:262:ILE:HA   | 2.00                     | 0.43              |
| 40:LA:6:U:H2'      | 40:LA:7:U:C6       | 2.54                     | 0.43              |
| 40:LA:74:OMG:H1'   | 40:LA:74:OMG:HM23  | 1.67                     | 0.43              |
| 42:LC:363:G:H2'    | 42:LC:364:C:C5     | 2.54                     | 0.43              |
| 42:LC:610:G:OP1    | 45:LF:1799:U:O2'   | 2.31                     | 0.43              |
| 44:LE:766:G:H2'    | 44:LE:767:C:C6     | 2.54                     | 0.43              |
| 44:LE:815:C:C2     | 44:LE:831:G:N2     | 2.87                     | 0.43              |
| 44:LE:1095:U:H2'   | 44:LE:1096:U:C6    | 2.54                     | 0.43              |
| 47:LH:2405:A:N1    | 47:LH:2587:C:O2'   | 2.50                     | 0.43              |
| 48:LI:3167:PSU:H2' | 48:LI:3168:C:C6    | 2.54                     | 0.43              |
| 48:LI:3298:U:H2'   | 48:LI:3299:C:C6    | 2.54                     | 0.43              |
| 48:LI:3530:G:H2'   | 48:LI:3531:PSU:O4' | 2.19                     | 0.43              |
| 51:LL:3903:A:H3'   | 87:Lv:63:ARG:HG3   | 2.01                     | 0.43              |
| 52:LM:3926:C:O2    | 74:Li:71:ARG:HD2   | 2.18                     | 0.43              |
| 55:LP:107:MET:HE2  | 55:LP:166:ILE:HD11 | 2.01                     | 0.43              |
| 56:LQ:57:VAL:HG11  | 78:Lm:1:MET:HG3    | 2.00                     | 0.43              |
| 67:Lb:26:ARG:HA    | 67:Lb:29:GLU:HG2   | 2.01                     | 0.43              |
| 73:Lh:43:VAL:HG11  | 73:Lh:97:ARG:NH2   | 2.34                     | 0.43              |
| 83:Lr:146:ARG:HG2  | 83:Lr:185:ILE:HG21 | 2.00                     | 0.43              |
| 85:Lt:49:SER:HB3   | 85:Lt:149:ILE:HD13 | 2.00                     | 0.43              |
| 86:Lu:13:LYS:O     | 86:Lu:17:LYS:HG2   | 2.17                     | 0.43              |
| 92:L1:23:ILE:HG22  | 92:L1:24:PRO:O     | 2.17                     | 0.43              |
| 1:S1:34:U:O4       | 1:S1:698:G:H2'     | 2.19                     | 0.43              |
| 1:S1:1377:G:H4'    | 1:S1:2282:A:H4'    | 2.01                     | 0.43              |
| 1:S1:2219:C:H2'    | 1:S1:2220:C:C6     | 2.53                     | 0.43              |
| 1:S1:2224:C:H2'    | 1:S1:2225:C:C6     | 2.54                     | 0.43              |
| 4:S4:9:A:C4        | 4:S4:46:G:H1'      | 2.54                     | 0.43              |
| 7:SB:158:ASP:OD1   | 30:SY:59:ARG:NE    | 2.52                     | 0.43              |
| 12:SG:27:LEU:HD23  | 12:SG:30:LYS:HG3   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:SO:100:ALA:N    | 20:SO:134:THR:HG22 | 2.17                     | 0.43              |
| 42:LC:541:OMG:HM23 | 42:LC:541:OMG:H1'  | 1.45                     | 0.43              |
| 42:LC:594:A2M:H8   | 42:LC:594:A2M:O5'  | 2.18                     | 0.43              |
| 43:LD:734:G:H2'    | 43:LD:735:C:C6     | 2.54                     | 0.43              |
| 44:LE:949:OMC:HM23 | 44:LE:949:OMC:H1'  | 1.64                     | 0.43              |
| 44:LE:1431:A:O2'   | 44:LE:1432:C:P     | 2.76                     | 0.43              |
| 45:LF:1678:G:O2'   | 45:LF:1679:G:H5''  | 2.19                     | 0.43              |
| 45:LF:1862:C:H2'   | 45:LF:1863:A:N9    | 2.33                     | 0.43              |
| 47:LH:2370:U:H2'   | 47:LH:2371:G:O4'   | 2.18                     | 0.43              |
| 47:LH:2956:A:N6    | 48:LI:2976:C:H41   | 2.16                     | 0.43              |
| 48:LI:3304:U:H2'   | 48:LI:3305:A:C8    | 2.54                     | 0.43              |
| 49:LJ:3634:A:O3'   | 56:LQ:13:ASN:HB2   | 2.19                     | 0.43              |
| 52:LM:3940:C:OP1   | 85:Lt:110:ARG:NH1  | 2.52                     | 0.43              |
| 52:LM:3945:A:OP2   | 56:LQ:380:LYS:NZ   | 2.37                     | 0.43              |
| 55:LP:206:PRO:HD3  | 55:LP:213:GLY:HA3  | 2.01                     | 0.43              |
| 58:LS:23:ARG:NH2   | 58:LS:142:GLU:OE2  | 2.35                     | 0.43              |
| 60:LU:37:GLU:HG2   | 60:LU:38:HIS:N     | 2.33                     | 0.43              |
| 61:LV:106:LEU:HD12 | 67:Lb:25:ILE:HD11  | 2.00                     | 0.43              |
| 73:Lh:100:ARG:HD3  | 98:L7:18:TYR:HB2   | 2.01                     | 0.43              |
| 79:Ln:75:VAL:CG1   | 79:Ln:80:LEU:HD21  | 2.49                     | 0.43              |
| 83:Lr:90:ILE:O     | 83:Lr:217:LYS:HE2  | 2.18                     | 0.43              |
| 1:S1:2087:G:N7     | 17:SL:22:LYS:HE2   | 2.33                     | 0.43              |
| 1:S1:2230:U:H4'    | 78:Lm:51:ARG:NH1   | 2.34                     | 0.43              |
| 4:S4:22:G:C5       | 4:S4:46:G:N2       | 2.86                     | 0.43              |
| 7:SB:60:LEU:O      | 7:SB:64:VAL:HG23   | 2.19                     | 0.43              |
| 10:SE:185:SER:OG   | 10:SE:186:GLY:N    | 2.51                     | 0.43              |
| 10:SE:239:LEU:HD12 | 10:SE:240:PRO:HD2  | 2.01                     | 0.43              |
| 12:SG:111:LEU:HD23 | 12:SG:111:LEU:HA   | 1.79                     | 0.43              |
| 13:SH:169:GLY:C    | 13:SH:171:SER:H    | 2.26                     | 0.43              |
| 22:SQ:68:ALA:HA    | 22:SQ:71:ARG:HG2   | 2.00                     | 0.43              |
| 25:ST:26:LEU:HD11  | 25:ST:59:GLY:O     | 2.19                     | 0.43              |
| 26:SU:41:LYS:HE3   | 26:SU:64:PRO:O     | 2.19                     | 0.43              |
| 29:SX:27:LYS:HE2   | 29:SX:27:LYS:HB3   | 1.84                     | 0.43              |
| 38:Sg:236:ARG:HH21 | 38:Sg:239:SER:HB2  | 1.84                     | 0.43              |
| 40:LA:16:PSU:H2'   | 40:LA:17:G:C8      | 2.53                     | 0.43              |
| 40:LA:62:G:H4'     | 81:Lp:52:ARG:CZ    | 2.49                     | 0.43              |
| 40:LA:74:OMG:H5'   | 92:L1:30:LYS:HA    | 2.00                     | 0.43              |
| 41:LB:275:G:C6     | 81:Lp:116:MET:HG2  | 2.54                     | 0.43              |
| 42:LC:349:G:H2'    | 42:LC:350:G:C8     | 2.54                     | 0.43              |
| 44:LE:1004:A:H2'   | 44:LE:1005:G:C8    | 2.54                     | 0.43              |
| 44:LE:1310:U:H2'   | 44:LE:1311:C:H6    | 1.84                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 44:LE:1386:C:O2     | 73:Lh:126:ARG:NH1  | 2.35                     | 0.43              |
| 44:LE:1403:C:H2'    | 44:LE:1404:U:C6    | 2.54                     | 0.43              |
| 46:LG:2009:OMG:HM23 | 46:LG:2009:OMG:H1' | 1.69                     | 0.43              |
| 47:LH:2887:A2M:HM'3 | 47:LH:2887:A2M:H1' | 1.68                     | 0.43              |
| 48:LI:3005:U:H2'    | 48:LI:3006:U:C6    | 2.54                     | 0.43              |
| 49:LJ:3681:A:O2'    | 49:LJ:3683:C:H2'   | 2.19                     | 0.43              |
| 53:LN:3969:PSU:H2'  | 53:LN:3970:C:C6    | 2.54                     | 0.43              |
| 68:Lc:55:MET:HB2    | 68:Lc:162:ARG:HG2  | 1.99                     | 0.43              |
| 71:Lf:72:LEU:HD23   | 71:Lf:72:LEU:HA    | 1.90                     | 0.43              |
| 72:Lg:64:ILE:HG23   | 72:Lg:65:ARG:H     | 1.84                     | 0.43              |
| 74:Li:26:VAL:HG11   | 74:Li:89:SER:HA    | 2.01                     | 0.43              |
| 81:Lp:29:ALA:O      | 81:Lp:33:VAL:HG23  | 2.19                     | 0.43              |
| 1:S1:84:A:O2'       | 31:SZ:124:GLY:HA2  | 2.19                     | 0.42              |
| 1:S1:171:A:O2'      | 1:S1:173:A:N7      | 2.44                     | 0.42              |
| 1:S1:1601:B8N:O2    | 1:S1:2140:C:N4     | 2.52                     | 0.42              |
| 1:S1:1637:G:O3'     | 22:SQ:42:GLY:HA2   | 2.18                     | 0.42              |
| 1:S1:1900:A2M:HM'3  | 1:S1:1900:A2M:H1'  | 1.84                     | 0.42              |
| 6:SA:121:ALA:HB1    | 6:SA:167:PHE:HE1   | 1.84                     | 0.42              |
| 11:SF:142:ARG:HG2   | 11:SF:194:VAL:HG12 | 2.01                     | 0.42              |
| 15:SJ:77:PRO:HD3    | 21:SP:6:GLY:H      | 1.84                     | 0.42              |
| 23:SR:13:ILE:HD12   | 58:LS:127:ASP:OD2  | 2.19                     | 0.42              |
| 35:Sd:20:ILE:HD11   | 35:Sd:36:ARG:HG2   | 2.01                     | 0.42              |
| 35:Sd:49:ILE:HD12   | 35:Sd:51:ARG:HD3   | 2.01                     | 0.42              |
| 37:Sf:124:HIS:NE2   | 37:Sf:147:LEU:HD13 | 2.33                     | 0.42              |
| 42:LC:556:A:N7      | 92:L1:35:GLN:HG2   | 2.34                     | 0.42              |
| 45:LF:1689:A:H5''   | 62:LW:133:ARG:HH12 | 1.84                     | 0.42              |
| 45:LF:1789:U:O2'    | 86:Lu:60:VAL:HG13  | 2.19                     | 0.42              |
| 45:LF:1924:C:H2'    | 45:LF:1925:G:C8    | 2.54                     | 0.42              |
| 46:LG:2014:U:H5'    | 46:LG:2133:G:H1'   | 2.01                     | 0.42              |
| 46:LG:2130:C:H2'    | 46:LG:2219:A:C8    | 2.55                     | 0.42              |
| 46:LG:2131:C:O2'    | 46:LG:2132:U:H5'   | 2.19                     | 0.42              |
| 47:LH:2242:OMC:HM23 | 47:LH:2242:OMC:H1' | 1.56                     | 0.42              |
| 47:LH:2673:G:H5'    | 55:LP:219:ILE:HD11 | 2.00                     | 0.42              |
| 47:LH:2849:A2M:H8   | 47:LH:2849:A2M:O5' | 2.19                     | 0.42              |
| 47:LH:2922:U:H4'    | 47:LH:2923:G:O5'   | 2.19                     | 0.42              |
| 48:LI:3257:C:H2'    | 48:LI:3258:C:H6    | 1.80                     | 0.42              |
| 48:LI:3273:C:H2'    | 48:LI:3274:C:C6    | 2.54                     | 0.42              |
| 49:LJ:3695:A:H2'    | 49:LJ:3696:C:C6    | 2.54                     | 0.42              |
| 54:LO:55:A:H4'      | 58:LS:162:HIS:HB2  | 2.01                     | 0.42              |
| 55:LP:176:GLU:OE1   | 55:LP:176:GLU:N    | 2.52                     | 0.42              |
| 58:LS:167:LYS:HE3   | 58:LS:167:LYS:HB2  | 1.74                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 63:LX:204:VAL:O    | 63:LX:208:ILE:HG13  | 2.19                     | 0.42              |
| 71:Lf:106:MET:SD   | 71:Lf:136:LYS:HG3   | 2.59                     | 0.42              |
| 86:Lu:96:ASN:OD1   | 86:Lu:96:ASN:N      | 2.52                     | 0.42              |
| 92:L1:43:HIS:HB3   | 92:L1:46:ARG:HG3    | 2.01                     | 0.42              |
| 1:S1:393:OMC:HM23  | 1:S1:393:OMC:H1'    | 1.70                     | 0.42              |
| 1:S1:774:G:C6      | 1:S1:828:G:O6       | 2.71                     | 0.42              |
| 1:S1:943:C:H4'     | 1:S1:944:U:H5'      | 2.01                     | 0.42              |
| 1:S1:1035:A:H2'    | 1:S1:1036:A:H8      | 1.83                     | 0.42              |
| 1:S1:1343:U:H2'    | 1:S1:1344:C:C6      | 2.54                     | 0.42              |
| 1:S1:1350:G:H2'    | 1:S1:1351:U:H6      | 1.84                     | 0.42              |
| 1:S1:1603:A:H5'    | 18:SM:76:THR:HG23   | 2.00                     | 0.42              |
| 1:S1:2246:C:H2'    | 1:S1:2247:A:C8      | 2.54                     | 0.42              |
| 4:S4:72:C:H2'      | 4:S4:73:A:O4'       | 2.19                     | 0.42              |
| 7:SB:110:ASN:HB3   | 7:SB:113:GLN:HB2    | 2.01                     | 0.42              |
| 7:SB:118:GLN:NE2   | 11:SF:37:THR:OG1    | 2.45                     | 0.42              |
| 8:SC:195:ASP:OD2   | 8:SC:199:LYS:N      | 2.52                     | 0.42              |
| 10:SE:87:MET:HG2   | 10:SE:123:LEU:O     | 2.19                     | 0.42              |
| 11:SF:231:TRP:N    | 11:SF:232:PRO:HD2   | 2.33                     | 0.42              |
| 14:SI:77:LYS:O     | 14:SI:81:ILE:HG13   | 2.19                     | 0.42              |
| 19:SN:88:SER:HA    | 19:SN:91:LYS:CG     | 2.49                     | 0.42              |
| 20:SO:44:HIS:CD2   | 20:SO:56:ARG:HB3    | 2.54                     | 0.42              |
| 28:SW:49:LYS:HD3   | 28:SW:89:VAL:HG23   | 2.01                     | 0.42              |
| 31:SZ:29:ILE:HD11  | 31:SZ:62:LEU:HD22   | 2.00                     | 0.42              |
| 41:LB:205:A:OP2    | 67:Lb:85:LYS:HD3    | 2.19                     | 0.42              |
| 42:LC:497:U:H2'    | 42:LC:498:PSU:O4'   | 2.19                     | 0.42              |
| 42:LC:626:C:OP2    | 42:LC:627:G:O2'     | 2.33                     | 0.42              |
| 43:LD:653:A:H2'    | 43:LD:654:A:C8      | 2.54                     | 0.42              |
| 44:LE:926:U:H2'    | 44:LE:927:C:C6      | 2.54                     | 0.42              |
| 44:LE:1402:G:H2'   | 44:LE:1403:C:C6     | 2.54                     | 0.42              |
| 44:LE:1452:OMU:H1' | 44:LE:1452:OMU:HM23 | 1.80                     | 0.42              |
| 45:LF:1811:C:H4'   | 57:LR:36:THR:HB     | 2.01                     | 0.42              |
| 46:LG:2085:U:H2'   | 46:LG:2086:C:C6     | 2.55                     | 0.42              |
| 47:LH:2293:U:H2'   | 47:LH:2294:G:O4'    | 2.19                     | 0.42              |
| 48:LI:3273:C:H5''  | 73:Lh:17:LYS:HG2    | 2.00                     | 0.42              |
| 51:LL:3827:G:H2'   | 51:LL:3828:C:C6     | 2.55                     | 0.42              |
| 56:LQ:208:ASP:HB3  | 56:LQ:287:ILE:HG21  | 2.00                     | 0.42              |
| 60:LU:101:ARG:HD3  | 60:LU:101:ARG:H     | 1.84                     | 0.42              |
| 62:LW:156:LYS:HE3  | 62:LW:156:LYS:HB3   | 1.72                     | 0.42              |
| 62:LW:208:SER:O    | 62:LW:209:LEU:HB3   | 2.18                     | 0.42              |
| 66:La:92:GLU:OE2   | 66:La:93:GLN:HG3    | 2.19                     | 0.42              |
| 1:S1:356:U:OP1     | 100:SG:301:HOH:O    | 2.21                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:S1:742:U:O2'      | 14:SI:109:GLN:NE2  | 2.32                     | 0.42              |
| 1:S1:896:C:H2'      | 1:S1:897:C:N1      | 2.34                     | 0.42              |
| 1:S1:1557:A:O2'     | 1:S1:2139:C:OP2    | 2.28                     | 0.42              |
| 1:S1:1951:A:H2'     | 1:S1:1952:C:C6     | 2.54                     | 0.42              |
| 1:S1:2265:C:H2'     | 1:S1:2266:G:O4'    | 2.20                     | 0.42              |
| 3:S3:24:G:H2'       | 3:S3:25:C:O4'      | 2.19                     | 0.42              |
| 11:SF:67:VAL:CG2    | 11:SF:134:LYS:HB3  | 2.50                     | 0.42              |
| 13:SH:106:GLY:HA3   | 13:SH:132:ARG:HG2  | 2.00                     | 0.42              |
| 14:SI:71:PRO:HD2    | 14:SI:74:PHE:HE1   | 1.84                     | 0.42              |
| 38:Sg:253:ALA:O     | 38:Sg:256:THR:OG1  | 2.33                     | 0.42              |
| 41:LB:189:C:OP1     | 67:Lb:190:ALA:HB2  | 2.19                     | 0.42              |
| 42:LC:305:G:H1      | 90:Ly:81:ASP:CG    | 2.27                     | 0.42              |
| 42:LC:568:C:OP2     | 90:Ly:56:ARG:NH1   | 2.48                     | 0.42              |
| 44:LE:1163:G:H2'    | 44:LE:1164:U:O2    | 2.19                     | 0.42              |
| 44:LE:1329:A:H2'    | 44:LE:1330:G:C8    | 2.55                     | 0.42              |
| 44:LE:1372:A:H5''   | 44:LE:1373:C:H5''  | 2.00                     | 0.42              |
| 47:LH:2368:A:H2'    | 47:LH:2369:C:H6    | 1.83                     | 0.42              |
| 47:LH:2842:PSU:H2'  | 47:LH:2843:G:C8    | 2.54                     | 0.42              |
| 48:LI:3306:C:H2'    | 48:LI:3307:G:O4'   | 2.19                     | 0.42              |
| 48:LI:3377:OMG:HM23 | 48:LI:3377:OMG:H1' | 1.87                     | 0.42              |
| 51:LL:3871:G:N7     | 100:LL:4001:HOH:O  | 2.36                     | 0.42              |
| 61:LV:156:ASP:N     | 61:LV:157:PRO:HD2  | 2.34                     | 0.42              |
| 62:LW:204:ILE:HD12  | 65:LZ:112:GLU:HG3  | 2.01                     | 0.42              |
| 69:Ld:230:LYS:O     | 69:Ld:233:GLU:HG2  | 2.19                     | 0.42              |
| 70:Le:67:LEU:HD23   | 70:Le:67:LEU:HA    | 1.81                     | 0.42              |
| 84:Ls:30:TYR:HA     | 84:Ls:92:MET:HG3   | 2.02                     | 0.42              |
| 1:S1:34:U:H2'       | 1:S1:35:G:C8       | 2.52                     | 0.42              |
| 1:S1:432:C:H2'      | 1:S1:433:G:O4'     | 2.19                     | 0.42              |
| 1:S1:493:G:O6       | 16:SK:26:LYS:HE3   | 2.19                     | 0.42              |
| 1:S1:495:G:P        | 16:SK:49:ARG:HH22  | 2.41                     | 0.42              |
| 1:S1:583:C:H2'      | 1:S1:584:C:C6      | 2.54                     | 0.42              |
| 1:S1:1249:G:H3'     | 1:S1:1250:A:C2     | 2.54                     | 0.42              |
| 6:SA:191:ILE:H      | 6:SA:191:ILE:HD12  | 1.83                     | 0.42              |
| 7:SB:78:SER:HB3     | 7:SB:87:ILE:HD13   | 2.01                     | 0.42              |
| 7:SB:141:ASN:OD1    | 30:SY:29:HIS:HA    | 2.20                     | 0.42              |
| 10:SE:223:ASP:OD1   | 10:SE:223:ASP:N    | 2.46                     | 0.42              |
| 11:SF:43:VAL:HG21   | 11:SF:66:ILE:HG12  | 2.00                     | 0.42              |
| 12:SG:58:LYS:O      | 12:SG:59:GLN:HB2   | 2.19                     | 0.42              |
| 12:SG:68:LEU:HD23   | 12:SG:102:CYS:SG   | 2.59                     | 0.42              |
| 16:SK:67:PHE:O      | 16:SK:75:ALA:HA    | 2.19                     | 0.42              |
| 26:SU:17:ILE:HD13   | 26:SU:17:ILE:HA    | 1.93                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:SV:45:ARG:O     | 27:SV:49:LYS:HG3   | 2.19                     | 0.42              |
| 28:SW:98:MET:SD    | 28:SW:111:GLU:HB2  | 2.58                     | 0.42              |
| 29:SX:21:TYR:CD1   | 29:SX:137:ILE:HD12 | 2.55                     | 0.42              |
| 42:LC:413:C:H41    | 45:LF:1775:G:H2'   | 1.84                     | 0.42              |
| 42:LC:475:U:H2'    | 42:LC:476:A:H8     | 1.84                     | 0.42              |
| 42:LC:609:U:H4'    | 45:LF:1800:U:H4'   | 2.01                     | 0.42              |
| 44:LE:913:U:H2'    | 44:LE:914:G:H8     | 1.84                     | 0.42              |
| 44:LE:929:C:H2'    | 44:LE:930:G:O4'    | 2.19                     | 0.42              |
| 44:LE:1022:A:H4'   | 44:LE:1277:C:O5'   | 2.19                     | 0.42              |
| 44:LE:1179:G:O6    | 44:LE:1182:A:H5'   | 2.19                     | 0.42              |
| 55:LP:104:LEU:HD12 | 55:LP:107:MET:SD   | 2.59                     | 0.42              |
| 56:LQ:90:VAL:HG23  | 56:LQ:161:ARG:HB2  | 2.00                     | 0.42              |
| 56:LQ:221:GLY:HA3  | 56:LQ:340:MET:SD   | 2.60                     | 0.42              |
| 56:LQ:289:LYS:HA   | 56:LQ:289:LYS:HD3  | 1.71                     | 0.42              |
| 58:LS:9:SER:O      | 58:LS:13:LYS:HG2   | 2.19                     | 0.42              |
| 70:Le:65:ILE:HD13  | 70:Le:138:ILE:HD11 | 2.01                     | 0.42              |
| 83:Lr:63:LEU:O     | 83:Lr:67:ARG:HG3   | 2.18                     | 0.42              |
| 92:L1:44:TRP:CZ3   | 92:L1:45:ARG:HD3   | 2.54                     | 0.42              |
| 1:S1:2:A:H3'       | 11:SF:180:VAL:HG11 | 2.01                     | 0.42              |
| 1:S1:182:C:H4'     | 12:SG:133:ARG:HD3  | 2.01                     | 0.42              |
| 1:S1:404:C:H2'     | 1:S1:405:U:C6      | 2.55                     | 0.42              |
| 1:S1:1686:U:OP1    | 8:SC:148:ARG:HG3   | 2.19                     | 0.42              |
| 1:S1:1954:A:H2'    | 1:S1:1955:C:C6     | 2.55                     | 0.42              |
| 1:S1:2034:G:H2'    | 1:S1:2035:A:H8     | 1.83                     | 0.42              |
| 2:S2:28:G:P        | 36:Se:3:LYS:HZ3    | 2.42                     | 0.42              |
| 2:S2:37:MIA:H2'    | 2:S2:38:A:H8       | 1.83                     | 0.42              |
| 3:S3:6:G:O2'       | 3:S3:7:A:OP1       | 2.34                     | 0.42              |
| 4:S4:53:G:H2'      | 4:S4:55:U:OP2      | 2.19                     | 0.42              |
| 8:SC:160:ILE:HG12  | 8:SC:191:MET:SD    | 2.60                     | 0.42              |
| 9:SD:170:GLY:O     | 9:SD:174:ARG:HB3   | 2.19                     | 0.42              |
| 12:SG:75:LEU:O     | 12:SG:96:ARG:HA    | 2.20                     | 0.42              |
| 12:SG:168:ASP:OD1  | 12:SG:168:ASP:N    | 2.53                     | 0.42              |
| 13:SH:60:ASN:HA    | 13:SH:63:MET:HG2   | 2.00                     | 0.42              |
| 14:SI:104:ARG:CZ   | 14:SI:129:ASN:HB3  | 2.49                     | 0.42              |
| 16:SK:295:LYS:O    | 16:SK:299:LYS:HG2  | 2.20                     | 0.42              |
| 28:SW:72:ALA:HB1   | 28:SW:76:GLU:HG2   | 2.01                     | 0.42              |
| 38:Sg:240:GLU:O    | 38:Sg:244:LYS:HG3  | 2.19                     | 0.42              |
| 40:LA:65:C:H2'     | 40:LA:66:G:H8      | 1.85                     | 0.42              |
| 42:LC:396:C:H2'    | 42:LC:397:C:C5     | 2.54                     | 0.42              |
| 42:LC:402:A:H4'    | 42:LC:404:A:N7     | 2.35                     | 0.42              |
| 44:LE:1027:G:H2'   | 44:LE:1028:C:O4'   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:LF:1696:U:H4'   | 72:Lg:4:PHE:HE2    | 1.85                     | 0.42              |
| 45:LF:1845:C:H5'   | 85:Lt:91:ILE:O     | 2.20                     | 0.42              |
| 45:LF:1939:A:OP1   | 76:Lk:113:LYS:NZ   | 2.42                     | 0.42              |
| 47:LH:2253:C:O2    | 88:Lw:67:ARG:NH1   | 2.52                     | 0.42              |
| 47:LH:2360:G:OP1   | 100:LH:3013:HOH:O  | 2.22                     | 0.42              |
| 55:LP:44:VAL:HG22  | 55:LP:87:TYR:HE1   | 1.84                     | 0.42              |
| 56:LQ:292:LEU:HD11 | 56:LQ:322:ARG:HB2  | 2.00                     | 0.42              |
| 59:LT:18:VAL:HG22  | 59:LT:27:VAL:HG22  | 2.01                     | 0.42              |
| 60:LU:86:ARG:C     | 60:LU:88:LYS:H     | 2.27                     | 0.42              |
| 60:LU:127:LYS:HE2  | 60:LU:140:GLU:OE1  | 2.20                     | 0.42              |
| 61:LV:295:LYS:HB2  | 61:LV:295:LYS:HE2  | 1.76                     | 0.42              |
| 69:Ld:94:PHE:CG    | 69:Ld:196:ARG:HG2  | 2.55                     | 0.42              |
| 70:Le:188:ALA:O    | 70:Le:189:PHE:HB3  | 2.19                     | 0.42              |
| 75:Lj:63:TYR:CD1   | 75:Lj:152:THR:HA   | 2.55                     | 0.42              |
| 82:Lq:61:GLU:HG2   | 82:Lq:65:LYS:HD3   | 2.01                     | 0.42              |
| 86:Lu:81:PHE:HB3   | 86:Lu:92:LEU:HD11  | 2.00                     | 0.42              |
| 90:Ly:21:ARG:HH11  | 90:Ly:39:TYR:HA    | 1.84                     | 0.42              |
| 1:S1:740:C:H5''    | 15:SJ:31:SER:OG    | 2.20                     | 0.42              |
| 1:S1:1414:C:C2     | 1:S1:1415:G:C8     | 3.07                     | 0.42              |
| 1:S1:1726:C:O2'    | 27:SV:10:LYS:HE3   | 2.19                     | 0.42              |
| 1:S1:1748:C:H1'    | 1:S1:1895:A:C5     | 2.55                     | 0.42              |
| 1:S1:1935:C:H2'    | 1:S1:1936:C:C6     | 2.54                     | 0.42              |
| 1:S1:1954:A:H4'    | 1:S1:2044:G:H4'    | 2.01                     | 0.42              |
| 1:S1:2087:G:O2'    | 1:S1:2113:G:O6     | 2.36                     | 0.42              |
| 3:S3:53:G:H2'      | 3:S3:53:G:N3       | 2.34                     | 0.42              |
| 3:S3:59:U:H2'      | 3:S3:60:U:O4'      | 2.19                     | 0.42              |
| 13:SH:88:LEU:HD21  | 32:Sa:102:VAL:HG21 | 2.01                     | 0.42              |
| 23:SR:17:LEU:HD11  | 23:SR:100:VAL:HG12 | 2.02                     | 0.42              |
| 39:Sh:91:MET:HB2   | 39:Sh:105:PHE:HB2  | 2.01                     | 0.42              |
| 39:Sh:289:GLU:O    | 39:Sh:291:ILE:HG13 | 2.20                     | 0.42              |
| 41:LB:169:C:H2'    | 41:LB:170:U:O4'    | 2.20                     | 0.42              |
| 42:LC:313:U:H2'    | 42:LC:314:G:O4'    | 2.20                     | 0.42              |
| 44:LE:765:C:H1'    | 83:Lr:43:LYS:NZ    | 2.35                     | 0.42              |
| 45:LF:1503:G:N3    | 48:LI:3214:6MZ:H2  | 2.33                     | 0.42              |
| 45:LF:1913:C:H2'   | 45:LF:1914:A:C8    | 2.54                     | 0.42              |
| 46:LG:2110:C:H2'   | 46:LG:2111:U:C6    | 2.55                     | 0.42              |
| 47:LH:2954:G:H8    | 48:LI:2979:G:H21   | 1.67                     | 0.42              |
| 49:LJ:3674:U:H2'   | 49:LJ:3675:G:O4'   | 2.20                     | 0.42              |
| 54:LO:69:C:H2'     | 54:LO:70:A:H8      | 1.82                     | 0.42              |
| 57:LR:301:ARG:C    | 57:LR:303:ASN:H    | 2.27                     | 0.42              |
| 62:LW:83:LYS:HD2   | 62:LW:86:GLU:OE2   | 2.19                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 62:LW:185:ALA:HB2   | 65:LZ:190:CYS:SG   | 2.60                     | 0.42              |
| 65:LZ:33:ILE:HG21   | 72:Lg:2:PRO:HD3    | 2.02                     | 0.42              |
| 67:Lb:14:LYS:HA     | 67:Lb:19:MET:HG2   | 2.01                     | 0.42              |
| 67:Lb:175:ARG:HD3   | 67:Lb:175:ARG:HA   | 1.92                     | 0.42              |
| 83:Lr:99:LYS:HB3    | 83:Lr:100:PRO:HD3  | 2.02                     | 0.42              |
| 86:Lu:102:VAL:HG22  | 86:Lu:127:THR:OG1  | 2.19                     | 0.42              |
| 87:Lv:14:MET:HA     | 87:Lv:31:LEU:HD23  | 2.01                     | 0.42              |
| 89:Lx:16:SER:C      | 89:Lx:18:VAL:H     | 2.27                     | 0.42              |
| 1:S1:327:A:H2'      | 1:S1:328:G:O4'     | 2.20                     | 0.42              |
| 1:S1:347:C:H4'      | 16:SK:279:ARG:HH11 | 1.83                     | 0.42              |
| 1:S1:587:G:H2'      | 1:S1:588:U:C6      | 2.55                     | 0.42              |
| 1:S1:1376:A:H4'     | 1:S1:2292:G:N2     | 2.34                     | 0.42              |
| 2:S2:34:G:HO2'      | 2:S2:35:A:P        | 2.43                     | 0.42              |
| 3:S3:9:A:N3         | 3:S3:45:U:H2'      | 2.34                     | 0.42              |
| 7:SB:10:PRO:HD3     | 7:SB:55:TRP:CD1    | 2.54                     | 0.42              |
| 9:SD:93:LEU:HA      | 9:SD:96:VAL:HG12   | 2.02                     | 0.42              |
| 10:SE:34:GLY:H      | 10:SE:83:PRO:HG3   | 1.84                     | 0.42              |
| 13:SH:169:GLY:O     | 13:SH:171:SER:N    | 2.53                     | 0.42              |
| 16:SK:45:VAL:HG12   | 16:SK:57:TRP:HE3   | 1.84                     | 0.42              |
| 25:ST:12:SER:O      | 25:ST:12:SER:OG    | 2.33                     | 0.42              |
| 33:Sb:79:ALA:HB1    | 33:Sb:85:VAL:HG22  | 2.01                     | 0.42              |
| 41:LB:201:G:N2      | 48:LI:3389:A:H62   | 2.17                     | 0.42              |
| 42:LC:495:G:H5''    | 67:Lb:98:MET:HE3   | 2.02                     | 0.42              |
| 43:LD:711:A:OP2     | 43:LD:714:A:N6     | 2.52                     | 0.42              |
| 44:LE:1088:A:H2'    | 44:LE:1089:A:H8    | 1.84                     | 0.42              |
| 45:LF:1763:U:H2'    | 45:LF:1764:G:H8    | 1.85                     | 0.42              |
| 46:LG:2062:G:O6     | 79:Ln:17:ARG:HD3   | 2.20                     | 0.42              |
| 46:LG:2190:C:O2     | 47:LH:2225:A:O2'   | 2.26                     | 0.42              |
| 47:LH:2605:OMU:HM22 | 47:LH:2606:G:O4'   | 2.20                     | 0.42              |
| 47:LH:2754:PSU:H2'  | 47:LH:2755:C:C6    | 2.54                     | 0.42              |
| 47:LH:2901:A:H2'    | 47:LH:2902:G:H8    | 1.84                     | 0.42              |
| 49:LJ:3674:U:O2'    | 52:LM:3947:U:OP1   | 2.32                     | 0.42              |
| 49:LJ:3743:U:H2'    | 49:LJ:3744:G:H8    | 1.85                     | 0.42              |
| 49:LJ:3744:G:H4'    | 56:LQ:130:PHE:CD1  | 2.54                     | 0.42              |
| 51:LL:3881:C:H2'    | 51:LL:3882:A:H8    | 1.84                     | 0.42              |
| 51:LL:3897:C:H4'    | 51:LL:3900:A:C6    | 2.55                     | 0.42              |
| 55:LP:245:ARG:H     | 55:LP:245:ARG:HG3  | 1.64                     | 0.42              |
| 58:LS:168:GLU:HA    | 58:LS:171:LYS:HG2  | 2.02                     | 0.42              |
| 60:LU:33:LEU:HD11   | 60:LU:44:THR:HG22  | 2.01                     | 0.42              |
| 66:La:13:GLN:HG3    | 66:La:14:LYS:N     | 2.34                     | 0.42              |
| 67:Lb:60:VAL:HG23   | 67:Lb:134:LEU:HB2  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:Lj:63:TYR:HD1   | 75:Lj:152:THR:HA   | 1.84                     | 0.42              |
| 77:Ll:30:MET:HB3   | 77:Ll:100:PRO:HG3  | 2.01                     | 0.42              |
| 79:Ln:68:LEU:O     | 79:Ln:68:LEU:HD23  | 2.20                     | 0.42              |
| 1:S1:322:G:C2      | 26:SU:45:LEU:HG    | 2.54                     | 0.42              |
| 1:S1:1134:G:H2'    | 1:S1:1134:G:N3     | 2.35                     | 0.42              |
| 1:S1:1157:G:H2'    | 1:S1:1158:U:C6     | 2.55                     | 0.42              |
| 1:S1:1635:C:H2'    | 1:S1:1636:U:O4'    | 2.20                     | 0.42              |
| 1:S1:2175:U:H2'    | 1:S1:2176:C:H6     | 1.85                     | 0.42              |
| 1:S1:2265:C:H4'    | 47:LH:2751:C:O2'   | 2.19                     | 0.42              |
| 5:S5:10:C:H2'      | 5:S5:11:A:O4'      | 2.19                     | 0.42              |
| 10:SE:265:LYS:HB2  | 10:SE:265:LYS:HE3  | 1.87                     | 0.42              |
| 11:SF:34:ILE:HD12  | 11:SF:35:PRO:HD2   | 2.01                     | 0.42              |
| 16:SK:47:ARG:HB3   | 16:SK:57:TRP:CZ3   | 2.54                     | 0.42              |
| 29:SX:8:VAL:HG12   | 29:SX:9:VAL:O      | 2.20                     | 0.42              |
| 34:Sc:12:PRO:HA    | 34:Sc:13:PRO:HD3   | 1.93                     | 0.42              |
| 38:Sg:137:TRP:HB2  | 38:Sg:214:LYS:CE   | 2.50                     | 0.42              |
| 38:Sg:236:ARG:N    | 38:Sg:237:PRO:HD2  | 2.35                     | 0.42              |
| 40:LA:83:U:O2'     | 77:Ll:112:LYS:HB2  | 2.19                     | 0.42              |
| 40:LA:135:C:H2'    | 40:LA:136:C:O4'    | 2.20                     | 0.42              |
| 42:LC:585:U:H2'    | 42:LC:586:C:H6     | 1.84                     | 0.42              |
| 43:LD:744:C:O2'    | 43:LD:750:G:OP1    | 2.33                     | 0.42              |
| 44:LE:1243:U:OP1   | 66:La:22:VAL:HA    | 2.20                     | 0.42              |
| 45:LF:1772:G:OP2   | 57:LR:198:ARG:NH2  | 2.43                     | 0.42              |
| 46:LG:2061:U:H2'   | 46:LG:2062:G:C8    | 2.54                     | 0.42              |
| 47:LH:2240:U:H2'   | 47:LH:2241:U:H6    | 1.85                     | 0.42              |
| 48:LI:3120:G:H2'   | 48:LI:3121:U:C6    | 2.55                     | 0.42              |
| 48:LI:3362:U:O4    | 66:La:67:ARG:NH1   | 2.53                     | 0.42              |
| 49:LJ:3588:G:H2'   | 49:LJ:3589:C:C6    | 2.55                     | 0.42              |
| 55:LP:180:LEU:HD23 | 55:LP:180:LEU:HA   | 1.75                     | 0.42              |
| 70:Le:22:PRO:HB2   | 80:Lo:21:VAL:HG22  | 2.02                     | 0.42              |
| 71:Lf:106:MET:SD   | 71:Lf:139:LEU:HD22 | 2.60                     | 0.42              |
| 73:Lh:109:VAL:O    | 73:Lh:113:GLU:HG2  | 2.19                     | 0.42              |
| 77:Ll:54:GLU:OE1   | 77:Ll:54:GLU:N     | 2.53                     | 0.42              |
| 78:Lm:64:LYS:HB2   | 78:Lm:64:LYS:HE2   | 1.83                     | 0.42              |
| 82:Lq:62:LYS:O     | 82:Lq:66:LYS:HG2   | 2.20                     | 0.42              |
| 85:Lt:130:TYR:HE1  | 85:Lt:132:VAL:HG13 | 1.84                     | 0.42              |
| 90:Ly:18:LEU:HG    | 92:L1:51:MET:O     | 2.20                     | 0.42              |
| 1:S1:622:G:O2'     | 1:S1:623:C:H5'     | 2.20                     | 0.42              |
| 1:S1:1058:C:H2'    | 1:S1:1059:C:O4'    | 2.19                     | 0.42              |
| 1:S1:1387:C:H2'    | 1:S1:1388:A:O4'    | 2.20                     | 0.42              |
| 1:S1:1966:OMU:HM23 | 1:S1:1966:OMU:H1'  | 1.43                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:1969:A:H2'    | 1:S1:1970:G:N3     | 2.35                     | 0.42              |
| 1:S1:1977:A:O2'    | 1:S1:1978:C:H6     | 2.03                     | 0.42              |
| 10:SE:213:ALA:HB3  | 10:SE:245:VAL:HG22 | 2.02                     | 0.42              |
| 12:SG:57:ASP:HB2   | 12:SG:107:ASP:O    | 2.20                     | 0.42              |
| 13:SH:153:LYS:HE3  | 13:SH:157:GLU:HB3  | 2.02                     | 0.42              |
| 15:SJ:37:PHE:CD1   | 15:SJ:41:MET:HE2   | 2.55                     | 0.42              |
| 18:SM:56:VAL:HB    | 18:SM:90:LEU:HB2   | 2.01                     | 0.42              |
| 21:SP:89:GLY:C     | 21:SP:91:LEU:H     | 2.28                     | 0.42              |
| 22:SQ:102:TYR:O    | 22:SQ:104:SER:N    | 2.52                     | 0.42              |
| 31:SZ:41:LYS:HE3   | 31:SZ:41:LYS:HB2   | 1.90                     | 0.42              |
| 31:SZ:45:GLN:HE21  | 31:SZ:57:GLU:C     | 2.28                     | 0.42              |
| 31:SZ:126:LYS:HB3  | 31:SZ:126:LYS:HE2  | 1.80                     | 0.42              |
| 34:Sc:66:ALA:HB1   | 34:Sc:73:ALA:HB1   | 2.01                     | 0.42              |
| 39:Sh:16:HIS:CG    | 39:Sh:37:SER:HB2   | 2.55                     | 0.42              |
| 42:LC:324:A:HO2'   | 61:LV:139:SER:HG   | 1.67                     | 0.42              |
| 42:LC:382:A:H2'    | 42:LC:383:G:H8     | 1.82                     | 0.42              |
| 43:LD:680:G:H2'    | 43:LD:681:C:H6     | 1.84                     | 0.42              |
| 44:LE:1200:C:H2'   | 44:LE:1201:OMG:H8  | 1.84                     | 0.42              |
| 44:LE:1411:C:H2'   | 44:LE:1412:C:C6    | 2.55                     | 0.42              |
| 46:LG:2023:G:H2'   | 46:LG:2024:A:O4'   | 2.20                     | 0.42              |
| 47:LH:2928:A:H2'   | 47:LH:2929:C:H6    | 1.85                     | 0.42              |
| 48:LI:3025:C:H4'   | 48:LI:3026:A:H5'   | 2.01                     | 0.42              |
| 48:LI:3533:A2M:OP1 | 100:LI:3610:HOH:O  | 2.22                     | 0.42              |
| 52:LM:3963:PSU:H2' | 52:LM:3964:U:C6    | 2.55                     | 0.42              |
| 57:LR:8:THR:HG22   | 57:LR:143:GLU:CD   | 2.45                     | 0.42              |
| 58:LS:59:LYS:HA    | 58:LS:74:LYS:HA    | 2.01                     | 0.42              |
| 60:LU:161:GLU:HB2  | 60:LU:162:PRO:HD3  | 2.02                     | 0.42              |
| 63:LX:147:THR:HG22 | 63:LX:150:ASP:OD2  | 2.20                     | 0.42              |
| 64:LY:13:LYS:HB2   | 64:LY:128:ILE:HD11 | 2.02                     | 0.42              |
| 75:Lj:109:ILE:HG22 | 75:Lj:111:GLY:N    | 2.34                     | 0.42              |
| 82:Lq:14:TYR:O     | 82:Lq:18:ARG:HG2   | 2.19                     | 0.42              |
| 90:Ly:93:GLU:OE1   | 90:Ly:93:GLU:N     | 2.51                     | 0.42              |
| 96:L4:47:GLN:OE1   | 96:L4:54:THR:OG1   | 2.26                     | 0.42              |
| 1:S1:198:C:H2'     | 1:S1:199:C:O4'     | 2.20                     | 0.42              |
| 1:S1:414:A:N1      | 1:S1:446:C:O2'     | 2.51                     | 0.42              |
| 1:S1:434:G:H1'     | 1:S1:436:C:OP2     | 2.20                     | 0.42              |
| 1:S1:461:A:OP1     | 1:S1:1077:A:N6     | 2.53                     | 0.42              |
| 1:S1:1027:C:H2'    | 1:S1:1028:C:C6     | 2.55                     | 0.42              |
| 1:S1:1557:A:H2'    | 1:S1:1558:C:C6     | 2.55                     | 0.42              |
| 1:S1:1767:U:H2'    | 1:S1:1768:C:C6     | 2.55                     | 0.42              |
| 1:S1:1870:G:H4'    | 1:S1:1871:C:O4'    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:2035:A:C5     | 1:S1:2036:C:C5     | 3.08                     | 0.42              |
| 3:S3:23:A:H2'      | 3:S3:24:G:C8       | 2.55                     | 0.42              |
| 4:S4:18:G:H5'      | 4:S4:60:U:N3       | 2.35                     | 0.42              |
| 4:S4:28:G:H2'      | 4:S4:29:G:C8       | 2.55                     | 0.42              |
| 6:SA:54:ASN:ND2    | 6:SA:56:THR:OG1    | 2.53                     | 0.42              |
| 8:SC:35:GLY:HA3    | 8:SC:55:THR:HB     | 2.01                     | 0.42              |
| 10:SE:63:MET:HE2   | 31:SZ:22:MET:HE1   | 2.01                     | 0.42              |
| 14:SI:46:LEU:C     | 14:SI:48:PRO:HD2   | 2.45                     | 0.42              |
| 21:SP:69:CYS:HB3   | 21:SP:83:ALA:O     | 2.20                     | 0.42              |
| 22:SQ:23:MET:HG2   | 22:SQ:96:TRP:CH2   | 2.55                     | 0.42              |
| 24:SS:35:LEU:HD21  | 24:SS:42:PHE:CD1   | 2.55                     | 0.42              |
| 31:SZ:10:ARG:O     | 31:SZ:31:ILE:HA    | 2.19                     | 0.42              |
| 34:Sc:50:SER:OG    | 34:Sc:51:HIS:HD2   | 2.03                     | 0.42              |
| 38:Sg:57:LYS:HA    | 38:Sg:89:THR:O     | 2.20                     | 0.42              |
| 42:LC:537:OMC:HM23 | 42:LC:537:OMC:H1'  | 1.89                     | 0.42              |
| 44:LE:917:C:C2     | 44:LE:918:U:C5     | 3.07                     | 0.42              |
| 45:LF:1489:A:H2'   | 45:LF:1490:U:C6    | 2.54                     | 0.42              |
| 45:LF:1528:G:H2'   | 45:LF:1529:A:C8    | 2.55                     | 0.42              |
| 45:LF:1550:U:O4    | 62:LW:26:ALA:HB3   | 2.19                     | 0.42              |
| 45:LF:1585:C:H2'   | 45:LF:1586:PSU:H6  | 1.85                     | 0.42              |
| 45:LF:1832:G:N7    | 74:Li:29:LYS:HB2   | 2.35                     | 0.42              |
| 48:LI:3141:A:O4'   | 76:Lk:42:ASN:HB2   | 2.20                     | 0.42              |
| 48:LI:3170:A:H2'   | 48:LI:3171:OMU:H6  | 2.02                     | 0.42              |
| 48:LI:3366:U:H2'   | 48:LI:3367:A2M:H8  | 2.02                     | 0.42              |
| 51:LL:3834:A:C8    | 62:LW:161:LEU:HD22 | 2.55                     | 0.42              |
| 53:LN:4011:G:N1    | 53:LN:4019:U:N3    | 2.67                     | 0.42              |
| 54:LO:23:A:H2'     | 54:LO:24:U:C6      | 2.55                     | 0.42              |
| 54:LO:92:C:H2'     | 54:LO:93:A:H8      | 1.85                     | 0.42              |
| 56:LQ:10:ARG:NH2   | 56:LQ:14:MET:SD    | 2.92                     | 0.42              |
| 58:LS:102:LYS:HG2  | 58:LS:105:ASN:OD1  | 2.19                     | 0.42              |
| 59:LT:34:LEU:HD11  | 59:LT:151:ASN:HB3  | 2.02                     | 0.42              |
| 64:LY:43:LYS:HD2   | 64:LY:43:LYS:HA    | 1.73                     | 0.42              |
| 68:Lc:101:LYS:O    | 68:Lc:101:LYS:HG3  | 2.18                     | 0.42              |
| 83:Lr:103:ILE:HB   | 83:Lr:131:VAL:HG11 | 2.01                     | 0.42              |
| 1:S1:865:A:H2'     | 1:S1:866:C:C6      | 2.54                     | 0.41              |
| 1:S1:1249:G:O2'    | 1:S1:1250:A:OP1    | 2.34                     | 0.41              |
| 1:S1:1304:A:H2'    | 1:S1:1305:U:C6     | 2.54                     | 0.41              |
| 1:S1:1359:C:H2'    | 1:S1:1360:G:O4'    | 2.20                     | 0.41              |
| 1:S1:2067:C:H2'    | 1:S1:2068:C:H6     | 1.85                     | 0.41              |
| 2:S2:10:G:N2       | 2:S2:11:C:C2       | 2.88                     | 0.41              |
| 6:SA:134:ARG:HG3   | 6:SA:216:LEU:HD21  | 2.01                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 13:SH:107:PRO:O     | 13:SH:132:ARG:HG3  | 2.20                     | 0.41              |
| 14:SI:59:ILE:HD12   | 14:SI:59:ILE:H     | 1.84                     | 0.41              |
| 14:SI:135:LEU:HB3   | 14:SI:174:ILE:HD13 | 2.02                     | 0.41              |
| 16:SK:91:GLU:HG2    | 16:SK:94:ARG:HH21  | 1.85                     | 0.41              |
| 16:SK:247:LYS:HD3   | 26:SU:23:ASN:ND2   | 2.35                     | 0.41              |
| 20:SO:133:VAL:O     | 20:SO:133:VAL:CG1  | 2.57                     | 0.41              |
| 33:Sb:23:CYS:HB3    | 33:Sb:28:ARG:H     | 1.85                     | 0.41              |
| 35:Sd:16:LEU:H      | 35:Sd:16:LEU:HD23  | 1.85                     | 0.41              |
| 38:Sg:95:SER:OG     | 38:Sg:97:GLU:OE1   | 2.32                     | 0.41              |
| 42:LC:426:C:O3'     | 42:LC:430:A:N6     | 2.45                     | 0.41              |
| 43:LD:698:C:H3'     | 59:LT:50:LYS:HD3   | 2.02                     | 0.41              |
| 44:LE:882:C:H2'     | 44:LE:883:A:O4'    | 2.19                     | 0.41              |
| 44:LE:1076:U:H2'    | 44:LE:1077:C:C6    | 2.56                     | 0.41              |
| 44:LE:1132:G:H2'    | 44:LE:1133:U:O4'   | 2.20                     | 0.41              |
| 45:LF:1728:C:N4     | 70:Le:33:PHE:HE2   | 2.17                     | 0.41              |
| 47:LH:2288:C:OP1    | 76:Lk:141:LYS:NZ   | 2.45                     | 0.41              |
| 48:LI:3561:U:H2'    | 48:LI:3562:PSU:H6  | 1.85                     | 0.41              |
| 49:LJ:3630:U:H2'    | 49:LJ:3631:G:C8    | 2.54                     | 0.41              |
| 52:LM:3948:G:H21    | 53:LN:3981:A:H2    | 1.68                     | 0.41              |
| 52:LM:3957:OMC:HM23 | 52:LM:3957:OMC:H1' | 1.81                     | 0.41              |
| 54:LO:7:G:P         | 69:Ld:49:ARG:HH22  | 2.43                     | 0.41              |
| 54:LO:54:A:C8       | 58:LS:17:ASN:ND2   | 2.88                     | 0.41              |
| 56:LQ:232:ILE:HD13  | 56:LQ:237:VAL:HG23 | 2.00                     | 0.41              |
| 58:LS:135:MET:HE2   | 58:LS:135:MET:HB3  | 1.98                     | 0.41              |
| 61:LV:112:ILE:HD11  | 67:Lb:18:VAL:HG13  | 2.02                     | 0.41              |
| 61:LV:131:ALA:HB2   | 61:LV:236:PHE:HZ   | 1.85                     | 0.41              |
| 65:LZ:183:GLU:OE1   | 65:LZ:183:GLU:N    | 2.51                     | 0.41              |
| 72:Lg:83:ARG:HE     | 72:Lg:90:VAL:HG11  | 1.85                     | 0.41              |
| 74:Li:42:THR:HA     | 74:Li:115:PHE:HA   | 2.02                     | 0.41              |
| 77:Ll:69:VAL:HG13   | 77:Ll:79:VAL:HG13  | 2.01                     | 0.41              |
| 80:Lo:31:SER:O      | 80:Lo:31:SER:OG    | 2.33                     | 0.41              |
| 80:Lo:40:HIS:C      | 80:Lo:42:ALA:H     | 2.28                     | 0.41              |
| 96:L4:24:LYS:HB2    | 96:L4:24:LYS:HE3   | 1.83                     | 0.41              |
| 1:S1:128:G:C6       | 1:S1:136:G:C5      | 3.08                     | 0.41              |
| 1:S1:509:U:H2'      | 1:S1:510:A:C8      | 2.54                     | 0.41              |
| 1:S1:697:G:H4'      | 1:S1:699:G:H4'     | 2.02                     | 0.41              |
| 1:S1:1892:U:H2'     | 1:S1:1893:G:C8     | 2.56                     | 0.41              |
| 4:S4:13:C:H2'       | 4:S4:14:A:N7       | 2.35                     | 0.41              |
| 11:SF:84:ILE:HD11   | 11:SF:126:ILE:HD11 | 2.02                     | 0.41              |
| 12:SG:52:ILE:HA     | 12:SG:113:LEU:HD23 | 2.01                     | 0.41              |
| 13:SH:136:ALA:O     | 13:SH:140:ILE:HG13 | 2.20                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:SO:46:THR:HG22  | 20:SO:53:THR:HA   | 2.02                     | 0.41              |
| 21:SP:59:ALA:HB1   | 21:SP:114:ASP:HB3 | 2.02                     | 0.41              |
| 22:SQ:40:ALA:HB2   | 22:SQ:120:LYS:NZ  | 2.35                     | 0.41              |
| 22:SQ:102:TYR:C    | 22:SQ:104:SER:H   | 2.28                     | 0.41              |
| 23:SR:142:ARG:HA   | 23:SR:142:ARG:HD3 | 1.84                     | 0.41              |
| 30:SY:46:ILE:O     | 30:SY:48:GLU:N    | 2.49                     | 0.41              |
| 32:Sa:107:ASN:O    | 32:Sa:108:CYS:C   | 2.63                     | 0.41              |
| 40:LA:94:C:H6      | 40:LA:94:C:H2'    | 1.74                     | 0.41              |
| 42:LC:466:A:H1'    | 42:LC:467:U:C5'   | 2.50                     | 0.41              |
| 42:LC:569:G:OP2    | 90:Ly:52:LYS:NZ   | 2.27                     | 0.41              |
| 43:LD:702:A:H2'    | 43:LD:703:C:C6    | 2.55                     | 0.41              |
| 44:LE:818:C:H2'    | 44:LE:819:G:C8    | 2.55                     | 0.41              |
| 44:LE:1082:G:H5''  | 44:LE:1083:C:H5'  | 2.01                     | 0.41              |
| 44:LE:1301:C:O2'   | 44:LE:1302:U:H5'  | 2.20                     | 0.41              |
| 44:LE:1319:G:H2'   | 44:LE:1320:C:C6   | 2.55                     | 0.41              |
| 45:LF:1684:U:H2'   | 45:LF:1685:G:O4'  | 2.20                     | 0.41              |
| 45:LF:1748:U:O3'   | 70:Le:5:LYS:HD3   | 2.20                     | 0.41              |
| 46:LG:2014:U:H2'   | 46:LG:2015:G:C8   | 2.55                     | 0.41              |
| 48:LI:3036:U:H2'   | 48:LI:3037:G:H1'  | 2.00                     | 0.41              |
| 48:LI:3233:A:H2'   | 48:LI:3234:U:H6   | 1.85                     | 0.41              |
| 48:LI:3527:A:OP2   | 56:LQ:2:SER:N     | 2.54                     | 0.41              |
| 54:LO:120:U:H2'    | 97:L6:33:TYR:CZ   | 2.55                     | 0.41              |
| 63:LX:180:LYS:HD3  | 66:La:102:GLU:HG3 | 2.03                     | 0.41              |
| 64:LY:14:PHE:CD1   | 64:LY:91:LYS:HE3  | 2.55                     | 0.41              |
| 69:Ld:38:GLN:HA    | 69:Ld:47:LYS:HE3  | 2.02                     | 0.41              |
| 73:Lh:75:LEU:HD11  | 82:Lq:30:ILE:HD13 | 2.02                     | 0.41              |
| 76:Lk:43:LYS:HE2   | 76:Lk:43:LYS:HB2  | 1.90                     | 0.41              |
| 77:Ll:59:ARG:HA    | 77:Ll:59:ARG:HD3  | 1.81                     | 0.41              |
| 83:Lr:166:ASN:HD22 | 83:Lr:180:CYS:HA  | 1.85                     | 0.41              |
| 1:S1:10:G:O2'      | 11:SF:88:GLN:OE1  | 2.26                     | 0.41              |
| 1:S1:369:U:C4      | 1:S1:370:G:C6     | 3.09                     | 0.41              |
| 1:S1:396:A:N3      | 10:SE:33:ALA:HB1  | 2.35                     | 0.41              |
| 1:S1:487:G:N3      | 1:S1:487:G:H5''   | 2.34                     | 0.41              |
| 1:S1:497:G:H5''    | 16:SK:24:LYS:O    | 2.20                     | 0.41              |
| 1:S1:531:G:OP1     | 21:SP:76:LYS:HA   | 2.20                     | 0.41              |
| 1:S1:546:C:OP1     | 10:SE:81:LYS:HD3  | 2.21                     | 0.41              |
| 1:S1:693:C:H2'     | 1:S1:694:C:H6     | 1.85                     | 0.41              |
| 1:S1:928:U:H3'     | 1:S1:929:U:H5''   | 2.01                     | 0.41              |
| 1:S1:965:G:C8      | 1:S1:965:G:OP2    | 2.73                     | 0.41              |
| 1:S1:1030:U:H2'    | 1:S1:1031:G:C8    | 2.56                     | 0.41              |
| 1:S1:1317:U:H2'    | 1:S1:1318:G:N3    | 2.35                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:S1:1663:U:H2'     | 1:S1:1664:U:C6     | 2.56                     | 0.41              |
| 1:S1:1691:G:O3'     | 18:SM:76:THR:OG1   | 2.31                     | 0.41              |
| 1:S1:1968:A:H2'     | 1:S1:1969:A:C8     | 2.55                     | 0.41              |
| 1:S1:2284:G:O6      | 94:L3:21:ARG:NH2   | 2.52                     | 0.41              |
| 4:S4:53:G:C5        | 4:S4:54:U:H1'      | 2.55                     | 0.41              |
| 7:SB:52:HIS:O       | 7:SB:56:GLN:HG2    | 2.20                     | 0.41              |
| 10:SE:175:PHE:CG    | 10:SE:175:PHE:O    | 2.73                     | 0.41              |
| 13:SH:35:LEU:HD23   | 13:SH:35:LEU:HA    | 1.95                     | 0.41              |
| 15:SJ:30:CYS:N      | 15:SJ:59:ASN:O     | 2.53                     | 0.41              |
| 21:SP:61:GLN:OE1    | 100:SP:201:HOH:O   | 2.22                     | 0.41              |
| 27:SV:77:GLU:O      | 27:SV:80:LYS:HG3   | 2.20                     | 0.41              |
| 38:Sg:58:LEU:HB2    | 38:Sg:89:THR:OG1   | 2.20                     | 0.41              |
| 40:LA:25:C:H2'      | 40:LA:26:C:C6      | 2.55                     | 0.41              |
| 41:LB:254:G:OP2     | 66:La:60:PHE:HA    | 2.20                     | 0.41              |
| 42:LC:589:C:H2'     | 42:LC:590:G:O4'    | 2.20                     | 0.41              |
| 44:LE:779:C:H2'     | 44:LE:780:U:H6     | 1.84                     | 0.41              |
| 44:LE:779:C:H2'     | 44:LE:780:U:C6     | 2.55                     | 0.41              |
| 44:LE:1342:G:H2'    | 44:LE:1343:G:C8    | 2.55                     | 0.41              |
| 45:LF:1578:G:OP1    | 68:Lc:157:TYR:OH   | 2.39                     | 0.41              |
| 46:LG:2094:C:O2     | 88:Lw:19:ARG:NH2   | 2.49                     | 0.41              |
| 47:LH:2625:OMU:HM23 | 47:LH:2629:U:O4    | 2.20                     | 0.41              |
| 48:LI:3106:C:H2'    | 48:LI:3107:A:C8    | 2.55                     | 0.41              |
| 53:LN:4049:G:O6     | 56:LQ:124:ARG:NH2  | 2.46                     | 0.41              |
| 55:LP:137:ILE:CD1   | 55:LP:155:LYS:HE3  | 2.50                     | 0.41              |
| 60:LU:33:LEU:HB3    | 60:LU:76:LEU:HD12  | 2.02                     | 0.41              |
| 60:LU:34:LYS:HE2    | 60:LU:36:LEU:HD23  | 2.02                     | 0.41              |
| 61:LV:109:PRO:HG2   | 61:LV:112:ILE:HG13 | 2.02                     | 0.41              |
| 67:Lb:51:LEU:HD13   | 67:Lb:117:ASN:HB3  | 2.02                     | 0.41              |
| 68:Lc:87:ILE:HG12   | 68:Lc:138:ILE:HG12 | 2.01                     | 0.41              |
| 74:Li:65:TYR:OH     | 74:Li:123:ARG:NH2  | 2.53                     | 0.41              |
| 76:Lk:58:THR:OG1    | 76:Lk:59:LYS:N     | 2.52                     | 0.41              |
| 77:Ll:33:ARG:HH11   | 77:Ll:39:ARG:NH1   | 2.19                     | 0.41              |
| 83:Lr:211:ARG:O     | 83:Lr:240:LYS:HD3  | 2.20                     | 0.41              |
| 95:L5:29:ILE:HD12   | 95:L5:69:TRP:CD1   | 2.55                     | 0.41              |
| 1:S1:60:U:O2'       | 1:S1:62:A:N7       | 2.44                     | 0.41              |
| 1:S1:280:PSU:OP2    | 1:S1:280:PSU:H6    | 2.03                     | 0.41              |
| 1:S1:365:U:H2'      | 1:S1:377:G:P       | 2.60                     | 0.41              |
| 1:S1:430:A:N6       | 16:SK:27:PHE:HB2   | 2.34                     | 0.41              |
| 1:S1:1392:A:H2'     | 1:S1:1393:PSU:O4'  | 2.19                     | 0.41              |
| 1:S1:1435:G:H2'     | 1:S1:1436:C:H6     | 1.85                     | 0.41              |
| 1:S1:1624:PSU:OP1   | 1:S1:1656:C:O2'    | 2.28                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:SA:221:PHE:CE2   | 6:SA:223:PRO:HB3  | 2.56                     | 0.41              |
| 8:SC:37:SER:OG     | 8:SC:99:SER:OG    | 2.27                     | 0.41              |
| 8:SC:99:SER:HB3    | 8:SC:102:ALA:HB3  | 2.02                     | 0.41              |
| 10:SE:151:ASP:OD2  | 10:SE:153:ASN:OD1 | 2.39                     | 0.41              |
| 10:SE:191:ARG:HD2  | 10:SE:246:LYS:HD2 | 2.03                     | 0.41              |
| 11:SF:164:GLY:HA3  | 11:SF:210:ASN:ND2 | 2.35                     | 0.41              |
| 12:SG:44:LYS:HG3   | 12:SG:45:TRP:CD1  | 2.55                     | 0.41              |
| 13:SH:59:VAL:HG13  | 13:SH:72:LYS:HE3  | 1.99                     | 0.41              |
| 20:SO:30:GLY:O     | 20:SO:94:LEU:HA   | 2.21                     | 0.41              |
| 20:SO:76:MET:HE3   | 20:SO:80:GLN:NE2  | 2.35                     | 0.41              |
| 35:Sd:17:ALA:HB1   | 35:Sd:38:LYS:O    | 2.20                     | 0.41              |
| 37:Sf:133:MET:HG2  | 37:Sf:142:CYS:HB2 | 2.01                     | 0.41              |
| 39:Sh:176:LYS:HD2  | 39:Sh:197:GLY:N   | 2.36                     | 0.41              |
| 40:LA:87:A:H2'     | 40:LA:88:U:O4'    | 2.20                     | 0.41              |
| 42:LC:347:U:H2'    | 42:LC:348:U:C6    | 2.55                     | 0.41              |
| 42:LC:413:C:N4     | 45:LF:1775:G:H2'  | 2.35                     | 0.41              |
| 42:LC:538:C:O2     | 90:Ly:82:GLN:NE2  | 2.54                     | 0.41              |
| 44:LE:766:G:H2'    | 44:LE:767:C:H6    | 1.85                     | 0.41              |
| 44:LE:916:U:H2'    | 44:LE:917:C:C6    | 2.56                     | 0.41              |
| 44:LE:972:G:N7     | 44:LE:973:C:N4    | 2.69                     | 0.41              |
| 44:LE:1216:G:O6    | 47:LH:2903:U:H5'  | 2.20                     | 0.41              |
| 44:LE:1441:U:H2'   | 44:LE:1442:C:C6   | 2.56                     | 0.41              |
| 47:LH:2808:A:H2    | 95:L5:16:THR:HG22 | 1.85                     | 0.41              |
| 48:LI:3468:U:H2'   | 48:LI:3469:U:H6   | 1.83                     | 0.41              |
| 48:LI:3518:5MC:H2' | 48:LI:3519:C:O4'  | 2.20                     | 0.41              |
| 50:LK:3758:A:H2'   | 50:LK:3759:G:O4'  | 2.20                     | 0.41              |
| 52:LM:3913:C:H2'   | 52:LM:3914:A:H8   | 1.84                     | 0.41              |
| 53:LN:3998:U:H2'   | 53:LN:3999:C:C6   | 2.55                     | 0.41              |
| 58:LS:142:GLU:OE1  | 58:LS:150:ARG:NH2 | 2.53                     | 0.41              |
| 59:LT:16:VAL:HG11  | 59:LT:81:ILE:HD12 | 2.02                     | 0.41              |
| 62:LW:65:LYS:O     | 62:LW:77:HIS:HE1  | 2.02                     | 0.41              |
| 63:LX:195:ARG:HD2  | 63:LX:195:ARG:HA  | 1.69                     | 0.41              |
| 69:Ld:207:LYS:HG2  | 69:Ld:231:PRO:HB2 | 2.03                     | 0.41              |
| 70:Le:181:ARG:HA   | 70:Le:187:ARG:HB3 | 2.02                     | 0.41              |
| 73:Lh:122:LYS:HG3  | 73:Lh:122:LYS:O   | 2.21                     | 0.41              |
| 90:Ly:14:ARG:HD3   | 90:Ly:14:ARG:HA   | 1.93                     | 0.41              |
| 95:L5:27:LYS:O     | 95:L5:31:ILE:HG13 | 2.20                     | 0.41              |
| 1:S1:378:C:H2'     | 1:S1:379:A:C8     | 2.56                     | 0.41              |
| 1:S1:610:C:H2'     | 1:S1:611:U:H6     | 1.83                     | 0.41              |
| 1:S1:1052:G:H5''   | 10:SE:23:LEU:HD13 | 2.02                     | 0.41              |
| 1:S1:1310:A:N3     | 47:LH:2694:G:C2   | 2.87                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:1597:UR3:H6   | 1:S1:1597:UR3:O5'  | 2.20                     | 0.41              |
| 1:S1:1918:G:H21    | 24:SS:41:GLU:CD    | 2.29                     | 0.41              |
| 1:S1:2067:C:H1'    | 23:SR:88:LYS:NZ    | 2.35                     | 0.41              |
| 1:S1:2116:PSU:C4   | 1:S1:2117:G:C8     | 3.09                     | 0.41              |
| 1:S1:2293:C:H2'    | 1:S1:2294:A:C8     | 2.56                     | 0.41              |
| 13:SH:94:PRO:HA    | 13:SH:97:VAL:HG12  | 2.03                     | 0.41              |
| 14:SI:173:ALA:O    | 14:SI:177:VAL:HG23 | 2.20                     | 0.41              |
| 15:SJ:111:MET:HE3  | 15:SJ:111:MET:HB2  | 1.99                     | 0.41              |
| 22:SQ:65:THR:HG22  | 22:SQ:66:GLU:N     | 2.29                     | 0.41              |
| 28:SW:35:ASN:HA    | 28:SW:38:LEU:HB2   | 2.01                     | 0.41              |
| 32:Sa:96:GLU:OE2   | 32:Sa:98:LEU:HD13  | 2.20                     | 0.41              |
| 38:Sg:99:ALA:HA    | 38:Sg:102:CYS:HB3  | 2.01                     | 0.41              |
| 39:Sh:286:MET:HE3  | 39:Sh:286:MET:HB3  | 1.94                     | 0.41              |
| 41:LB:296:U:H2'    | 42:LC:297:C:C6     | 2.55                     | 0.41              |
| 42:LC:474:G:OP2    | 67:Lb:44:ARG:NH1   | 2.52                     | 0.41              |
| 42:LC:618:A:H2'    | 42:LC:619:A:C8     | 2.55                     | 0.41              |
| 44:LE:1045:C:OP1   | 82:Lq:44:LYS:HE2   | 2.21                     | 0.41              |
| 46:LG:2103:G:H2'   | 46:LG:2104:A:C8    | 2.56                     | 0.41              |
| 47:LH:2917:G:H2'   | 47:LH:2918:A:H8    | 1.85                     | 0.41              |
| 49:LJ:3600:C:O2'   | 49:LJ:3601:A:H2'   | 2.19                     | 0.41              |
| 49:LJ:3718:OMU:O2' | 49:LJ:3719:G:H5'   | 2.20                     | 0.41              |
| 50:LK:3800:G:H1'   | 65:LZ:102:GLN:NE2  | 2.35                     | 0.41              |
| 53:LN:4023:C:H2'   | 53:LN:4024:C:C6    | 2.56                     | 0.41              |
| 56:LQ:48:CYS:HB2   | 56:LQ:79:MET:HB3   | 2.02                     | 0.41              |
| 58:LS:158:VAL:CG1  | 58:LS:162:HIS:HB3  | 2.50                     | 0.41              |
| 60:LU:80:GLU:HG2   | 60:LU:81:ALA:N     | 2.36                     | 0.41              |
| 62:LW:84:MET:O     | 62:LW:88:VAL:HG23  | 2.20                     | 0.41              |
| 64:LY:35:LYS:HE3   | 64:LY:67:LYS:HG2   | 2.02                     | 0.41              |
| 65:LZ:40:ALA:HB3   | 65:LZ:49:MET:HE1   | 2.01                     | 0.41              |
| 65:LZ:41:ASP:HB2   | 65:LZ:51:ARG:HG3   | 2.02                     | 0.41              |
| 83:Lr:90:ILE:HD13  | 83:Lr:226:ASP:O    | 2.21                     | 0.41              |
| 85:Lt:60:VAL:HG23  | 85:Lt:60:VAL:O     | 2.20                     | 0.41              |
| 85:Lt:79:PHE:O     | 85:Lt:83:VAL:HG23  | 2.20                     | 0.41              |
| 89:Lx:45:VAL:O     | 89:Lx:49:VAL:HG22  | 2.21                     | 0.41              |
| 1:S1:145:G:H2'     | 1:S1:146:C:C6      | 2.55                     | 0.41              |
| 1:S1:325:U:O2'     | 26:SU:68:LYS:HE3   | 2.20                     | 0.41              |
| 1:S1:704:OMU:H2'   | 1:S1:705:A:C8      | 2.56                     | 0.41              |
| 1:S1:754:G:H8      | 1:S1:754:G:OP2     | 2.03                     | 0.41              |
| 1:S1:977:A:C8      | 38:Sg:217:LEU:HD11 | 2.56                     | 0.41              |
| 1:S1:1913:G:OP1    | 100:S1:2425:HOH:O  | 2.21                     | 0.41              |
| 1:S1:2170:U:H2'    | 1:S1:2171:A:C8     | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:S4:8:U:H2'       | 4:S4:13:C:N4       | 2.35                     | 0.41              |
| 4:S4:8:U:O4'       | 4:S4:48:C:O2'      | 2.26                     | 0.41              |
| 6:SA:103:LEU:HD23  | 6:SA:103:LEU:HA    | 1.97                     | 0.41              |
| 6:SA:188:LEU:O     | 6:SA:190:THR:HG23  | 2.21                     | 0.41              |
| 6:SA:195:ILE:HB    | 6:SA:208:VAL:HG11  | 2.02                     | 0.41              |
| 11:SF:51:LEU:HD21  | 11:SF:67:VAL:HG12  | 2.02                     | 0.41              |
| 11:SF:148:LYS:O    | 30:SY:4:ASP:HB2    | 2.21                     | 0.41              |
| 21:SP:32:LEU:HD12  | 21:SP:32:LEU:HA    | 1.85                     | 0.41              |
| 33:Sb:5:ARG:HB3    | 33:Sb:7:ASN:O      | 2.20                     | 0.41              |
| 41:LB:249:A:H2'    | 41:LB:250:U:H6     | 1.86                     | 0.41              |
| 44:LE:935:A2M:H1'  | 44:LE:935:A2M:HM'3 | 1.76                     | 0.41              |
| 44:LE:1084:U:O4    | 66:La:84:ARG:HD2   | 2.21                     | 0.41              |
| 44:LE:1305:U:H2'   | 44:LE:1306:U:H6    | 1.86                     | 0.41              |
| 45:LF:1833:U:H2'   | 45:LF:1834:A:C8    | 2.55                     | 0.41              |
| 46:LG:2101:G:H2'   | 46:LG:2102:U:C6    | 2.56                     | 0.41              |
| 46:LG:2168:A:P     | 71:Lf:104:ARG:HH22 | 2.43                     | 0.41              |
| 47:LH:2385:G:P     | 95:L5:6:VAL:H      | 2.43                     | 0.41              |
| 47:LH:2957:G:H2'   | 47:LH:2958:G:C4    | 2.55                     | 0.41              |
| 48:LI:3176:U:H2'   | 48:LI:3177:G:O4'   | 2.20                     | 0.41              |
| 48:LI:3503:PSU:N1  | 48:LI:3522:C:O2'   | 2.53                     | 0.41              |
| 48:LI:3535:OMC:H5' | 56:LQ:245:HIS:HB3  | 2.02                     | 0.41              |
| 54:LO:8:G:O2'      | 98:L7:16:TRP:NE1   | 2.53                     | 0.41              |
| 57:LR:283:ARG:HD2  | 57:LR:284:HIS:O    | 2.19                     | 0.41              |
| 58:LS:13:LYS:HA    | 58:LS:13:LYS:HD3   | 1.85                     | 0.41              |
| 65:LZ:31:ASP:OD1   | 65:LZ:32:ILE:N     | 2.53                     | 0.41              |
| 66:La:19:ARG:HA    | 66:La:19:ARG:HD3   | 1.80                     | 0.41              |
| 71:Lf:163:LYS:O    | 71:Lf:166:LYS:HB2  | 2.21                     | 0.41              |
| 89:Lx:54:TYR:O     | 89:Lx:58:MET:HG3   | 2.20                     | 0.41              |
| 91:Lz:26:LYS:HB3   | 91:Lz:33:LYS:HG3   | 2.03                     | 0.41              |
| 1:S1:151:A:H2'     | 1:S1:152:C:O4'     | 2.20                     | 0.41              |
| 1:S1:444:G:C5'     | 26:SU:85:MET:HE2   | 2.51                     | 0.41              |
| 1:S1:588:U:H2'     | 1:S1:589:C:H6      | 1.84                     | 0.41              |
| 1:S1:733:U:H2'     | 1:S1:734:A:H8      | 1.85                     | 0.41              |
| 1:S1:1158:U:C4     | 1:S1:1244:C:N3     | 2.87                     | 0.41              |
| 1:S1:1533:C:H2'    | 1:S1:1534:A:C8     | 2.55                     | 0.41              |
| 1:S1:2046:A2M:OP1  | 29:SX:89:GLY:HA3   | 2.21                     | 0.41              |
| 1:S1:2287:MA6:H92  | 1:S1:2288:MA6:H103 | 2.01                     | 0.41              |
| 6:SA:65:GLU:HG2    | 6:SA:81:ASN:HB3    | 2.03                     | 0.41              |
| 6:SA:191:ILE:O     | 6:SA:195:ILE:HG13  | 2.21                     | 0.41              |
| 10:SE:65:LEU:HD23  | 10:SE:65:LEU:HA    | 1.93                     | 0.41              |
| 11:SF:161:GLY:HA3  | 11:SF:214:ALA:O    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:SF:184:VAL:HB   | 11:SF:185:PRO:HD3   | 2.02                     | 0.41              |
| 13:SH:48:ARG:HG2   | 13:SH:51:GLN:NE2    | 2.35                     | 0.41              |
| 16:SK:69:TRP:O     | 16:SK:73:ASN:N      | 2.52                     | 0.41              |
| 19:SN:31:HIS:ND1   | 19:SN:32:PRO:O      | 2.54                     | 0.41              |
| 20:SO:79:ALA:HB3   | 20:SO:119:ALA:HB3   | 2.02                     | 0.41              |
| 21:SP:141:PRO:O    | 21:SP:142:ARG:HG2   | 2.21                     | 0.41              |
| 27:SV:114:ASP:O    | 27:SV:115:MET:HB2   | 2.20                     | 0.41              |
| 28:SW:61:LEU:HD22  | 28:SW:83:THR:HG21   | 2.02                     | 0.41              |
| 31:SZ:63:PHE:N     | 31:SZ:63:PHE:CD1    | 2.88                     | 0.41              |
| 39:Sh:15:GLY:HA3   | 39:Sh:45:TRP:CH2    | 2.56                     | 0.41              |
| 44:LE:846:G:H2'    | 44:LE:847:C:H6      | 1.85                     | 0.41              |
| 44:LE:1074:U:OP1   | 82:Lq:41:LYS:HE3    | 2.21                     | 0.41              |
| 44:LE:1379:A:H2'   | 44:LE:1380:U:O4'    | 2.20                     | 0.41              |
| 45:LF:1883:OMG:H1' | 45:LF:1883:OMG:HM23 | 1.76                     | 0.41              |
| 46:LG:2206:G:H2'   | 46:LG:2207:G:N9     | 2.35                     | 0.41              |
| 47:LH:2880:C:H2'   | 47:LH:2881:G:C4     | 2.55                     | 0.41              |
| 48:LI:3277:A:O2'   | 48:LI:3278:G:H5'    | 2.20                     | 0.41              |
| 48:LI:3435:C:H2'   | 48:LI:3436:G:H5'    | 2.03                     | 0.41              |
| 49:LJ:3602:U:O2    | 49:LJ:3602:U:H2'    | 2.20                     | 0.41              |
| 51:LL:3822:U:C2    | 51:LL:3823:G:C8     | 3.08                     | 0.41              |
| 55:LP:28:ARG:HB3   | 55:LP:123:ARG:HB3   | 2.01                     | 0.41              |
| 55:LP:185:ASN:HD21 | 55:LP:188:ARG:HH11  | 1.68                     | 0.41              |
| 59:LT:149:GLU:OE1  | 59:LT:149:GLU:N     | 2.54                     | 0.41              |
| 60:LU:104:ALA:HB3  | 60:LU:105:ILE:HD12  | 2.03                     | 0.41              |
| 61:LV:109:PRO:HG3  | 67:Lb:18:VAL:HA     | 2.03                     | 0.41              |
| 62:LW:184:ARG:O    | 62:LW:188:ARG:HG2   | 2.20                     | 0.41              |
| 63:LX:203:MET:HE3  | 63:LX:203:MET:HB3   | 1.97                     | 0.41              |
| 64:LY:30:ASP:OD1   | 64:LY:112:MET:HE3   | 2.20                     | 0.41              |
| 65:LZ:68:MET:HE3   | 65:LZ:72:LEU:HB2    | 2.02                     | 0.41              |
| 67:Lb:183:LYS:HD3  | 67:Lb:195:ARG:NH2   | 2.35                     | 0.41              |
| 69:Ld:20:ARG:O     | 69:Ld:24:GLU:HG3    | 2.21                     | 0.41              |
| 71:Lf:105:ARG:O    | 71:Lf:109:ARG:HG3   | 2.20                     | 0.41              |
| 85:Lt:51:GLU:HG3   | 85:Lt:149:ILE:HD11  | 2.02                     | 0.41              |
| 87:Lv:39:ARG:O     | 87:Lv:42:THR:OG1    | 2.37                     | 0.41              |
| 91:Lz:24:LYS:HB3   | 91:Lz:69:ILE:HD11   | 2.02                     | 0.41              |
| 1:S1:96:C:H1'      | 1:S1:523:G:H5'      | 2.01                     | 0.41              |
| 1:S1:208:A:H2'     | 1:S1:209:U:C6       | 2.56                     | 0.41              |
| 1:S1:341:U:H2'     | 1:S1:342:G:N9       | 2.36                     | 0.41              |
| 1:S1:600:G:H8      | 1:S1:600:G:O5'      | 2.03                     | 0.41              |
| 1:S1:777:G:H2'     | 1:S1:778:U:C4'      | 2.51                     | 0.41              |
| 1:S1:882:G:HO2'    | 1:S1:883:A:P        | 2.44                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:S1:957:C:H2'    | 1:S1:958:A:O4'     | 2.21                     | 0.41              |
| 1:S1:1027:C:H4'   | 15:SJ:80:ASP:CG    | 2.45                     | 0.41              |
| 1:S1:1641:OMU:H1' | 1:S1:1641:OMU:HM23 | 1.85                     | 0.41              |
| 1:S1:1659:U:H2'   | 1:S1:1660:PSU:O4'  | 2.21                     | 0.41              |
| 1:S1:1672:U:H2'   | 1:S1:1673:G:H8     | 1.84                     | 0.41              |
| 1:S1:1840:C:H2'   | 1:S1:1841:G:C8     | 2.56                     | 0.41              |
| 6:SA:188:LEU:O    | 6:SA:190:THR:N     | 2.53                     | 0.41              |
| 10:SE:151:ASP:CG  | 10:SE:153:ASN:OD1  | 2.64                     | 0.41              |
| 13:SH:48:ARG:C    | 13:SH:50:ALA:H     | 2.29                     | 0.41              |
| 14:SI:52:ASN:HB2  | 14:SI:69:PHE:O     | 2.21                     | 0.41              |
| 21:SP:87:LYS:HD2  | 21:SP:87:LYS:HA    | 1.78                     | 0.41              |
| 23:SR:41:PHE:HA   | 23:SR:84:PHE:HE2   | 1.85                     | 0.41              |
| 32:Sa:100:LYS:HG2 | 32:Sa:112:THR:HG22 | 2.03                     | 0.41              |
| 42:LC:350:G:H2'   | 42:LC:351:C:C6     | 2.56                     | 0.41              |
| 42:LC:532:A:O3'   | 63:LX:29:ARG:NH2   | 2.53                     | 0.41              |
| 43:LD:651:C:OP1   | 86:Lu:13:LYS:HG2   | 2.20                     | 0.41              |
| 44:LE:1286:A:H2'  | 44:LE:1287:A:H8    | 1.86                     | 0.41              |
| 45:LF:1522:C:N4   | 45:LF:1523:U:O4    | 2.54                     | 0.41              |
| 45:LF:1676:A:O2'  | 48:LI:3470:C:O2    | 2.36                     | 0.41              |
| 45:LF:1687:C:OP2  | 62:LW:49:SER:HB2   | 2.21                     | 0.41              |
| 45:LF:1793:C:H2'  | 45:LF:1794:C:C6    | 2.56                     | 0.41              |
| 45:LF:1810:C:H2'  | 45:LF:1811:C:C6    | 2.56                     | 0.41              |
| 46:LG:2166:A:N6   | 71:Lf:129:LYS:HD2  | 2.35                     | 0.41              |
| 47:LH:2358:A2M:C2 | 47:LH:2365:C:H41   | 2.31                     | 0.41              |
| 48:LI:3011:U:H2'  | 48:LI:3012:A:H8    | 1.86                     | 0.41              |
| 48:LI:3207:A:H4'  | 48:LI:3208:OMC:O5' | 2.21                     | 0.41              |
| 48:LI:3278:G:N3   | 48:LI:3278:G:H2'   | 2.36                     | 0.41              |
| 54:LO:49:A:H5''   | 69:Ld:222:SER:OG   | 2.20                     | 0.41              |
| 62:LW:199:TYR:CE2 | 65:LZ:105:LYS:HG2  | 2.56                     | 0.41              |
| 76:Lk:96:LYS:HB3  | 76:Lk:102:THR:OG1  | 2.20                     | 0.41              |
| 77:Ll:68:LYS:O    | 77:Ll:82:ASP:N     | 2.54                     | 0.41              |
| 79:Ln:57:MET:HG2  | 79:Ln:61:LYS:HE3   | 2.03                     | 0.41              |
| 84:Ls:54:MET:HE1  | 88:Lw:96:ARG:NH2   | 2.35                     | 0.41              |
| 88:Lw:108:ARG:O   | 88:Lw:111:LYS:HG2  | 2.21                     | 0.41              |
| 89:Lx:87:LYS:HD2  | 89:Lx:87:LYS:HA    | 1.88                     | 0.41              |
| 1:S1:336:C:H42    | 1:S1:341:U:H3      | 1.68                     | 0.41              |
| 1:S1:516:G:OP1    | 12:SG:72:ARG:NH1   | 2.54                     | 0.41              |
| 1:S1:606:G:H2'    | 1:S1:607:G:C8      | 2.56                     | 0.41              |
| 1:S1:828:G:H3'    | 1:S1:829:G:C8      | 2.56                     | 0.41              |
| 1:S1:896:C:H2'    | 1:S1:897:C:C6      | 2.56                     | 0.41              |
| 1:S1:902:G:H2'    | 1:S1:903:U:C6      | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:1078:U:C2     | 1:S1:1079:C:C6     | 3.08                     | 0.41              |
| 1:S1:1596:U:H2'    | 1:S1:1597:UR3:O4'  | 2.20                     | 0.41              |
| 1:S1:1651:G:H1'    | 28:SW:84:HIS:CD2   | 2.56                     | 0.41              |
| 1:S1:1717:U:H5''   | 100:S1:2424:HOH:O  | 2.20                     | 0.41              |
| 1:S1:2001:G:H2'    | 1:S1:2002:C:C6     | 2.56                     | 0.41              |
| 1:S1:2034:G:C4     | 1:S1:2035:A:C8     | 3.09                     | 0.41              |
| 2:S2:9:A:N6        | 2:S2:22:G:N7       | 2.69                     | 0.41              |
| 3:S3:50:U:H3       | 3:S3:64:A:H61      | 1.68                     | 0.41              |
| 6:SA:66:LEU:HD21   | 20:SO:48:ILE:HG21  | 2.03                     | 0.41              |
| 6:SA:68:LEU:HD23   | 6:SA:68:LEU:HA     | 1.90                     | 0.41              |
| 7:SB:71:PRO:HB3    | 7:SB:186:ARG:HH22  | 1.86                     | 0.41              |
| 9:SD:106:GLU:HG2   | 9:SD:115:LYS:HZ2   | 1.86                     | 0.41              |
| 12:SG:56:CYS:O     | 12:SG:108:ILE:HG23 | 2.20                     | 0.41              |
| 13:SH:111:SER:OG   | 13:SH:122:ARG:HD3  | 2.21                     | 0.41              |
| 14:SI:50:TYR:OH    | 14:SI:73:ARG:NH2   | 2.40                     | 0.41              |
| 16:SK:37:LYS:O     | 16:SK:61:ARG:HA    | 2.21                     | 0.41              |
| 29:SX:79:ARG:HB3   | 29:SX:97:LYS:HB3   | 2.03                     | 0.41              |
| 31:SZ:91:GLU:CD    | 31:SZ:92:PRO:HD2   | 2.46                     | 0.41              |
| 38:Sg:73:LYS:HB2   | 38:Sg:84:ARG:CG    | 2.51                     | 0.41              |
| 38:Sg:219:ARG:HH21 | 38:Sg:220:ARG:HG3  | 1.84                     | 0.41              |
| 39:Sh:22:ALA:HB2   | 39:Sh:72:ASP:HA    | 2.03                     | 0.41              |
| 39:Sh:174:TRP:HA   | 39:Sh:198:TYR:HB2  | 2.03                     | 0.41              |
| 41:LB:240:G:H2'    | 41:LB:241:C:H6     | 1.86                     | 0.41              |
| 42:LC:316:A:H2'    | 42:LC:317:A:C8     | 2.56                     | 0.41              |
| 42:LC:339:U:OP2    | 89:Lx:26:ARG:HB2   | 2.21                     | 0.41              |
| 42:LC:350:G:C2     | 42:LC:459:U:C2     | 3.09                     | 0.41              |
| 42:LC:504:G:H2'    | 42:LC:505:U:C6     | 2.55                     | 0.41              |
| 42:LC:545:C:H2'    | 42:LC:546:G:O4'    | 2.21                     | 0.41              |
| 44:LE:960:G:H2'    | 44:LE:961:C:C6     | 2.56                     | 0.41              |
| 44:LE:1003:A:OP1   | 70:Le:184:ARG:NH2  | 2.37                     | 0.41              |
| 44:LE:1151:U:C5    | 95:L5:2:ALA:HA     | 2.56                     | 0.41              |
| 44:LE:1454:A:OP1   | 73:Lh:35:LYS:NZ    | 2.38                     | 0.41              |
| 45:LF:1536:U:H2'   | 45:LF:1537:U:O4'   | 2.21                     | 0.41              |
| 45:LF:1781:G:H2'   | 45:LF:1782:U:C6    | 2.56                     | 0.41              |
| 45:LF:1806:G:H2'   | 45:LF:1807:U:C6    | 2.55                     | 0.41              |
| 45:LF:1863:A:H1'   | 45:LF:1870:C:H42   | 1.85                     | 0.41              |
| 47:LH:2320:U:OP2   | 100:LH:3014:HOH:O  | 2.22                     | 0.41              |
| 47:LH:2642:PSU:H2' | 47:LH:2643:G:H8    | 1.85                     | 0.41              |
| 47:LH:2783:A:N3    | 48:LI:3516:C:O2'   | 2.49                     | 0.41              |
| 47:LH:2887:A2M:O2' | 47:LH:2888:G:H5'   | 2.21                     | 0.41              |
| 48:LI:2988:U:O2'   | 48:LI:2989:A:OP2   | 2.39                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 48:LI:3214:6MZ:H8   | 48:LI:3214:6MZ:OP1 | 2.20                     | 0.41              |
| 48:LI:3233:A:H2'    | 48:LI:3234:U:C6    | 2.56                     | 0.41              |
| 48:LI:3509:OMG:O4'  | 48:LI:3538:G:O2'   | 2.33                     | 0.41              |
| 49:LJ:3694:OMU:HM23 | 49:LJ:3694:OMU:H1' | 1.86                     | 0.41              |
| 50:LK:3795:A:H5''   | 65:LZ:5:LYS:HD2    | 2.02                     | 0.41              |
| 50:LK:3805:G:OP2    | 65:LZ:120:ARG:NH2  | 2.53                     | 0.41              |
| 51:LL:3879:U:H3     | 65:LZ:171:LYS:HE3  | 1.86                     | 0.41              |
| 51:LL:3903:A:C4     | 87:Lv:64:LYS:HG3   | 2.55                     | 0.41              |
| 54:LO:91:C:H2'      | 54:LO:92:C:C6      | 2.56                     | 0.41              |
| 55:LP:32:LEU:HD12   | 55:LP:121:ALA:HA   | 2.03                     | 0.41              |
| 55:LP:49:VAL:HG11   | 55:LP:60:LYS:HE3   | 2.01                     | 0.41              |
| 55:LP:82:MET:HE3    | 55:LP:82:MET:HB2   | 1.91                     | 0.41              |
| 55:LP:120:VAL:C     | 55:LP:122:ASP:H    | 2.28                     | 0.41              |
| 57:LR:108:LYS:HE2   | 67:Lb:203:TYR:HB3  | 2.02                     | 0.41              |
| 57:LR:324:ASN:HA    | 57:LR:330:ARG:HG2  | 2.03                     | 0.41              |
| 60:LU:20:LEU:O      | 60:LU:27:GLY:N     | 2.41                     | 0.41              |
| 60:LU:48:LYS:HE2    | 60:LU:48:LYS:HB2   | 1.90                     | 0.41              |
| 62:LW:189:LEU:HD13  | 65:LZ:183:GLU:HG3  | 2.03                     | 0.41              |
| 63:LX:63:PRO:HG3    | 63:LX:81:GLY:O     | 2.21                     | 0.41              |
| 63:LX:83:THR:HG22   | 63:LX:109:ARG:HB3  | 2.03                     | 0.41              |
| 63:LX:160:ASP:OD1   | 63:LX:160:ASP:N    | 2.54                     | 0.41              |
| 64:LY:8:LYS:HD3     | 64:LY:8:LYS:HA     | 1.76                     | 0.41              |
| 65:LZ:14:VAL:HG11   | 65:LZ:64:MET:HE3   | 2.03                     | 0.41              |
| 65:LZ:29:ILE:HG12   | 65:LZ:38:ILE:HD12  | 2.03                     | 0.41              |
| 68:Lc:16:ALA:O      | 68:Lc:18:PRO:HD3   | 2.20                     | 0.41              |
| 72:Lg:79:SER:HB2    | 72:Lg:132:LEU:HD11 | 2.02                     | 0.41              |
| 75:Lj:84:PHE:CD2    | 75:Lj:114:VAL:HG21 | 2.55                     | 0.41              |
| 82:Lq:80:ALA:O      | 82:Lq:83:PRO:HD2   | 2.20                     | 0.41              |
| 84:Ls:28:LEU:HD21   | 84:Ls:84:CYS:SG    | 2.60                     | 0.41              |
| 84:Ls:50:ASN:ND2    | 95:L5:41:TRP:O     | 2.54                     | 0.41              |
| 1:S1:109:C:H2'      | 1:S1:110:A2M:O4'   | 2.20                     | 0.41              |
| 1:S1:1435:G:H2'     | 1:S1:1436:C:C6     | 2.56                     | 0.41              |
| 1:S1:1611:G:H21     | 1:S1:2103:A:H5'    | 1.85                     | 0.41              |
| 6:SA:86:VAL:HG22    | 6:SA:96:THR:HG22   | 2.01                     | 0.41              |
| 8:SC:52:ILE:O       | 8:SC:90:ALA:HA     | 2.21                     | 0.41              |
| 9:SD:85:LEU:C       | 9:SD:86:LEU:HD12   | 2.46                     | 0.41              |
| 10:SE:128:LYS:HB3   | 10:SE:140:VAL:HB   | 2.02                     | 0.41              |
| 10:SE:160:VAL:HG11  | 10:SE:169:ILE:HG12 | 2.03                     | 0.41              |
| 14:SI:15:LYS:HA     | 14:SI:18:ARG:HB2   | 2.02                     | 0.41              |
| 26:SU:81:ILE:HG13   | 26:SU:92:ARG:HB2   | 2.03                     | 0.41              |
| 26:SU:85:MET:HB2    | 26:SU:88:THR:HB    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:SV:27:ASP:HB3   | 27:SV:30:THR:HG22  | 2.03                     | 0.41              |
| 31:SZ:115:LYS:HG2  | 31:SZ:119:MET:HE2  | 2.03                     | 0.41              |
| 39:Sh:257:GLU:HB2  | 39:Sh:289:GLU:OE1  | 2.21                     | 0.41              |
| 40:LA:20:U:OP2     | 57:LR:190:ARG:HD2  | 2.21                     | 0.41              |
| 44:LE:927:C:H2'    | 44:LE:928:U:O4'    | 2.21                     | 0.41              |
| 44:LE:1000:G:H2'   | 44:LE:1001:U:C6    | 2.56                     | 0.41              |
| 45:LF:1467:A:OP2   | 73:Lh:126:ARG:HB3  | 2.21                     | 0.41              |
| 45:LF:1863:A:H1'   | 45:LF:1870:C:N4    | 2.35                     | 0.41              |
| 45:LF:1894:G:N2    | 47:LH:2329:C:C5    | 2.89                     | 0.41              |
| 46:LG:2012:A:H1'   | 46:LG:2013:G:C8    | 2.55                     | 0.41              |
| 46:LG:2123:G:N2    | 46:LG:2125:PSU:O4  | 2.54                     | 0.41              |
| 47:LH:2938:G:H5''  | 47:LH:2946:C:C4    | 2.56                     | 0.41              |
| 48:LI:3303:G:H5''  | 73:Lh:83:ARG:NH1   | 2.36                     | 0.41              |
| 48:LI:3573:U:H2'   | 48:LI:3574:C:H6    | 1.86                     | 0.41              |
| 57:LR:128:PRO:HG3  | 80:Lo:72:GLU:HB2   | 2.02                     | 0.41              |
| 58:LS:85:LYS:HB3   | 58:LS:85:LYS:HE2   | 1.83                     | 0.41              |
| 59:LT:2:ARG:HH12   | 59:LT:63:LYS:HE2   | 1.86                     | 0.41              |
| 73:Lh:152:VAL:HG11 | 73:Lh:155:GLU:HG3  | 2.02                     | 0.41              |
| 75:Lj:88:LEU:O     | 75:Lj:92:ILE:HG12  | 2.21                     | 0.41              |
| 76:Lk:89:THR:HG22  | 76:Lk:162:ILE:HG23 | 2.03                     | 0.41              |
| 80:Lo:12:CYS:O     | 80:Lo:14:ALA:N     | 2.53                     | 0.41              |
| 83:Lr:82:PRO:HG3   | 83:Lr:139:TYR:CE2  | 2.56                     | 0.41              |
| 92:L1:13:TYR:CE1   | 92:L1:51:MET:HE3   | 2.55                     | 0.41              |
| 1:S1:600:G:H2'     | 1:S1:601:C:H6      | 1.85                     | 0.40              |
| 1:S1:749:U:H5''    | 1:S1:750:G:H8      | 1.86                     | 0.40              |
| 1:S1:1116:G:O2'    | 1:S1:1133:G:N2     | 2.55                     | 0.40              |
| 1:S1:1960:PSU:H2'  | 1:S1:1961:C:H6     | 1.87                     | 0.40              |
| 6:SA:165:LYS:HA    | 6:SA:165:LYS:HD2   | 1.84                     | 0.40              |
| 7:SB:190:PRO:HG2   | 7:SB:193:VAL:HB    | 2.04                     | 0.40              |
| 8:SC:68:ILE:HD12   | 8:SC:71:LEU:HD12   | 2.03                     | 0.40              |
| 8:SC:138:ILE:HG12  | 8:SC:188:VAL:HG22  | 2.03                     | 0.40              |
| 23:SR:2:SER:OG     | 23:SR:3:LEU:N      | 2.54                     | 0.40              |
| 27:SV:24:LEU:HB2   | 27:SV:58:MET:HE2   | 2.02                     | 0.40              |
| 30:SY:3:ASN:OD1    | 30:SY:7:ILE:HB     | 2.20                     | 0.40              |
| 38:Sg:163:VAL:HG12 | 38:Sg:174:VAL:HG22 | 2.03                     | 0.40              |
| 41:LB:185:G:H2'    | 42:LC:535:G:H4'    | 2.02                     | 0.40              |
| 44:LE:1203:C:OP2   | 90:Ly:30:GLN:HG2   | 2.21                     | 0.40              |
| 44:LE:1422:G:C2    | 82:Lq:85:TRP:HH2   | 2.38                     | 0.40              |
| 46:LG:2169:G:H2'   | 46:LG:2170:A:H5'   | 2.03                     | 0.40              |
| 46:LG:2186:U:H5'   | 88:Lw:61:ARG:HD2   | 2.03                     | 0.40              |
| 47:LH:2830:G:N3    | 49:LJ:3644:PSU:O2' | 2.54                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:LJ:3645:U:H1'   | 49:LJ:3647:C:OP2   | 2.21                     | 0.40              |
| 51:LL:3834:A:H4'   | 56:LQ:95:THR:HG22  | 2.03                     | 0.40              |
| 58:LS:120:ILE:H    | 58:LS:120:ILE:HG13 | 1.67                     | 0.40              |
| 60:LU:191:HIS:CD2  | 60:LU:192:LEU:HG   | 2.56                     | 0.40              |
| 62:LW:129:HIS:O    | 62:LW:133:ARG:HB2  | 2.21                     | 0.40              |
| 70:Le:45:ALA:HA    | 70:Le:48:LYS:HE3   | 2.04                     | 0.40              |
| 71:Lf:116:ILE:HG22 | 71:Lf:120:LEU:HD23 | 2.03                     | 0.40              |
| 81:Lp:14:LYS:HE2   | 81:Lp:18:LEU:HD11  | 2.01                     | 0.40              |
| 85:Lt:120:SER:C    | 85:Lt:122:ASP:H    | 2.29                     | 0.40              |
| 87:Lv:16:GLY:HA2   | 87:Lv:102:ILE:HG12 | 2.03                     | 0.40              |
| 1:S1:159:G:N7      | 12:SG:139:ARG:NH2  | 2.68                     | 0.40              |
| 1:S1:1767:U:O2'    | 29:SX:135:ASP:OD2  | 2.37                     | 0.40              |
| 1:S1:2041:OMU:H1'  | 1:S1:2041:OMU:HM22 | 1.46                     | 0.40              |
| 6:SA:22:MET:HE3    | 20:SO:89:CYS:HB3   | 2.02                     | 0.40              |
| 14:SI:15:LYS:HE2   | 14:SI:15:LYS:HB2   | 1.88                     | 0.40              |
| 22:SQ:66:GLU:O     | 22:SQ:69:TYR:N     | 2.55                     | 0.40              |
| 22:SQ:135:HIS:HA   | 22:SQ:138:ARG:HH11 | 1.86                     | 0.40              |
| 23:SR:131:ARG:HD3  | 23:SR:131:ARG:HA   | 1.91                     | 0.40              |
| 33:Sb:22:ARG:HD2   | 33:Sb:27:GLY:O     | 2.21                     | 0.40              |
| 37:Sf:88:ARG:HB2   | 37:Sf:89:PRO:HD2   | 2.02                     | 0.40              |
| 39:Sh:19:TRP:N     | 39:Sh:19:TRP:CD1   | 2.88                     | 0.40              |
| 42:LC:303:C:P      | 90:Ly:95:ARG:HH22  | 2.44                     | 0.40              |
| 42:LC:449:G:H2'    | 42:LC:450:G:C8     | 2.56                     | 0.40              |
| 44:LE:1375:G:H2'   | 44:LE:1375:G:N3    | 2.36                     | 0.40              |
| 45:LF:1515:C:H4'   | 45:LF:1709:C:C4    | 2.57                     | 0.40              |
| 45:LF:1587:U:H2'   | 45:LF:1588:A:H8    | 1.85                     | 0.40              |
| 45:LF:1833:U:H2'   | 45:LF:1834:A:H8    | 1.86                     | 0.40              |
| 47:LH:2661:U:H5''  | 55:LP:18:THR:HG23  | 2.03                     | 0.40              |
| 47:LH:2962:G:H4'   | 47:LH:2966:C:H42   | 1.85                     | 0.40              |
| 48:LI:3158:C:H2'   | 48:LI:3159:OMU:H6  | 2.03                     | 0.40              |
| 48:LI:3206:PSU:OP2 | 48:LI:3207:A:O2'   | 2.34                     | 0.40              |
| 51:LL:3846:G:H1    | 65:LZ:173:ASP:CB   | 2.33                     | 0.40              |
| 51:LL:3854:A:H3'   | 51:LL:3855:G:H8    | 1.86                     | 0.40              |
| 54:LO:63:C:H5''    | 68:Lc:205:ARG:HA   | 2.03                     | 0.40              |
| 55:LP:35:GLY:HA2   | 61:LV:73:VAL:HG13  | 2.02                     | 0.40              |
| 56:LQ:213:GLU:HG3  | 56:LQ:287:ILE:N    | 2.37                     | 0.40              |
| 72:Lg:96:GLU:HG3   | 72:Lg:142:ILE:HG13 | 2.03                     | 0.40              |
| 72:Lg:151:LYS:HE2  | 72:Lg:151:LYS:HB3  | 1.91                     | 0.40              |
| 76:Lk:77:LYS:HA    | 76:Lk:77:LYS:HD2   | 1.85                     | 0.40              |
| 83:Lr:84:ILE:HD13  | 83:Lr:188:LEU:O    | 2.21                     | 0.40              |
| 83:Lr:165:THR:O    | 83:Lr:169:ILE:HG13 | 2.20                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 83:Lr:236:GLN:O    | 83:Lr:240:LYS:HG3  | 2.20                     | 0.40              |
| 87:Lv:97:LEU:HD23  | 87:Lv:97:LEU:HA    | 1.81                     | 0.40              |
| 88:Lw:39:LYS:HB2   | 88:Lw:63:ARG:NH1   | 2.37                     | 0.40              |
| 89:Lx:93:GLU:O     | 89:Lx:97:LYS:HG2   | 2.20                     | 0.40              |
| 1:S1:12:U:H2'      | 1:S1:13:C:H6       | 1.83                     | 0.40              |
| 1:S1:68:A:O2'      | 1:S1:69:A:H3'      | 2.22                     | 0.40              |
| 1:S1:454:G:O2'     | 1:S1:455:U:H5'     | 2.21                     | 0.40              |
| 1:S1:1300:U:H1'    | 1:S1:1303:A:N7     | 2.37                     | 0.40              |
| 1:S1:1315:G:H21    | 20:SO:51:ARG:HA    | 1.87                     | 0.40              |
| 1:S1:1534:A:H2'    | 1:S1:1535:A:C8     | 2.57                     | 0.40              |
| 1:S1:2056:G:N1     | 1:S1:2059:A:OP2    | 2.53                     | 0.40              |
| 1:S1:2184:G:H4'    | 12:SG:65:GLN:NE2   | 2.35                     | 0.40              |
| 1:S1:2302:C:C6     | 33:Sb:93:ARG:HB3   | 2.57                     | 0.40              |
| 10:SE:32:ARG:NH2   | 10:SE:79:ASP:OD2   | 2.54                     | 0.40              |
| 13:SH:78:HIS:CD2   | 13:SH:155:PHE:CD2  | 2.98                     | 0.40              |
| 15:SJ:119:LYS:HB3  | 15:SJ:119:LYS:HE2  | 1.64                     | 0.40              |
| 17:SL:49:PRO:HG2   | 17:SL:52:LEU:HD12  | 2.02                     | 0.40              |
| 25:ST:34:VAL:HG21  | 25:ST:69:ARG:HH22  | 1.86                     | 0.40              |
| 29:SX:42:LEU:HA    | 29:SX:42:LEU:HD23  | 1.78                     | 0.40              |
| 30:SY:20:THR:HG22  | 30:SY:21:ASN:N     | 2.31                     | 0.40              |
| 31:SZ:40:PRO:O     | 31:SZ:44:ILE:HG13  | 2.21                     | 0.40              |
| 34:Sc:35:MET:HE2   | 34:Sc:50:SER:HA    | 2.03                     | 0.40              |
| 35:Sd:20:ILE:HG12  | 35:Sd:36:ARG:O     | 2.21                     | 0.40              |
| 38:Sg:133:CYS:HB3  | 38:Sg:214:LYS:O    | 2.22                     | 0.40              |
| 39:Sh:65:GLY:O     | 39:Sh:92:ARG:NH2   | 2.55                     | 0.40              |
| 39:Sh:182:SER:HB3  | 39:Sh:189:LEU:HD11 | 2.04                     | 0.40              |
| 39:Sh:224:ASP:H    | 39:Sh:231:LEU:HD23 | 1.86                     | 0.40              |
| 40:LA:150:G:OP1    | 67:Lb:38:ARG:HD3   | 2.21                     | 0.40              |
| 44:LE:914:G:H2'    | 44:LE:915:C:C6     | 2.56                     | 0.40              |
| 44:LE:937:G:H2'    | 44:LE:938:7MG:O4'  | 2.22                     | 0.40              |
| 44:LE:1196:A:H5'   | 55:LP:183:GLY:HA2  | 2.02                     | 0.40              |
| 46:LG:2064:C:H4'   | 79:Ln:75:VAL:HA    | 2.04                     | 0.40              |
| 47:LH:2232:G:H2'   | 47:LH:2233:U:C6    | 2.57                     | 0.40              |
| 47:LH:2671:A:O2'   | 55:LP:236:GLY:N    | 2.51                     | 0.40              |
| 48:LI:3033:C:H2'   | 48:LI:3034:G:H8    | 1.85                     | 0.40              |
| 48:LI:3207:A:H62   | 48:LI:3214:6MZ:C8  | 2.34                     | 0.40              |
| 48:LI:3527:A:N7    | 56:LQ:2:SER:N      | 2.70                     | 0.40              |
| 49:LJ:3624:C:H2'   | 49:LJ:3625:C:O4'   | 2.21                     | 0.40              |
| 50:LK:3752:G:O2'   | 50:LK:3754:A:OP2   | 2.38                     | 0.40              |
| 53:LN:3969:PSU:H2' | 53:LN:3970:C:H6    | 1.86                     | 0.40              |
| 54:LO:35:C:H5      | 54:LO:45:U:HO2'    | 1.66                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:LO:65:G:O2'     | 69:Ld:9:ARG:HG2    | 2.21                     | 0.40              |
| 68:Lc:35:ASP:HB3   | 68:Lc:39:ARG:HD2   | 2.04                     | 0.40              |
| 69:Ld:24:GLU:OE1   | 69:Ld:26:LYS:HD2   | 2.22                     | 0.40              |
| 69:Ld:157:ILE:H    | 69:Ld:157:ILE:HG12 | 1.69                     | 0.40              |
| 70:Le:74:LYS:HD3   | 70:Le:136:VAL:HG21 | 2.03                     | 0.40              |
| 70:Le:81:CYS:O     | 70:Le:101:ALA:HA   | 2.22                     | 0.40              |
| 75:Lj:84:PHE:HB2   | 75:Lj:134:TYR:CE2  | 2.56                     | 0.40              |
| 75:Lj:137:LYS:HD2  | 75:Lj:137:LYS:HA   | 1.73                     | 0.40              |
| 83:Lr:82:PRO:HG3   | 83:Lr:139:TYR:CZ   | 2.56                     | 0.40              |
| 83:Lr:187:GLN:O    | 83:Lr:191:CYS:HA   | 2.22                     | 0.40              |
| 85:Lt:90:ARG:HB2   | 85:Lt:132:VAL:HG12 | 2.04                     | 0.40              |
| 1:S1:521:C:H4'     | 1:S1:523:G:OP1     | 2.21                     | 0.40              |
| 1:S1:1015:C:H2'    | 1:S1:1016:C:H6     | 1.86                     | 0.40              |
| 1:S1:1671:G:H2'    | 1:S1:1672:U:C6     | 2.55                     | 0.40              |
| 1:S1:1866:A:H2'    | 1:S1:1867:G:O4'    | 2.21                     | 0.40              |
| 4:S4:34:G:OP1      | 35:Sd:29:ARG:NH1   | 2.55                     | 0.40              |
| 7:SB:85:ARG:HA     | 7:SB:85:ARG:HD2    | 1.96                     | 0.40              |
| 10:SE:54:TYR:CD1   | 31:SZ:17:MET:HE1   | 2.57                     | 0.40              |
| 10:SE:151:ASP:OD2  | 10:SE:172:TRP:CH2  | 2.74                     | 0.40              |
| 10:SE:228:ILE:HG13 | 10:SE:228:ILE:O    | 2.21                     | 0.40              |
| 13:SH:29:SER:OG    | 13:SH:50:ALA:O     | 2.24                     | 0.40              |
| 17:SL:54:LEU:HD23  | 17:SL:54:LEU:HA    | 1.89                     | 0.40              |
| 23:SR:102:ASN:HA   | 23:SR:105:GLU:OE2  | 2.20                     | 0.40              |
| 25:ST:56:ASP:O     | 34:Sc:48:VAL:HA    | 2.22                     | 0.40              |
| 27:SV:58:MET:HA    | 27:SV:61:ILE:HD12  | 2.03                     | 0.40              |
| 40:LA:68:PSU:H2'   | 40:LA:69:G:O4'     | 2.22                     | 0.40              |
| 42:LC:339:U:P      | 89:Lx:26:ARG:HH11  | 2.44                     | 0.40              |
| 42:LC:372:U:H3     | 42:LC:437:G:H22    | 1.69                     | 0.40              |
| 42:LC:571:A:H2'    | 42:LC:572:G:O4'    | 2.21                     | 0.40              |
| 45:LF:1859:PSU:H2' | 45:LF:1860:G:C8    | 2.57                     | 0.40              |
| 46:LG:2155:C:N4    | 46:LG:2156:G:C6    | 2.90                     | 0.40              |
| 47:LH:2367:A:H2'   | 47:LH:2368:A:H8    | 1.87                     | 0.40              |
| 47:LH:2674:U:H2'   | 47:LH:2675:G:O4'   | 2.20                     | 0.40              |
| 47:LH:2945:G:H2'   | 47:LH:2946:C:C5    | 2.56                     | 0.40              |
| 48:LI:3240:A:H2'   | 48:LI:3241:G:O4'   | 2.21                     | 0.40              |
| 48:LI:3385:A:H5''  | 48:LI:3386:G:O5'   | 2.22                     | 0.40              |
| 48:LI:3438:C:N3    | 68:Lc:158:LYS:NZ   | 2.44                     | 0.40              |
| 48:LI:3577:G:H5'   | 56:LQ:20:LYS:HB3   | 2.03                     | 0.40              |
| 49:LJ:3618:G:H2'   | 49:LJ:3619:A:C8    | 2.57                     | 0.40              |
| 51:LL:3818:U:O2'   | 65:LZ:129:VAL:HG11 | 2.21                     | 0.40              |
| 55:LP:65:HIS:HB3   | 55:LP:68:LYS:O     | 2.22                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:LQ:213:GLU:HG3  | 56:LQ:287:ILE:H    | 1.87                     | 0.40              |
| 56:LQ:383:PHE:CE2  | 78:Lm:12:PRO:HD3   | 2.57                     | 0.40              |
| 58:LS:119:HIS:O    | 58:LS:122:LEU:HB2  | 2.22                     | 0.40              |
| 59:LT:40:HIS:HD1   | 59:LT:41:VAL:HG13  | 1.86                     | 0.40              |
| 59:LT:63:LYS:HE3   | 59:LT:63:LYS:HB2   | 1.92                     | 0.40              |
| 61:LV:101:ILE:O    | 61:LV:105:ARG:HG2  | 2.21                     | 0.40              |
| 69:Ld:101:GLY:O    | 69:Ld:164:VAL:HG12 | 2.21                     | 0.40              |
| 71:Lf:26:ASP:HB3   | 71:Lf:29:GLU:HB2   | 2.02                     | 0.40              |
| 71:Lf:140:MET:HE3  | 71:Lf:140:MET:HB3  | 1.96                     | 0.40              |
| 83:Lr:237:LEU:HD11 | 83:Lr:241:MET:HE3  | 2.02                     | 0.40              |
| 1:S1:207:C:H2'     | 1:S1:208:A:C8      | 2.56                     | 0.40              |
| 1:S1:272:C:H2'     | 1:S1:273:C:H6      | 1.86                     | 0.40              |
| 1:S1:940:G:P       | 38:Sg:214:LYS:HG3  | 2.61                     | 0.40              |
| 1:S1:1074:U:C3'    | 1:S1:1075:C:H5''   | 2.48                     | 0.40              |
| 1:S1:1084:G:H21    | 15:SJ:107:SER:HB3  | 1.87                     | 0.40              |
| 1:S1:1095:C:H2'    | 25:ST:73:ARG:NH2   | 2.36                     | 0.40              |
| 1:S1:1114:U:HO2'   | 1:S1:1117:A:P      | 2.41                     | 0.40              |
| 1:S1:1141:U:H2'    | 1:S1:1143:U:C5     | 2.56                     | 0.40              |
| 1:S1:1725:U:O2     | 27:SV:4:VAL:HG11   | 2.21                     | 0.40              |
| 1:S1:1756:U:H5     | 1:S1:2019:A:OP1    | 2.05                     | 0.40              |
| 1:S1:2284:G:H2'    | 1:S1:2285:U:O4'    | 2.22                     | 0.40              |
| 4:S4:19:G:H4'      | 4:S4:20:U:C5       | 2.56                     | 0.40              |
| 4:S4:21:A:C6       | 4:S4:48:C:C2       | 3.09                     | 0.40              |
| 7:SB:36:ARG:O      | 34:Sc:2:SER:HA     | 2.21                     | 0.40              |
| 9:SD:110:GLN:NE2   | 9:SD:122:ILE:HG13  | 2.36                     | 0.40              |
| 11:SF:98:ARG:HE    | 11:SF:98:ARG:HB2   | 1.60                     | 0.40              |
| 13:SH:187:LYS:HE2  | 13:SH:187:LYS:HB3  | 1.94                     | 0.40              |
| 24:SS:35:LEU:HG    | 24:SS:37:MET:HG2   | 2.04                     | 0.40              |
| 25:ST:45:VAL:HG12  | 25:ST:49:GLN:HB2   | 2.03                     | 0.40              |
| 34:Sc:35:MET:HE3   | 34:Sc:48:VAL:HG23  | 2.04                     | 0.40              |
| 37:Sf:138:ASP:N    | 37:Sf:138:ASP:OD1  | 2.55                     | 0.40              |
| 38:Sg:236:ARG:HA   | 38:Sg:239:SER:OG   | 2.21                     | 0.40              |
| 42:LC:436:U:H2'    | 42:LC:437:G:H8     | 1.86                     | 0.40              |
| 42:LC:457:G:H2'    | 42:LC:458:C:O4'    | 2.21                     | 0.40              |
| 43:LD:732:U:C5     | 43:LD:742:G:C8     | 3.09                     | 0.40              |
| 44:LE:1006:G:H2'   | 44:LE:1007:C:O4'   | 2.22                     | 0.40              |
| 44:LE:1255:U:H2'   | 44:LE:1256:U:C6    | 2.57                     | 0.40              |
| 44:LE:1286:A:P     | 83:Lr:35:LYS:HE3   | 2.61                     | 0.40              |
| 45:LF:1501:C:H2'   | 45:LF:1502:A2M:H8  | 2.04                     | 0.40              |
| 46:LG:2038:G:H2'   | 46:LG:2039:G:H8    | 1.86                     | 0.40              |
| 47:LH:2287:C:H2'   | 47:LH:2288:C:C6    | 2.56                     | 0.40              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 47:LH:2377:G:H2'    | 47:LH:2378:C:C6    | 2.57                     | 0.40              |
| 47:LH:2610:OMG:HM23 | 47:LH:2610:OMG:H1' | 1.89                     | 0.40              |
| 47:LH:2637:A:N3     | 100:LH:3037:HOH:O  | 2.37                     | 0.40              |
| 48:LI:3139:U:H1'    | 48:LI:3140:C:H5    | 1.86                     | 0.40              |
| 48:LI:3163:A:H4'    | 48:LI:3165:C:C2    | 2.56                     | 0.40              |
| 56:LQ:228:PHE:CE2   | 56:LQ:270:GLY:HA2  | 2.57                     | 0.40              |
| 57:LR:194:ARG:HA    | 57:LR:194:ARG:HD2  | 1.89                     | 0.40              |
| 58:LS:171:LYS:HB2   | 58:LS:171:LYS:HE3  | 1.88                     | 0.40              |
| 69:Ld:230:LYS:HG2   | 69:Ld:231:PRO:HD2  | 2.02                     | 0.40              |
| 70:Le:82:VAL:HG22   | 70:Le:122:PHE:CZ   | 2.56                     | 0.40              |
| 73:Lh:75:LEU:HD23   | 73:Lh:88:LYS:HG2   | 2.02                     | 0.40              |
| 73:Lh:111:HIS:O     | 73:Lh:115:VAL:HG23 | 2.21                     | 0.40              |
| 74:Li:6:TYR:HE1     | 74:Li:20:ARG:HE    | 1.68                     | 0.40              |
| 83:Lr:230:ARG:CZ    | 83:Lr:237:LEU:HD22 | 2.51                     | 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 PDB entries followed by that with respect to all EM entries.

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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6   | SA    | 219/249 (88%) | 197 (90%) | 22 (10%) | 0        | 100         | 100 |
| 7   | SB    | 205/261 (78%) | 186 (91%) | 19 (9%)  | 0        | 100         | 100 |
| 8   | SC    | 210/220 (96%) | 196 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 9   | SD    | 175/196 (89%) | 166 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 10  | SE    | 263/271 (97%) | 243 (92%) | 20 (8%)  | 0        | 100         | 100 |
| 11  | SF    | 219/257 (85%) | 207 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 12  | SG    | 246/283 (87%) | 227 (92%) | 19 (8%)  | 0        | 100         | 100 |
| 13  | SH    | 178/190 (94%) | 154 (86%) | 23 (13%) | 1 (1%)   | 21          | 52  |
| 14  | SI    | 183/200 (92%) | 168 (92%) | 15 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 15  | SJ    | 127/130 (98%) | 116 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 16  | SK    | 195/304 (64%) | 182 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 17  | SL    | 141/151 (93%) | 132 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 18  | SM    | 99/121 (82%)  | 96 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 19  | SN    | 90/152 (59%)  | 86 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 20  | SO    | 133/152 (88%) | 125 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 21  | SP    | 139/143 (97%) | 132 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 22  | SQ    | 120/139 (86%) | 100 (83%) | 20 (17%) | 0        | 100         | 100 |
| 23  | SR    | 144/153 (94%) | 132 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 24  | SS    | 50/55 (91%)   | 44 (88%)  | 6 (12%)  | 0        | 100         | 100 |
| 25  | ST    | 144/151 (95%) | 129 (90%) | 15 (10%) | 0        | 100         | 100 |
| 26  | SU    | 146/164 (89%) | 135 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 27  | SV    | 123/145 (85%) | 113 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 28  | SW    | 123/150 (82%) | 117 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 29  | SX    | 141/148 (95%) | 130 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 30  | SY    | 80/96 (83%)   | 72 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 31  | SZ    | 125/137 (91%) | 116 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 32  | Sa    | 74/119 (62%)  | 69 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 33  | Sb    | 95/120 (79%)  | 89 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 34  | Sc    | 82/86 (95%)   | 78 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 35  | Sd    | 61/76 (80%)   | 50 (82%)  | 11 (18%) | 0        | 100         | 100 |
| 36  | Se    | 60/67 (90%)   | 53 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 37  | Sf    | 62/157 (40%)  | 57 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 38  | Sg    | 195/295 (66%) | 164 (84%) | 31 (16%) | 0        | 100         | 100 |
| 39  | Sh    | 309/317 (98%) | 270 (87%) | 39 (13%) | 0        | 100         | 100 |
| 55  | LP    | 247/264 (94%) | 232 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 56  | LQ    | 390/410 (95%) | 365 (94%) | 25 (6%)  | 0        | 100         | 100 |
| 57  | LR    | 363/375 (97%) | 338 (93%) | 25 (7%)  | 0        | 100         | 100 |
| 58  | LS    | 176/191 (92%) | 166 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 59  | LT    | 188/193 (97%) | 177 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 60  | LU    | 192/195 (98%) | 171 (89%) | 21 (11%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 61  | LV    | 236/295 (80%) | 228 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 62  | LW    | 206/209 (99%) | 194 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 63  | LX    | 217/226 (96%) | 196 (90%) | 21 (10%) | 0        | 100         | 100 |
| 64  | LY    | 132/140 (94%) | 120 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 65  | LZ    | 215/219 (98%) | 198 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 66  | La    | 149/152 (98%) | 138 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 67  | Lb    | 201/204 (98%) | 191 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 68  | Lc    | 199/215 (93%) | 183 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 69  | Ld    | 258/260 (99%) | 242 (94%) | 16 (6%)  | 0        | 100         | 100 |
| 70  | Le    | 190/193 (98%) | 176 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 71  | Lf    | 168/250 (67%) | 157 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 72  | Lg    | 179/182 (98%) | 160 (89%) | 19 (11%) | 0        | 100         | 100 |
| 73  | Lh    | 156/159 (98%) | 141 (90%) | 15 (10%) | 0        | 100         | 100 |
| 74  | Li    | 153/164 (93%) | 147 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 75  | Lj    | 99/170 (58%)  | 94 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 76  | Lk    | 129/163 (79%) | 114 (88%) | 15 (12%) | 0        | 100         | 100 |
| 77  | Ll    | 122/146 (84%) | 112 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 78  | Lm    | 64/157 (41%)  | 62 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 79  | Ln    | 131/134 (98%) | 122 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 80  | Lo    | 54/72 (75%)   | 48 (89%)  | 6 (11%)  | 0        | 100         | 100 |
| 81  | Lp    | 119/123 (97%) | 115 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 82  | Lq    | 89/117 (76%)  | 83 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 83  | Lr    | 216/242 (89%) | 208 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 84  | Ls    | 95/109 (87%)  | 92 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 85  | Lt    | 109/151 (72%) | 98 (90%)  | 11 (10%) | 0        | 100         | 100 |
| 86  | Lu    | 126/139 (91%) | 121 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 87  | Lv    | 112/115 (97%) | 106 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 88  | Lw    | 112/128 (88%) | 99 (88%)  | 13 (12%) | 0        | 100         | 100 |
| 89  | Lx    | 100/106 (94%) | 96 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 90  | Ly    | 104/117 (89%) | 95 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 91  | Lz    | 68/82 (83%)   | 66 (97%)  | 2 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 92  | L1    | 48/51 (94%)       | 44 (92%)    | 4 (8%)   | 0        | 100         | 100 |
| 93  | L2    | 49/126 (39%)      | 48 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 94  | L3    | 31/34 (91%)       | 27 (87%)    | 4 (13%)  | 0        | 100         | 100 |
| 95  | L5    | 88/92 (96%)       | 82 (93%)    | 6 (7%)   | 0        | 100         | 100 |
| 96  | L4    | 95/106 (90%)      | 87 (92%)    | 8 (8%)   | 0        | 100         | 100 |
| 97  | L6    | 57/69 (83%)       | 53 (93%)    | 4 (7%)   | 0        | 100         | 100 |
| 98  | L7    | 52/64 (81%)       | 51 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 11440/13164 (87%) | 10574 (92%) | 865 (8%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | SH    | 64  | TYR  |

### 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 PDB entries followed by that with respect to all EM entries.

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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 6   | SA    | 204/224 (91%) | 204 (100%) | 0        | 100         | 100 |
| 7   | SB    | 179/215 (83%) | 179 (100%) | 0        | 100         | 100 |
| 8   | SC    | 177/184 (96%) | 177 (100%) | 0        | 100         | 100 |
| 9   | SD    | 155/169 (92%) | 155 (100%) | 0        | 100         | 100 |
| 10  | SE    | 231/237 (98%) | 231 (100%) | 0        | 100         | 100 |
| 11  | SF    | 184/206 (89%) | 184 (100%) | 0        | 100         | 100 |
| 12  | SG    | 217/231 (94%) | 217 (100%) | 0        | 100         | 100 |
| 13  | SH    | 160/166 (96%) | 160 (100%) | 0        | 100         | 100 |
| 14  | SI    | 165/176 (94%) | 165 (100%) | 0        | 100         | 100 |
| 15  | SJ    | 115/116 (99%) | 115 (100%) | 0        | 100         | 100 |
| 16  | SK    | 169/258 (66%) | 169 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 17  | SL    | 119/125 (95%)  | 119 (100%) | 0        | 100         | 100 |
| 18  | SM    | 91/104 (88%)   | 91 (100%)  | 0        | 100         | 100 |
| 19  | SN    | 83/119 (70%)   | 83 (100%)  | 0        | 100         | 100 |
| 20  | SO    | 104/119 (87%)  | 103 (99%)  | 1 (1%)   | 68          | 76  |
| 21  | SP    | 118/120 (98%)  | 118 (100%) | 0        | 100         | 100 |
| 22  | SQ    | 97/113 (86%)   | 97 (100%)  | 0        | 100         | 100 |
| 23  | SR    | 129/135 (96%)  | 128 (99%)  | 1 (1%)   | 73          | 78  |
| 24  | SS    | 43/45 (96%)    | 43 (100%)  | 0        | 100         | 100 |
| 25  | ST    | 129/131 (98%)  | 129 (100%) | 0        | 100         | 100 |
| 26  | SU    | 132/146 (90%)  | 132 (100%) | 0        | 100         | 100 |
| 27  | SV    | 111/125 (89%)  | 111 (100%) | 0        | 100         | 100 |
| 28  | SW    | 104/127 (82%)  | 104 (100%) | 0        | 100         | 100 |
| 29  | SX    | 114/117 (97%)  | 114 (100%) | 0        | 100         | 100 |
| 30  | SY    | 63/76 (83%)    | 63 (100%)  | 0        | 100         | 100 |
| 31  | SZ    | 113/121 (93%)  | 113 (100%) | 0        | 100         | 100 |
| 32  | Sa    | 70/99 (71%)    | 70 (100%)  | 0        | 100         | 100 |
| 33  | Sb    | 85/97 (88%)    | 85 (100%)  | 0        | 100         | 100 |
| 34  | Sc    | 75/77 (97%)    | 75 (100%)  | 0        | 100         | 100 |
| 35  | Sd    | 55/65 (85%)    | 55 (100%)  | 0        | 100         | 100 |
| 36  | Se    | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 37  | Sf    | 55/136 (40%)   | 55 (100%)  | 0        | 100         | 100 |
| 38  | Sg    | 169/241 (70%)  | 169 (100%) | 0        | 100         | 100 |
| 39  | Sh    | 261/267 (98%)  | 261 (100%) | 0        | 100         | 100 |
| 55  | LP    | 195/208 (94%)  | 195 (100%) | 0        | 100         | 100 |
| 56  | LQ    | 329/344 (96%)  | 329 (100%) | 0        | 100         | 100 |
| 57  | LR    | 305/314 (97%)  | 305 (100%) | 0        | 100         | 100 |
| 58  | LS    | 154/166 (93%)  | 154 (100%) | 0        | 100         | 100 |
| 59  | LT    | 166/168 (99%)  | 166 (100%) | 0        | 100         | 100 |
| 60  | LU    | 173/174 (99%)  | 173 (100%) | 0        | 100         | 100 |
| 61  | LV    | 206/242 (85%)  | 206 (100%) | 0        | 100         | 100 |
| 62  | LW    | 182/183 (100%) | 182 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 63  | LX    | 187/192 (97%)  | 187 (100%) | 0        | 100         | 100 |
| 64  | LY    | 104/109 (95%)  | 104 (100%) | 0        | 100         | 100 |
| 65  | LZ    | 190/192 (99%)  | 189 (100%) | 1 (0%)   | 81          | 82  |
| 66  | La    | 123/124 (99%)  | 123 (100%) | 0        | 100         | 100 |
| 67  | Lb    | 174/175 (99%)  | 174 (100%) | 0        | 100         | 100 |
| 68  | Lc    | 167/175 (95%)  | 167 (100%) | 0        | 100         | 100 |
| 69  | Ld    | 213/213 (100%) | 213 (100%) | 0        | 100         | 100 |
| 70  | Le    | 162/163 (99%)  | 162 (100%) | 0        | 100         | 100 |
| 71  | Lf    | 142/208 (68%)  | 142 (100%) | 0        | 100         | 100 |
| 72  | Lg    | 164/165 (99%)  | 164 (100%) | 0        | 100         | 100 |
| 73  | Lh    | 140/141 (99%)  | 140 (100%) | 0        | 100         | 100 |
| 74  | Li    | 131/139 (94%)  | 130 (99%)  | 1 (1%)   | 73          | 78  |
| 75  | Lj    | 90/144 (62%)   | 90 (100%)  | 0        | 100         | 100 |
| 76  | Lk    | 117/139 (84%)  | 117 (100%) | 0        | 100         | 100 |
| 77  | Ll    | 110/129 (85%)  | 110 (100%) | 0        | 100         | 100 |
| 78  | Lm    | 62/135 (46%)   | 62 (100%)  | 0        | 100         | 100 |
| 79  | Ln    | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 80  | Lo    | 48/59 (81%)    | 48 (100%)  | 0        | 100         | 100 |
| 81  | Lp    | 111/113 (98%)  | 111 (100%) | 0        | 100         | 100 |
| 82  | Lq    | 81/102 (79%)   | 81 (100%)  | 0        | 100         | 100 |
| 83  | Lr    | 193/215 (90%)  | 193 (100%) | 0        | 100         | 100 |
| 84  | Ls    | 84/94 (89%)    | 84 (100%)  | 0        | 100         | 100 |
| 85  | Lt    | 101/138 (73%)  | 101 (100%) | 0        | 100         | 100 |
| 86  | Lu    | 113/121 (93%)  | 113 (100%) | 0        | 100         | 100 |
| 87  | Lv    | 97/98 (99%)    | 97 (100%)  | 0        | 100         | 100 |
| 88  | Lw    | 101/113 (89%)  | 101 (100%) | 0        | 100         | 100 |
| 89  | Lx    | 86/90 (96%)    | 86 (100%)  | 0        | 100         | 100 |
| 90  | Ly    | 89/96 (93%)    | 89 (100%)  | 0        | 100         | 100 |
| 91  | Lz    | 67/76 (88%)    | 67 (100%)  | 0        | 100         | 100 |
| 92  | L1    | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |
| 93  | L2    | 47/108 (44%)   | 47 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 94  | L3    | 31/32 (97%)      | 31 (100%)   | 0        | 100         | 100 |
| 95  | L5    | 74/76 (97%)      | 74 (100%)   | 0        | 100         | 100 |
| 96  | L4    | 86/94 (92%)      | 86 (100%)   | 0        | 100         | 100 |
| 97  | L6    | 54/61 (88%)      | 54 (100%)   | 0        | 100         | 100 |
| 98  | L7    | 46/53 (87%)      | 46 (100%)   | 0        | 100         | 100 |
| All | All   | 9982/11183 (89%) | 9978 (100%) | 4 (0%)   | 100         | 100 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | SO    | 139 | ASP  |
| 23  | SR    | 96  | PHE  |
| 65  | LZ    | 116 | ILE  |
| 74  | Li    | 26  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | SA    | 187 | GLN  |
| 6   | SA    | 209 | HIS  |
| 7   | SB    | 24  | HIS  |
| 7   | SB    | 70  | ASN  |
| 8   | SC    | 147 | GLN  |
| 8   | SC    | 181 | GLN  |
| 9   | SD    | 110 | GLN  |
| 10  | SE    | 62  | HIS  |
| 12  | SG    | 214 | HIS  |
| 13  | SH    | 25  | GLN  |
| 13  | SH    | 165 | ASN  |
| 13  | SH    | 189 | ASN  |
| 14  | SI    | 30  | GLN  |
| 14  | SI    | 47  | GLN  |
| 14  | SI    | 79  | HIS  |
| 14  | SI    | 82  | HIS  |
| 14  | SI    | 97  | GLN  |
| 14  | SI    | 154 | GLN  |
| 14  | SI    | 197 | GLN  |
| 15  | SJ    | 56  | HIS  |
| 15  | SJ    | 59  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | SK    | 21  | HIS  |
| 16  | SK    | 54  | ASN  |
| 16  | SK    | 246 | GLN  |
| 17  | SL    | 13  | GLN  |
| 17  | SL    | 40  | ASN  |
| 17  | SL    | 70  | ASN  |
| 18  | SM    | 94  | HIS  |
| 19  | SN    | 80  | HIS  |
| 20  | SO    | 80  | GLN  |
| 21  | SP    | 5   | HIS  |
| 21  | SP    | 61  | GLN  |
| 22  | SQ    | 135 | HIS  |
| 23  | SR    | 12  | HIS  |
| 24  | SS    | 10  | HIS  |
| 26  | SU    | 23  | ASN  |
| 26  | SU    | 115 | HIS  |
| 26  | SU    | 132 | GLN  |
| 26  | SU    | 143 | ASN  |
| 27  | SV    | 26  | GLN  |
| 27  | SV    | 94  | GLN  |
| 28  | SW    | 87  | ASN  |
| 29  | SX    | 70  | ASN  |
| 35  | Sd    | 34  | GLN  |
| 35  | Sd    | 43  | ASN  |
| 35  | Sd    | 52  | ASN  |
| 36  | Se    | 61  | GLN  |
| 37  | Sf    | 124 | HIS  |
| 38  | Sg    | 106 | ASN  |
| 38  | Sg    | 153 | HIS  |
| 38  | Sg    | 189 | GLN  |
| 38  | Sg    | 234 | ASN  |
| 55  | LP    | 62  | GLN  |
| 55  | LP    | 211 | HIS  |
| 56  | LQ    | 167 | GLN  |
| 56  | LQ    | 351 | ASN  |
| 57  | LR    | 224 | ASN  |
| 57  | LR    | 279 | GLN  |
| 57  | LR    | 367 | GLN  |
| 58  | LS    | 6   | ASN  |
| 58  | LS    | 17  | ASN  |
| 58  | LS    | 109 | ASN  |
| 59  | LT    | 8   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | LT    | 165 | GLN  |
| 60  | LU    | 38  | HIS  |
| 60  | LU    | 156 | GLN  |
| 61  | LV    | 113 | ASN  |
| 65  | LZ    | 47  | ASN  |
| 65  | LZ    | 102 | GLN  |
| 65  | LZ    | 150 | ASN  |
| 66  | La    | 56  | HIS  |
| 67  | Lb    | 196 | ASN  |
| 69  | Ld    | 240 | ASN  |
| 71  | Lf    | 21  | ASN  |
| 72  | Lg    | 107 | HIS  |
| 73  | Lh    | 22  | HIS  |
| 73  | Lh    | 158 | ASN  |
| 74  | Li    | 27  | HIS  |
| 74  | Li    | 127 | GLN  |
| 74  | Li    | 139 | ASN  |
| 75  | Lj    | 86  | GLN  |
| 75  | Lj    | 150 | ASN  |
| 76  | Lk    | 100 | ASN  |
| 77  | Ll    | 80  | HIS  |
| 79  | Ln    | 86  | ASN  |
| 80  | Lo    | 51  | ASN  |
| 82  | Lq    | 9   | ASN  |
| 82  | Lq    | 28  | ASN  |
| 83  | Lr    | 114 | ASN  |
| 83  | Lr    | 142 | HIS  |
| 84  | Ls    | 9   | GLN  |
| 84  | Ls    | 14  | ASN  |
| 85  | Lt    | 45  | ASN  |
| 85  | Lt    | 57  | HIS  |
| 86  | Lu    | 32  | HIS  |
| 86  | Lu    | 130 | ASN  |
| 87  | Lv    | 41  | HIS  |
| 87  | Lv    | 71  | ASN  |
| 88  | Lw    | 46  | HIS  |
| 88  | Lw    | 66  | GLN  |
| 93  | L2    | 107 | ASN  |
| 96  | L4    | 73  | GLN  |
| 96  | L4    | 82  | GLN  |
| 97  | L6    | 23  | GLN  |
| 97  | L6    | 54  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 98  | L7    | 43  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | S1    | 2004/2315 (86%) | 484 (24%)         | 16 (0%)         |
| 2   | S2    | 75/76 (98%)     | 41 (54%)          | 2 (2%)          |
| 3   | S3    | 75/76 (98%)     | 25 (33%)          | 2 (2%)          |
| 4   | S4    | 75/76 (98%)     | 41 (54%)          | 3 (4%)          |
| 40  | LA    | 158/163 (96%)   | 31 (19%)          | 0               |
| 41  | LB    | 132/133 (99%)   | 22 (16%)          | 1 (0%)          |
| 42  | LC    | 349/350 (99%)   | 79 (22%)          | 5 (1%)          |
| 43  | LD    | 108/116 (93%)   | 30 (27%)          | 1 (0%)          |
| 44  | LE    | 641/698 (91%)   | 106 (16%)         | 4 (0%)          |
| 45  | LF    | 445/527 (84%)   | 87 (19%)          | 1 (0%)          |
| 46  | LG    | 203/234 (86%)   | 38 (18%)          | 0               |
| 47  | LH    | 556/744 (74%)   | 119 (21%)         | 7 (1%)          |
| 48  | LI    | 568/617 (92%)   | 137 (24%)         | 1 (0%)          |
| 49  | LJ    | 162/164 (98%)   | 27 (16%)          | 0               |
| 5   | S5    | 11/12 (91%)     | 1 (9%)            | 0               |
| 50  | LK    | 59/64 (92%)     | 16 (27%)          | 0               |
| 51  | LL    | 90/95 (94%)     | 13 (14%)          | 0               |
| 52  | LM    | 52/58 (89%)     | 6 (11%)           | 0               |
| 53  | LN    | 76/86 (88%)     | 16 (21%)          | 0               |
| 54  | LO    | 119/120 (99%)   | 15 (12%)          | 0               |
| All | All   | 5958/6724 (88%) | 1334 (22%)        | 43 (0%)         |

All (1334) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S1    | 2   | A    |
| 1   | S1    | 3   | U    |
| 1   | S1    | 4   | C    |
| 1   | S1    | 17  | C    |
| 1   | S1    | 34  | U    |
| 1   | S1    | 42  | OMG  |
| 1   | S1    | 45  | U    |
| 1   | S1    | 47  | A    |
| 1   | S1    | 50  | C    |
| 1   | S1    | 57  | OMG  |
| 1   | S1    | 69  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S1    | 75  | U    |
| 1   | S1    | 76  | G    |
| 1   | S1    | 93  | U    |
| 1   | S1    | 103 | OMC  |
| 1   | S1    | 113 | C    |
| 1   | S1    | 114 | A    |
| 1   | S1    | 115 | U    |
| 1   | S1    | 122 | G    |
| 1   | S1    | 128 | G    |
| 1   | S1    | 131 | U    |
| 1   | S1    | 140 | C    |
| 1   | S1    | 141 | A    |
| 1   | S1    | 142 | C    |
| 1   | S1    | 144 | U    |
| 1   | S1    | 145 | G    |
| 1   | S1    | 149 | G    |
| 1   | S1    | 155 | C    |
| 1   | S1    | 156 | A    |
| 1   | S1    | 157 | U    |
| 1   | S1    | 161 | A    |
| 1   | S1    | 163 | A    |
| 1   | S1    | 169 | C    |
| 1   | S1    | 174 | C    |
| 1   | S1    | 176 | PSU  |
| 1   | S1    | 180 | OMG  |
| 1   | S1    | 185 | A    |
| 1   | S1    | 193 | U    |
| 1   | S1    | 194 | C    |
| 1   | S1    | 196 | A    |
| 1   | S1    | 200 | A    |
| 1   | S1    | 211 | C    |
| 1   | S1    | 213 | A    |
| 1   | S1    | 217 | U    |
| 1   | S1    | 220 | G    |
| 1   | S1    | 222 | A    |
| 1   | S1    | 251 | C    |
| 1   | S1    | 257 | G    |
| 1   | S1    | 267 | U    |
| 1   | S1    | 268 | A    |
| 1   | S1    | 269 | U    |
| 1   | S1    | 280 | PSU  |
| 1   | S1    | 282 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S1    | 283 | G    |
| 1   | S1    | 284 | A    |
| 1   | S1    | 287 | A    |
| 1   | S1    | 289 | C    |
| 1   | S1    | 291 | G    |
| 1   | S1    | 297 | G    |
| 1   | S1    | 299 | A    |
| 1   | S1    | 304 | C    |
| 1   | S1    | 305 | A    |
| 1   | S1    | 306 | G    |
| 1   | S1    | 308 | G    |
| 1   | S1    | 309 | U    |
| 1   | S1    | 318 | G    |
| 1   | S1    | 326 | C    |
| 1   | S1    | 327 | A    |
| 1   | S1    | 334 | C    |
| 1   | S1    | 335 | C    |
| 1   | S1    | 347 | C    |
| 1   | S1    | 348 | A    |
| 1   | S1    | 352 | C    |
| 1   | S1    | 353 | U    |
| 1   | S1    | 354 | G    |
| 1   | S1    | 362 | U    |
| 1   | S1    | 363 | C    |
| 1   | S1    | 365 | U    |
| 1   | S1    | 378 | C    |
| 1   | S1    | 381 | G    |
| 1   | S1    | 382 | C    |
| 1   | S1    | 384 | C    |
| 1   | S1    | 394 | G    |
| 1   | S1    | 398 | G    |
| 1   | S1    | 404 | C    |
| 1   | S1    | 412 | U    |
| 1   | S1    | 413 | C    |
| 1   | S1    | 415 | G    |
| 1   | S1    | 419 | G    |
| 1   | S1    | 434 | G    |
| 1   | S1    | 435 | A    |
| 1   | S1    | 442 | U    |
| 1   | S1    | 456 | A    |
| 1   | S1    | 457 | A    |
| 1   | S1    | 458 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S1    | 465 | PSU  |
| 1   | S1    | 477 | U    |
| 1   | S1    | 485 | OMG  |
| 1   | S1    | 487 | G    |
| 1   | S1    | 491 | C    |
| 1   | S1    | 497 | G    |
| 1   | S1    | 498 | A    |
| 1   | S1    | 499 | C    |
| 1   | S1    | 510 | A    |
| 1   | S1    | 514 | A    |
| 1   | S1    | 516 | G    |
| 1   | S1    | 518 | G    |
| 1   | S1    | 520 | G    |
| 1   | S1    | 521 | C    |
| 1   | S1    | 523 | G    |
| 1   | S1    | 525 | A    |
| 1   | S1    | 531 | G    |
| 1   | S1    | 536 | U    |
| 1   | S1    | 541 | C    |
| 1   | S1    | 542 | C    |
| 1   | S1    | 545 | G    |
| 1   | S1    | 549 | A    |
| 1   | S1    | 550 | G    |
| 1   | S1    | 551 | A    |
| 1   | S1    | 555 | U    |
| 1   | S1    | 565 | A2M  |
| 1   | S1    | 569 | A    |
| 1   | S1    | 570 | C    |
| 1   | S1    | 578 | A    |
| 1   | S1    | 582 | A    |
| 1   | S1    | 588 | U    |
| 1   | S1    | 594 | U    |
| 1   | S1    | 600 | G    |
| 1   | S1    | 602 | C    |
| 1   | S1    | 605 | U    |
| 1   | S1    | 615 | A    |
| 1   | S1    | 621 | OMC  |
| 1   | S1    | 624 | U    |
| 1   | S1    | 625 | A    |
| 1   | S1    | 639 | G    |
| 1   | S1    | 641 | OMG  |
| 1   | S1    | 643 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S1    | 646 | U    |
| 1   | S1    | 649 | A2M  |
| 1   | S1    | 653 | G    |
| 1   | S1    | 655 | G    |
| 1   | S1    | 661 | G    |
| 1   | S1    | 668 | G    |
| 1   | S1    | 669 | C    |
| 1   | S1    | 672 | G    |
| 1   | S1    | 681 | G    |
| 1   | S1    | 682 | OMU  |
| 1   | S1    | 683 | A    |
| 1   | S1    | 698 | G    |
| 1   | S1    | 714 | G    |
| 1   | S1    | 715 | C    |
| 1   | S1    | 723 | A2M  |
| 1   | S1    | 724 | A    |
| 1   | S1    | 725 | A    |
| 1   | S1    | 726 | A    |
| 1   | S1    | 727 | C    |
| 1   | S1    | 732 | G    |
| 1   | S1    | 743 | A    |
| 1   | S1    | 744 | C    |
| 1   | S1    | 745 | G    |
| 1   | S1    | 747 | G    |
| 1   | S1    | 750 | G    |
| 1   | S1    | 751 | C    |
| 1   | S1    | 755 | U    |
| 1   | S1    | 757 | U    |
| 1   | S1    | 759 | C    |
| 1   | S1    | 762 | G    |
| 1   | S1    | 763 | G    |
| 1   | S1    | 764 | U    |
| 1   | S1    | 767 | C    |
| 1   | S1    | 769 | G    |
| 1   | S1    | 770 | G    |
| 1   | S1    | 771 | U    |
| 1   | S1    | 772 | U    |
| 1   | S1    | 773 | U    |
| 1   | S1    | 774 | G    |
| 1   | S1    | 776 | U    |
| 1   | S1    | 777 | G    |
| 1   | S1    | 778 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S1    | 782 | U    |
| 1   | S1    | 784 | U    |
| 1   | S1    | 785 | G    |
| 1   | S1    | 786 | G    |
| 1   | S1    | 789 | A    |
| 1   | S1    | 812 | U    |
| 1   | S1    | 814 | U    |
| 1   | S1    | 815 | G    |
| 1   | S1    | 817 | U    |
| 1   | S1    | 819 | G    |
| 1   | S1    | 820 | G    |
| 1   | S1    | 823 | G    |
| 1   | S1    | 824 | C    |
| 1   | S1    | 826 | A    |
| 1   | S1    | 827 | C    |
| 1   | S1    | 830 | C    |
| 1   | S1    | 832 | G    |
| 1   | S1    | 833 | G    |
| 1   | S1    | 855 | C    |
| 1   | S1    | 857 | C    |
| 1   | S1    | 861 | G    |
| 1   | S1    | 862 | C    |
| 1   | S1    | 865 | A    |
| 1   | S1    | 883 | A    |
| 1   | S1    | 884 | G    |
| 1   | S1    | 905 | U    |
| 1   | S1    | 921 | A    |
| 1   | S1    | 924 | G    |
| 1   | S1    | 926 | G    |
| 1   | S1    | 929 | U    |
| 1   | S1    | 931 | A    |
| 1   | S1    | 932 | U    |
| 1   | S1    | 934 | C    |
| 1   | S1    | 940 | G    |
| 1   | S1    | 941 | C    |
| 1   | S1    | 944 | U    |
| 1   | S1    | 945 | G    |
| 1   | S1    | 950 | C    |
| 1   | S1    | 951 | G    |
| 1   | S1    | 959 | A    |
| 1   | S1    | 961 | A    |
| 1   | S1    | 965 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 966  | A    |
| 1   | S1    | 967  | C    |
| 1   | S1    | 968  | C    |
| 1   | S1    | 970  | A    |
| 1   | S1    | 978  | G    |
| 1   | S1    | 979  | C    |
| 1   | S1    | 980  | U    |
| 1   | S1    | 983  | G    |
| 1   | S1    | 984  | U    |
| 1   | S1    | 994  | C    |
| 1   | S1    | 996  | G    |
| 1   | S1    | 997  | G    |
| 1   | S1    | 1002 | C    |
| 1   | S1    | 1003 | C    |
| 1   | S1    | 1018 | U    |
| 1   | S1    | 1035 | A    |
| 1   | S1    | 1045 | G    |
| 1   | S1    | 1046 | C    |
| 1   | S1    | 1061 | C    |
| 1   | S1    | 1062 | G    |
| 1   | S1    | 1063 | A2M  |
| 1   | S1    | 1065 | G    |
| 1   | S1    | 1068 | PSU  |
| 1   | S1    | 1071 | A    |
| 1   | S1    | 1074 | U    |
| 1   | S1    | 1075 | C    |
| 1   | S1    | 1076 | C    |
| 1   | S1    | 1077 | A    |
| 1   | S1    | 1078 | U    |
| 1   | S1    | 1079 | C    |
| 1   | S1    | 1085 | A    |
| 1   | S1    | 1090 | C    |
| 1   | S1    | 1093 | G    |
| 1   | S1    | 1096 | A2M  |
| 1   | S1    | 1098 | C    |
| 1   | S1    | 1101 | C    |
| 1   | S1    | 1104 | A    |
| 1   | S1    | 1106 | U    |
| 1   | S1    | 1109 | G    |
| 1   | S1    | 1110 | G    |
| 1   | S1    | 1112 | A    |
| 1   | S1    | 1113 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 1114 | U    |
| 1   | S1    | 1115 | G    |
| 1   | S1    | 1116 | G    |
| 1   | S1    | 1117 | A    |
| 1   | S1    | 1122 | U    |
| 1   | S1    | 1126 | G    |
| 1   | S1    | 1129 | C    |
| 1   | S1    | 1130 | U    |
| 1   | S1    | 1134 | G    |
| 1   | S1    | 1135 | G    |
| 1   | S1    | 1136 | C    |
| 1   | S1    | 1139 | A    |
| 1   | S1    | 1140 | C    |
| 1   | S1    | 1141 | U    |
| 1   | S1    | 1142 | C    |
| 1   | S1    | 1144 | G    |
| 1   | S1    | 1145 | G    |
| 1   | S1    | 1148 | A    |
| 1   | S1    | 1149 | A    |
| 1   | S1    | 1151 | C    |
| 1   | S1    | 1152 | U    |
| 1   | S1    | 1153 | G    |
| 1   | S1    | 1159 | G    |
| 1   | S1    | 1244 | C    |
| 1   | S1    | 1246 | A    |
| 1   | S1    | 1247 | U    |
| 1   | S1    | 1248 | C    |
| 1   | S1    | 1249 | G    |
| 1   | S1    | 1250 | A    |
| 1   | S1    | 1251 | U    |
| 1   | S1    | 1252 | C    |
| 1   | S1    | 1253 | G    |
| 1   | S1    | 1254 | U    |
| 1   | S1    | 1255 | A    |
| 1   | S1    | 1256 | A    |
| 1   | S1    | 1257 | G    |
| 1   | S1    | 1260 | A    |
| 1   | S1    | 1273 | G    |
| 1   | S1    | 1283 | U    |
| 1   | S1    | 1293 | C    |
| 1   | S1    | 1296 | G    |
| 1   | S1    | 1310 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 1311 | G    |
| 1   | S1    | 1329 | U    |
| 1   | S1    | 1330 | G    |
| 1   | S1    | 1331 | C    |
| 1   | S1    | 1339 | G    |
| 1   | S1    | 1342 | U    |
| 1   | S1    | 1356 | G    |
| 1   | S1    | 1363 | G    |
| 1   | S1    | 1367 | A    |
| 1   | S1    | 1371 | A2M  |
| 1   | S1    | 1385 | A    |
| 1   | S1    | 1389 | A    |
| 1   | S1    | 1400 | A    |
| 1   | S1    | 1417 | C    |
| 1   | S1    | 1418 | C    |
| 1   | S1    | 1422 | G    |
| 1   | S1    | 1424 | A    |
| 1   | S1    | 1425 | A    |
| 1   | S1    | 1427 | C    |
| 1   | S1    | 1429 | A    |
| 1   | S1    | 1453 | A    |
| 1   | S1    | 1454 | A    |
| 1   | S1    | 1455 | G    |
| 1   | S1    | 1457 | A    |
| 1   | S1    | 1458 | U    |
| 1   | S1    | 1459 | C    |
| 1   | S1    | 1461 | U    |
| 1   | S1    | 1463 | G    |
| 1   | S1    | 1495 | A    |
| 1   | S1    | 1500 | C    |
| 1   | S1    | 1502 | C    |
| 1   | S1    | 1507 | U    |
| 1   | S1    | 1508 | G    |
| 1   | S1    | 1510 | G    |
| 1   | S1    | 1524 | G    |
| 1   | S1    | 1536 | OMG  |
| 1   | S1    | 1548 | A    |
| 1   | S1    | 1549 | A2M  |
| 1   | S1    | 1560 | G    |
| 1   | S1    | 1568 | C    |
| 1   | S1    | 1595 | U    |
| 1   | S1    | 1604 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 1606 | G    |
| 1   | S1    | 1609 | G    |
| 1   | S1    | 1610 | G    |
| 1   | S1    | 1611 | G    |
| 1   | S1    | 1612 | A    |
| 1   | S1    | 1614 | U    |
| 1   | S1    | 1624 | PSU  |
| 1   | S1    | 1627 | G    |
| 1   | S1    | 1628 | G    |
| 1   | S1    | 1638 | G    |
| 1   | S1    | 1639 | G    |
| 1   | S1    | 1651 | G    |
| 1   | S1    | 1653 | G    |
| 1   | S1    | 1654 | A    |
| 1   | S1    | 1655 | G    |
| 1   | S1    | 1656 | C    |
| 1   | S1    | 1662 | C    |
| 1   | S1    | 1665 | G    |
| 1   | S1    | 1680 | G    |
| 1   | S1    | 1683 | G    |
| 1   | S1    | 1694 | C    |
| 1   | S1    | 1696 | U    |
| 1   | S1    | 1698 | A    |
| 1   | S1    | 1711 | PSU  |
| 1   | S1    | 1724 | U    |
| 1   | S1    | 1725 | U    |
| 1   | S1    | 1726 | C    |
| 1   | S1    | 1731 | A    |
| 1   | S1    | 1735 | A    |
| 1   | S1    | 1755 | C    |
| 1   | S1    | 1756 | U    |
| 1   | S1    | 1757 | A    |
| 1   | S1    | 1765 | G    |
| 1   | S1    | 1766 | C    |
| 1   | S1    | 1767 | U    |
| 1   | S1    | 1770 | C    |
| 1   | S1    | 1780 | G    |
| 1   | S1    | 1785 | G    |
| 1   | S1    | 1787 | C    |
| 1   | S1    | 1789 | G    |
| 1   | S1    | 1790 | C    |
| 1   | S1    | 1833 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 1835 | G    |
| 1   | S1    | 1841 | G    |
| 1   | S1    | 1842 | A    |
| 1   | S1    | 1843 | G    |
| 1   | S1    | 1849 | C    |
| 1   | S1    | 1850 | C    |
| 1   | S1    | 1852 | G    |
| 1   | S1    | 1853 | U    |
| 1   | S1    | 1854 | U    |
| 1   | S1    | 1855 | C    |
| 1   | S1    | 1856 | A    |
| 1   | S1    | 1860 | U    |
| 1   | S1    | 1865 | G    |
| 1   | S1    | 1872 | U    |
| 1   | S1    | 1880 | C    |
| 1   | S1    | 1882 | A    |
| 1   | S1    | 1885 | A    |
| 1   | S1    | 1897 | G    |
| 1   | S1    | 1898 | C    |
| 1   | S1    | 1899 | U    |
| 1   | S1    | 1900 | A2M  |
| 1   | S1    | 1903 | G    |
| 1   | S1    | 1906 | A    |
| 1   | S1    | 1907 | A    |
| 1   | S1    | 1910 | G    |
| 1   | S1    | 1912 | A    |
| 1   | S1    | 1913 | G    |
| 1   | S1    | 1917 | U    |
| 1   | S1    | 1918 | G    |
| 1   | S1    | 1920 | G    |
| 1   | S1    | 1944 | C    |
| 1   | S1    | 1946 | C    |
| 1   | S1    | 1956 | A    |
| 1   | S1    | 1957 | U    |
| 1   | S1    | 1958 | U    |
| 1   | S1    | 1959 | G    |
| 1   | S1    | 1960 | PSU  |
| 1   | S1    | 1975 | C    |
| 1   | S1    | 1977 | A    |
| 1   | S1    | 1978 | C    |
| 1   | S1    | 1979 | A    |
| 1   | S1    | 1992 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 1993 | G    |
| 1   | S1    | 2007 | A    |
| 1   | S1    | 2009 | A    |
| 1   | S1    | 2011 | G    |
| 1   | S1    | 2019 | A    |
| 1   | S1    | 2023 | U    |
| 1   | S1    | 2024 | G    |
| 1   | S1    | 2026 | A    |
| 1   | S1    | 2030 | C    |
| 1   | S1    | 2031 | U    |
| 1   | S1    | 2039 | A    |
| 1   | S1    | 2040 | C    |
| 1   | S1    | 2045 | G    |
| 1   | S1    | 2052 | G    |
| 1   | S1    | 2060 | C    |
| 1   | S1    | 2062 | G    |
| 1   | S1    | 2075 | OMG  |
| 1   | S1    | 2076 | U    |
| 1   | S1    | 2078 | 7MG  |
| 1   | S1    | 2085 | U    |
| 1   | S1    | 2093 | C    |
| 1   | S1    | 2101 | PSU  |
| 1   | S1    | 2102 | C    |
| 1   | S1    | 2103 | A    |
| 1   | S1    | 2104 | G    |
| 1   | S1    | 2110 | A    |
| 1   | S1    | 2119 | G    |
| 1   | S1    | 2124 | U    |
| 1   | S1    | 2138 | A    |
| 1   | S1    | 2144 | 5MC  |
| 1   | S1    | 2181 | G    |
| 1   | S1    | 2182 | G    |
| 1   | S1    | 2189 | U    |
| 1   | S1    | 2194 | G    |
| 1   | S1    | 2216 | C    |
| 1   | S1    | 2217 | A    |
| 1   | S1    | 2218 | U    |
| 1   | S1    | 2222 | A    |
| 1   | S1    | 2233 | G    |
| 1   | S1    | 2256 | A    |
| 1   | S1    | 2261 | A    |
| 1   | S1    | 2266 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 2268 | A    |
| 1   | S1    | 2272 | A    |
| 1   | S1    | 2275 | U    |
| 1   | S1    | 2286 | G    |
| 1   | S1    | 2288 | MA6  |
| 1   | S1    | 2298 | G    |
| 1   | S1    | 2299 | G    |
| 1   | S1    | 2300 | A    |
| 1   | S1    | 2301 | U    |
| 1   | S1    | 2302 | C    |
| 1   | S1    | 2305 | PSU  |
| 2   | S2    | 3    | G    |
| 2   | S2    | 5    | G    |
| 2   | S2    | 8    | U    |
| 2   | S2    | 9    | A    |
| 2   | S2    | 10   | G    |
| 2   | S2    | 12   | U    |
| 2   | S2    | 14   | A    |
| 2   | S2    | 16   | U    |
| 2   | S2    | 17   | C    |
| 2   | S2    | 19   | G    |
| 2   | S2    | 20   | U    |
| 2   | S2    | 22   | G    |
| 2   | S2    | 27   | G    |
| 2   | S2    | 29   | G    |
| 2   | S2    | 34   | G    |
| 2   | S2    | 35   | A    |
| 2   | S2    | 36   | A    |
| 2   | S2    | 38   | A    |
| 2   | S2    | 43   | C    |
| 2   | S2    | 44   | G    |
| 2   | S2    | 45   | U    |
| 2   | S2    | 46   | G    |
| 2   | S2    | 47   | U    |
| 2   | S2    | 49   | C    |
| 2   | S2    | 50   | U    |
| 2   | S2    | 51   | U    |
| 2   | S2    | 52   | G    |
| 2   | S2    | 54   | U    |
| 2   | S2    | 56   | C    |
| 2   | S2    | 57   | G    |
| 2   | S2    | 59   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 60  | U    |
| 2   | S2    | 61  | C    |
| 2   | S2    | 64  | A    |
| 2   | S2    | 66  | U    |
| 2   | S2    | 71  | G    |
| 2   | S2    | 72  | C    |
| 2   | S2    | 73  | A    |
| 2   | S2    | 74  | C    |
| 2   | S2    | 75  | C    |
| 2   | S2    | 76  | A    |
| 3   | S3    | 7   | A    |
| 3   | S3    | 14  | A    |
| 3   | S3    | 16  | U    |
| 3   | S3    | 17  | C    |
| 3   | S3    | 18  | G    |
| 3   | S3    | 19  | G    |
| 3   | S3    | 20  | U    |
| 3   | S3    | 21  | A    |
| 3   | S3    | 22  | G    |
| 3   | S3    | 34  | C    |
| 3   | S3    | 35  | A    |
| 3   | S3    | 38  | A    |
| 3   | S3    | 44  | G    |
| 3   | S3    | 48  | C    |
| 3   | S3    | 49  | C    |
| 3   | S3    | 54  | U    |
| 3   | S3    | 56  | C    |
| 3   | S3    | 57  | G    |
| 3   | S3    | 61  | C    |
| 3   | S3    | 67  | C    |
| 3   | S3    | 69  | G    |
| 3   | S3    | 71  | G    |
| 3   | S3    | 72  | C    |
| 3   | S3    | 74  | C    |
| 3   | S3    | 76  | A    |
| 4   | S4    | 2   | C    |
| 4   | S4    | 3   | G    |
| 4   | S4    | 6   | G    |
| 4   | S4    | 7   | A    |
| 4   | S4    | 8   | U    |
| 4   | S4    | 9   | A    |
| 4   | S4    | 10  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | S4    | 14  | A    |
| 4   | S4    | 15  | G    |
| 4   | S4    | 16  | U    |
| 4   | S4    | 17  | C    |
| 4   | S4    | 19  | G    |
| 4   | S4    | 20  | U    |
| 4   | S4    | 21  | A    |
| 4   | S4    | 30  | G    |
| 4   | S4    | 31  | A    |
| 4   | S4    | 33  | U    |
| 4   | S4    | 34  | G    |
| 4   | S4    | 35  | A    |
| 4   | S4    | 36  | A    |
| 4   | S4    | 37  | A    |
| 4   | S4    | 44  | G    |
| 4   | S4    | 45  | U    |
| 4   | S4    | 46  | G    |
| 4   | S4    | 47  | U    |
| 4   | S4    | 51  | U    |
| 4   | S4    | 52  | G    |
| 4   | S4    | 54  | U    |
| 4   | S4    | 55  | U    |
| 4   | S4    | 56  | C    |
| 4   | S4    | 57  | G    |
| 4   | S4    | 58  | A    |
| 4   | S4    | 59  | U    |
| 4   | S4    | 61  | C    |
| 4   | S4    | 67  | C    |
| 4   | S4    | 69  | G    |
| 4   | S4    | 70  | C    |
| 4   | S4    | 71  | G    |
| 4   | S4    | 73  | A    |
| 4   | S4    | 74  | C    |
| 4   | S4    | 76  | A    |
| 5   | S5    | 5   | A    |
| 40  | LA    | 6   | U    |
| 40  | LA    | 10  | G    |
| 40  | LA    | 14  | G    |
| 40  | LA    | 32  | C    |
| 40  | LA    | 36  | G    |
| 40  | LA    | 40  | G    |
| 40  | LA    | 41  | OMG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | LA    | 46  | A    |
| 40  | LA    | 49  | A    |
| 40  | LA    | 58  | A    |
| 40  | LA    | 61  | C    |
| 40  | LA    | 62  | G    |
| 40  | LA    | 74  | OMG  |
| 40  | LA    | 76  | A    |
| 40  | LA    | 77  | G    |
| 40  | LA    | 80  | U    |
| 40  | LA    | 84  | G    |
| 40  | LA    | 85  | U    |
| 40  | LA    | 86  | G    |
| 40  | LA    | 92  | G    |
| 40  | LA    | 93  | A    |
| 40  | LA    | 94  | C    |
| 40  | LA    | 95  | A    |
| 40  | LA    | 96  | A    |
| 40  | LA    | 97  | A2M  |
| 40  | LA    | 102 | C    |
| 40  | LA    | 110 | A    |
| 40  | LA    | 112 | C    |
| 40  | LA    | 122 | C    |
| 40  | LA    | 123 | A    |
| 40  | LA    | 156 | C    |
| 41  | LB    | 181 | G    |
| 41  | LB    | 185 | G    |
| 41  | LB    | 191 | C    |
| 41  | LB    | 200 | A    |
| 41  | LB    | 203 | A    |
| 41  | LB    | 209 | C    |
| 41  | LB    | 219 | G    |
| 41  | LB    | 220 | A    |
| 41  | LB    | 225 | C    |
| 41  | LB    | 226 | A    |
| 41  | LB    | 233 | C    |
| 41  | LB    | 234 | PSU  |
| 41  | LB    | 247 | OMU  |
| 41  | LB    | 252 | G    |
| 41  | LB    | 274 | C    |
| 41  | LB    | 275 | G    |
| 41  | LB    | 277 | C    |
| 41  | LB    | 278 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | LB    | 279 | C    |
| 41  | LB    | 288 | A    |
| 41  | LB    | 289 | A    |
| 41  | LB    | 290 | U    |
| 42  | LC    | 298 | U    |
| 42  | LC    | 302 | PSU  |
| 42  | LC    | 305 | G    |
| 42  | LC    | 306 | C    |
| 42  | LC    | 308 | PSU  |
| 42  | LC    | 312 | U    |
| 42  | LC    | 320 | C    |
| 42  | LC    | 323 | C    |
| 42  | LC    | 324 | A    |
| 42  | LC    | 330 | U    |
| 42  | LC    | 340 | G    |
| 42  | LC    | 354 | U    |
| 42  | LC    | 355 | G    |
| 42  | LC    | 358 | U    |
| 42  | LC    | 363 | G    |
| 42  | LC    | 375 | C    |
| 42  | LC    | 381 | G    |
| 42  | LC    | 382 | A    |
| 42  | LC    | 383 | G    |
| 42  | LC    | 384 | U    |
| 42  | LC    | 391 | A    |
| 42  | LC    | 392 | U    |
| 42  | LC    | 399 | A    |
| 42  | LC    | 400 | C    |
| 42  | LC    | 412 | A    |
| 42  | LC    | 413 | C    |
| 42  | LC    | 414 | U    |
| 42  | LC    | 420 | G    |
| 42  | LC    | 426 | C    |
| 42  | LC    | 428 | G    |
| 42  | LC    | 429 | A    |
| 42  | LC    | 430 | A    |
| 42  | LC    | 431 | C    |
| 42  | LC    | 432 | C    |
| 42  | LC    | 433 | G    |
| 42  | LC    | 434 | U    |
| 42  | LC    | 435 | G    |
| 42  | LC    | 448 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | LC    | 451 | G    |
| 42  | LC    | 452 | A    |
| 42  | LC    | 453 | U    |
| 42  | LC    | 457 | G    |
| 42  | LC    | 458 | C    |
| 42  | LC    | 466 | A    |
| 42  | LC    | 467 | U    |
| 42  | LC    | 469 | C    |
| 42  | LC    | 470 | C    |
| 42  | LC    | 474 | G    |
| 42  | LC    | 491 | OMU  |
| 42  | LC    | 500 | A    |
| 42  | LC    | 504 | G    |
| 42  | LC    | 505 | U    |
| 42  | LC    | 508 | C    |
| 42  | LC    | 510 | U    |
| 42  | LC    | 515 | C    |
| 42  | LC    | 528 | G    |
| 42  | LC    | 534 | A    |
| 42  | LC    | 535 | G    |
| 42  | LC    | 536 | A    |
| 42  | LC    | 537 | OMC  |
| 42  | LC    | 542 | G    |
| 42  | LC    | 551 | U    |
| 42  | LC    | 573 | G    |
| 42  | LC    | 577 | OMC  |
| 42  | LC    | 580 | A    |
| 42  | LC    | 581 | G    |
| 42  | LC    | 595 | G    |
| 42  | LC    | 602 | A    |
| 42  | LC    | 603 | A    |
| 42  | LC    | 605 | U    |
| 42  | LC    | 606 | C    |
| 42  | LC    | 607 | C    |
| 42  | LC    | 608 | C    |
| 42  | LC    | 611 | A    |
| 42  | LC    | 624 | A    |
| 42  | LC    | 626 | C    |
| 42  | LC    | 627 | G    |
| 42  | LC    | 634 | U    |
| 42  | LC    | 636 | C    |
| 43  | LD    | 661 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | LD    | 668 | A    |
| 43  | LD    | 675 | G    |
| 43  | LD    | 679 | G    |
| 43  | LD    | 680 | G    |
| 43  | LD    | 686 | G    |
| 43  | LD    | 687 | A    |
| 43  | LD    | 688 | G    |
| 43  | LD    | 689 | C    |
| 43  | LD    | 697 | U    |
| 43  | LD    | 700 | G    |
| 43  | LD    | 701 | G    |
| 43  | LD    | 705 | G    |
| 43  | LD    | 709 | U    |
| 43  | LD    | 713 | U    |
| 43  | LD    | 715 | U    |
| 43  | LD    | 727 | C    |
| 43  | LD    | 730 | G    |
| 43  | LD    | 731 | G    |
| 43  | LD    | 733 | G    |
| 43  | LD    | 734 | G    |
| 43  | LD    | 736 | A    |
| 43  | LD    | 738 | C    |
| 43  | LD    | 742 | G    |
| 43  | LD    | 746 | G    |
| 43  | LD    | 747 | C    |
| 43  | LD    | 749 | A    |
| 43  | LD    | 750 | G    |
| 43  | LD    | 751 | G    |
| 43  | LD    | 756 | G    |
| 44  | LE    | 765 | C    |
| 44  | LE    | 771 | U    |
| 44  | LE    | 772 | G    |
| 44  | LE    | 776 | G    |
| 44  | LE    | 778 | G    |
| 44  | LE    | 802 | G    |
| 44  | LE    | 805 | C    |
| 44  | LE    | 808 | G    |
| 44  | LE    | 809 | G    |
| 44  | LE    | 812 | C    |
| 44  | LE    | 813 | U    |
| 44  | LE    | 817 | C    |
| 44  | LE    | 826 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 44  | LE    | 831  | G    |
| 44  | LE    | 841  | U    |
| 44  | LE    | 842  | G    |
| 44  | LE    | 846  | G    |
| 44  | LE    | 850  | C    |
| 44  | LE    | 851  | G    |
| 44  | LE    | 858  | A    |
| 44  | LE    | 878  | U    |
| 44  | LE    | 883  | A    |
| 44  | LE    | 884  | G    |
| 44  | LE    | 888  | A    |
| 44  | LE    | 889  | G    |
| 44  | LE    | 896  | A    |
| 44  | LE    | 911  | G    |
| 44  | LE    | 923  | C    |
| 44  | LE    | 933  | A    |
| 44  | LE    | 935  | A2M  |
| 44  | LE    | 936  | OMC  |
| 44  | LE    | 946  | A    |
| 44  | LE    | 963  | A    |
| 44  | LE    | 968  | G    |
| 44  | LE    | 969  | A    |
| 44  | LE    | 974  | U    |
| 44  | LE    | 1006 | G    |
| 44  | LE    | 1016 | U    |
| 44  | LE    | 1030 | A    |
| 44  | LE    | 1032 | U    |
| 44  | LE    | 1038 | C    |
| 44  | LE    | 1046 | G    |
| 44  | LE    | 1047 | A    |
| 44  | LE    | 1075 | PSU  |
| 44  | LE    | 1076 | U    |
| 44  | LE    | 1080 | G    |
| 44  | LE    | 1084 | U    |
| 44  | LE    | 1098 | G    |
| 44  | LE    | 1101 | C    |
| 44  | LE    | 1104 | OMG  |
| 44  | LE    | 1111 | G    |
| 44  | LE    | 1114 | G    |
| 44  | LE    | 1116 | A    |
| 44  | LE    | 1129 | A    |
| 44  | LE    | 1160 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 44  | LE    | 1170 | U    |
| 44  | LE    | 1173 | U    |
| 44  | LE    | 1178 | U    |
| 44  | LE    | 1179 | G    |
| 44  | LE    | 1188 | G    |
| 44  | LE    | 1195 | G    |
| 44  | LE    | 1196 | A    |
| 44  | LE    | 1207 | G    |
| 44  | LE    | 1208 | OMG  |
| 44  | LE    | 1209 | G    |
| 44  | LE    | 1214 | A    |
| 44  | LE    | 1216 | G    |
| 44  | LE    | 1217 | OMG  |
| 44  | LE    | 1221 | A    |
| 44  | LE    | 1223 | C    |
| 44  | LE    | 1224 | G    |
| 44  | LE    | 1225 | A    |
| 44  | LE    | 1237 | G    |
| 44  | LE    | 1244 | C    |
| 44  | LE    | 1259 | C    |
| 44  | LE    | 1260 | PSU  |
| 44  | LE    | 1261 | C    |
| 44  | LE    | 1277 | C    |
| 44  | LE    | 1297 | G    |
| 44  | LE    | 1298 | U    |
| 44  | LE    | 1299 | G    |
| 44  | LE    | 1300 | A    |
| 44  | LE    | 1301 | C    |
| 44  | LE    | 1314 | G    |
| 44  | LE    | 1325 | C    |
| 44  | LE    | 1326 | A    |
| 44  | LE    | 1356 | C    |
| 44  | LE    | 1357 | U    |
| 44  | LE    | 1361 | C    |
| 44  | LE    | 1371 | A    |
| 44  | LE    | 1376 | U    |
| 44  | LE    | 1403 | C    |
| 44  | LE    | 1409 | U    |
| 44  | LE    | 1414 | C    |
| 44  | LE    | 1423 | G    |
| 44  | LE    | 1424 | C    |
| 44  | LE    | 1428 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 44  | LE    | 1430 | A    |
| 44  | LE    | 1431 | A    |
| 44  | LE    | 1432 | C    |
| 44  | LE    | 1438 | U    |
| 44  | LE    | 1440 | C    |
| 44  | LE    | 1445 | C    |
| 44  | LE    | 1451 | C    |
| 44  | LE    | 1452 | OMU  |
| 44  | LE    | 1453 | G    |
| 45  | LF    | 1466 | G    |
| 45  | LF    | 1467 | A    |
| 45  | LF    | 1477 | C    |
| 45  | LF    | 1486 | A    |
| 45  | LF    | 1491 | G    |
| 45  | LF    | 1492 | A    |
| 45  | LF    | 1493 | C    |
| 45  | LF    | 1500 | G    |
| 45  | LF    | 1504 | OMU  |
| 45  | LF    | 1513 | U    |
| 45  | LF    | 1522 | C    |
| 45  | LF    | 1530 | G    |
| 45  | LF    | 1537 | U    |
| 45  | LF    | 1549 | G    |
| 45  | LF    | 1550 | U    |
| 45  | LF    | 1551 | G    |
| 45  | LF    | 1555 | G    |
| 45  | LF    | 1564 | C    |
| 45  | LF    | 1565 | A    |
| 45  | LF    | 1568 | PSU  |
| 45  | LF    | 1569 | C    |
| 45  | LF    | 1572 | A    |
| 45  | LF    | 1573 | OMC  |
| 45  | LF    | 1581 | G    |
| 45  | LF    | 1590 | U    |
| 45  | LF    | 1662 | OMG  |
| 45  | LF    | 1664 | G    |
| 45  | LF    | 1665 | C    |
| 45  | LF    | 1666 | A    |
| 45  | LF    | 1667 | OMG  |
| 45  | LF    | 1674 | A    |
| 45  | LF    | 1677 | U    |
| 45  | LF    | 1679 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 45  | LF    | 1681 | OMU  |
| 45  | LF    | 1685 | G    |
| 45  | LF    | 1689 | A    |
| 45  | LF    | 1698 | U    |
| 45  | LF    | 1699 | G    |
| 45  | LF    | 1702 | U    |
| 45  | LF    | 1703 | C    |
| 45  | LF    | 1704 | C    |
| 45  | LF    | 1708 | A    |
| 45  | LF    | 1710 | A    |
| 45  | LF    | 1727 | G    |
| 45  | LF    | 1730 | G    |
| 45  | LF    | 1738 | A2M  |
| 45  | LF    | 1740 | A    |
| 45  | LF    | 1757 | A    |
| 45  | LF    | 1771 | A    |
| 45  | LF    | 1772 | G    |
| 45  | LF    | 1802 | A    |
| 45  | LF    | 1804 | G    |
| 45  | LF    | 1813 | A    |
| 45  | LF    | 1819 | OMG  |
| 45  | LF    | 1822 | OMC  |
| 45  | LF    | 1827 | U    |
| 45  | LF    | 1831 | A    |
| 45  | LF    | 1835 | OMG  |
| 45  | LF    | 1840 | U    |
| 45  | LF    | 1852 | A    |
| 45  | LF    | 1853 | G    |
| 45  | LF    | 1854 | A    |
| 45  | LF    | 1856 | OMG  |
| 45  | LF    | 1857 | A    |
| 45  | LF    | 1858 | G    |
| 45  | LF    | 1862 | C    |
| 45  | LF    | 1874 | G    |
| 45  | LF    | 1881 | G    |
| 45  | LF    | 1895 | G    |
| 45  | LF    | 1902 | G    |
| 45  | LF    | 1910 | C    |
| 45  | LF    | 1916 | C    |
| 45  | LF    | 1917 | A    |
| 45  | LF    | 1918 | A    |
| 45  | LF    | 1922 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 45  | LF    | 1925 | G    |
| 45  | LF    | 1926 | PSU  |
| 45  | LF    | 1937 | U    |
| 45  | LF    | 1938 | C    |
| 45  | LF    | 1940 | A    |
| 45  | LF    | 1946 | C    |
| 45  | LF    | 1947 | G    |
| 45  | LF    | 1961 | A    |
| 45  | LF    | 1971 | A    |
| 45  | LF    | 1976 | OMC  |
| 45  | LF    | 1979 | A    |
| 45  | LF    | 1980 | A    |
| 46  | LG    | 1997 | A    |
| 46  | LG    | 2004 | A    |
| 46  | LG    | 2005 | A2M  |
| 46  | LG    | 2006 | C    |
| 46  | LG    | 2011 | A    |
| 46  | LG    | 2016 | C    |
| 46  | LG    | 2018 | A    |
| 46  | LG    | 2020 | C    |
| 46  | LG    | 2022 | A2M  |
| 46  | LG    | 2024 | A    |
| 46  | LG    | 2025 | U    |
| 46  | LG    | 2032 | G    |
| 46  | LG    | 2067 | C    |
| 46  | LG    | 2071 | C    |
| 46  | LG    | 2094 | C    |
| 46  | LG    | 2120 | C    |
| 46  | LG    | 2143 | C    |
| 46  | LG    | 2145 | C    |
| 46  | LG    | 2146 | OMG  |
| 46  | LG    | 2155 | C    |
| 46  | LG    | 2161 | G    |
| 46  | LG    | 2169 | G    |
| 46  | LG    | 2170 | A    |
| 46  | LG    | 2171 | PSU  |
| 46  | LG    | 2173 | G    |
| 46  | LG    | 2182 | G    |
| 46  | LG    | 2188 | C    |
| 46  | LG    | 2195 | C    |
| 46  | LG    | 2196 | A    |
| 46  | LG    | 2197 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | LG    | 2198 | G    |
| 46  | LG    | 2207 | G    |
| 46  | LG    | 2208 | U    |
| 46  | LG    | 2209 | C    |
| 46  | LG    | 2210 | U    |
| 46  | LG    | 2216 | C    |
| 46  | LG    | 2220 | U    |
| 46  | LG    | 2221 | G    |
| 47  | LH    | 2226 | G    |
| 47  | LH    | 2239 | G    |
| 47  | LH    | 2241 | U    |
| 47  | LH    | 2248 | A    |
| 47  | LH    | 2263 | U    |
| 47  | LH    | 2282 | U    |
| 47  | LH    | 2295 | C    |
| 47  | LH    | 2296 | A    |
| 47  | LH    | 2297 | U    |
| 47  | LH    | 2299 | A    |
| 47  | LH    | 2303 | C    |
| 47  | LH    | 2304 | A    |
| 47  | LH    | 2306 | C    |
| 47  | LH    | 2307 | C    |
| 47  | LH    | 2310 | U    |
| 47  | LH    | 2335 | C    |
| 47  | LH    | 2336 | A    |
| 47  | LH    | 2337 | C    |
| 47  | LH    | 2343 | A    |
| 47  | LH    | 2344 | A    |
| 47  | LH    | 2349 | A2M  |
| 47  | LH    | 2352 | U    |
| 47  | LH    | 2364 | G    |
| 47  | LH    | 2365 | C    |
| 47  | LH    | 2366 | A    |
| 47  | LH    | 2383 | U    |
| 47  | LH    | 2583 | G    |
| 47  | LH    | 2588 | G    |
| 47  | LH    | 2590 | G    |
| 47  | LH    | 2598 | G    |
| 47  | LH    | 2599 | U    |
| 47  | LH    | 2601 | G    |
| 47  | LH    | 2602 | OMC  |
| 47  | LH    | 2610 | OMG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | LH    | 2619 | A    |
| 47  | LH    | 2624 | PSU  |
| 47  | LH    | 2628 | U    |
| 47  | LH    | 2632 | A    |
| 47  | LH    | 2634 | C    |
| 47  | LH    | 2646 | A    |
| 47  | LH    | 2648 | G    |
| 47  | LH    | 2657 | U    |
| 47  | LH    | 2667 | C    |
| 47  | LH    | 2685 | OMC  |
| 47  | LH    | 2694 | G    |
| 47  | LH    | 2695 | A    |
| 47  | LH    | 2696 | U    |
| 47  | LH    | 2697 | U    |
| 47  | LH    | 2713 | OMU  |
| 47  | LH    | 2732 | A    |
| 47  | LH    | 2737 | G    |
| 47  | LH    | 2744 | A2M  |
| 47  | LH    | 2745 | C    |
| 47  | LH    | 2760 | G    |
| 47  | LH    | 2761 | G    |
| 47  | LH    | 2768 | A2M  |
| 47  | LH    | 2769 | A2M  |
| 47  | LH    | 2776 | OMG  |
| 47  | LH    | 2785 | U    |
| 47  | LH    | 2786 | U    |
| 47  | LH    | 2791 | A    |
| 47  | LH    | 2794 | C    |
| 47  | LH    | 2795 | G    |
| 47  | LH    | 2798 | U    |
| 47  | LH    | 2801 | A    |
| 47  | LH    | 2802 | PSU  |
| 47  | LH    | 2803 | G    |
| 47  | LH    | 2822 | U    |
| 47  | LH    | 2824 | U    |
| 47  | LH    | 2844 | A    |
| 47  | LH    | 2852 | A    |
| 47  | LH    | 2853 | OMC  |
| 47  | LH    | 2854 | C    |
| 47  | LH    | 2860 | A    |
| 47  | LH    | 2861 | A    |
| 47  | LH    | 2862 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | LH    | 2863 | G    |
| 47  | LH    | 2881 | G    |
| 47  | LH    | 2882 | G    |
| 47  | LH    | 2885 | A    |
| 47  | LH    | 2890 | A    |
| 47  | LH    | 2891 | G    |
| 47  | LH    | 2892 | A    |
| 47  | LH    | 2893 | C    |
| 47  | LH    | 2899 | PSU  |
| 47  | LH    | 2900 | G    |
| 47  | LH    | 2906 | G    |
| 47  | LH    | 2907 | A    |
| 47  | LH    | 2923 | G    |
| 47  | LH    | 2925 | OMG  |
| 47  | LH    | 2932 | C    |
| 47  | LH    | 2933 | A    |
| 47  | LH    | 2934 | U    |
| 47  | LH    | 2935 | G    |
| 47  | LH    | 2936 | U    |
| 47  | LH    | 2937 | G    |
| 47  | LH    | 2938 | G    |
| 47  | LH    | 2939 | G    |
| 47  | LH    | 2940 | G    |
| 47  | LH    | 2941 | C    |
| 47  | LH    | 2942 | G    |
| 47  | LH    | 2943 | U    |
| 47  | LH    | 2944 | A    |
| 47  | LH    | 2947 | A    |
| 47  | LH    | 2948 | U    |
| 47  | LH    | 2949 | A    |
| 47  | LH    | 2950 | G    |
| 47  | LH    | 2951 | G    |
| 47  | LH    | 2952 | U    |
| 47  | LH    | 2953 | G    |
| 47  | LH    | 2954 | G    |
| 47  | LH    | 2955 | G    |
| 47  | LH    | 2956 | A    |
| 47  | LH    | 2957 | G    |
| 47  | LH    | 2959 | U    |
| 47  | LH    | 2961 | A    |
| 47  | LH    | 2962 | G    |
| 47  | LH    | 2963 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | LH    | 2965 | C    |
| 48  | LI    | 2971 | G    |
| 48  | LI    | 2972 | C    |
| 48  | LI    | 2973 | G    |
| 48  | LI    | 2975 | G    |
| 48  | LI    | 2978 | U    |
| 48  | LI    | 2981 | A    |
| 48  | LI    | 2983 | U    |
| 48  | LI    | 2986 | A    |
| 48  | LI    | 2987 | A    |
| 48  | LI    | 2988 | U    |
| 48  | LI    | 2989 | A    |
| 48  | LI    | 2990 | C    |
| 48  | LI    | 2991 | C    |
| 48  | LI    | 2993 | C    |
| 48  | LI    | 2994 | U    |
| 48  | LI    | 2995 | A    |
| 48  | LI    | 2996 | C    |
| 48  | LI    | 2998 | U    |
| 48  | LI    | 3000 | C    |
| 48  | LI    | 3001 | A    |
| 48  | LI    | 3003 | C    |
| 48  | LI    | 3004 | G    |
| 48  | LI    | 3015 | C    |
| 48  | LI    | 3023 | U    |
| 48  | LI    | 3035 | G    |
| 48  | LI    | 3037 | G    |
| 48  | LI    | 3038 | G    |
| 48  | LI    | 3039 | C    |
| 48  | LI    | 3040 | C    |
| 48  | LI    | 3041 | A    |
| 48  | LI    | 3042 | PSU  |
| 48  | LI    | 3084 | C    |
| 48  | LI    | 3091 | C    |
| 48  | LI    | 3092 | A    |
| 48  | LI    | 3093 | U    |
| 48  | LI    | 3100 | A    |
| 48  | LI    | 3110 | A    |
| 48  | LI    | 3111 | G    |
| 48  | LI    | 3130 | C    |
| 48  | LI    | 3139 | U    |
| 48  | LI    | 3140 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | LI    | 3141 | A    |
| 48  | LI    | 3143 | A    |
| 48  | LI    | 3150 | U    |
| 48  | LI    | 3157 | U    |
| 48  | LI    | 3158 | C    |
| 48  | LI    | 3164 | A    |
| 48  | LI    | 3167 | PSU  |
| 48  | LI    | 3171 | OMU  |
| 48  | LI    | 3178 | G    |
| 48  | LI    | 3179 | G    |
| 48  | LI    | 3186 | G    |
| 48  | LI    | 3191 | OMG  |
| 48  | LI    | 3198 | A    |
| 48  | LI    | 3200 | G    |
| 48  | LI    | 3207 | A    |
| 48  | LI    | 3208 | OMC  |
| 48  | LI    | 3214 | 6MZ  |
| 48  | LI    | 3220 | G    |
| 48  | LI    | 3223 | OMG  |
| 48  | LI    | 3224 | U    |
| 48  | LI    | 3228 | G    |
| 48  | LI    | 3229 | A    |
| 48  | LI    | 3247 | A    |
| 48  | LI    | 3250 | G    |
| 48  | LI    | 3262 | G    |
| 48  | LI    | 3264 | A    |
| 48  | LI    | 3269 | A    |
| 48  | LI    | 3277 | A    |
| 48  | LI    | 3278 | G    |
| 48  | LI    | 3279 | G    |
| 48  | LI    | 3287 | G    |
| 48  | LI    | 3290 | G    |
| 48  | LI    | 3302 | A    |
| 48  | LI    | 3303 | G    |
| 48  | LI    | 3312 | C    |
| 48  | LI    | 3314 | A    |
| 48  | LI    | 3315 | A2M  |
| 48  | LI    | 3316 | A    |
| 48  | LI    | 3324 | U    |
| 48  | LI    | 3327 | U    |
| 48  | LI    | 3328 | G    |
| 48  | LI    | 3330 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | LI    | 3336 | G    |
| 48  | LI    | 3353 | U    |
| 48  | LI    | 3354 | G    |
| 48  | LI    | 3355 | OMC  |
| 48  | LI    | 3356 | G    |
| 48  | LI    | 3359 | U    |
| 48  | LI    | 3362 | U    |
| 48  | LI    | 3368 | U    |
| 48  | LI    | 3374 | OMC  |
| 48  | LI    | 3377 | OMG  |
| 48  | LI    | 3382 | G    |
| 48  | LI    | 3385 | A    |
| 48  | LI    | 3386 | G    |
| 48  | LI    | 3387 | A    |
| 48  | LI    | 3388 | A    |
| 48  | LI    | 3390 | A    |
| 48  | LI    | 3393 | U    |
| 48  | LI    | 3396 | C    |
| 48  | LI    | 3400 | G    |
| 48  | LI    | 3401 | OMG  |
| 48  | LI    | 3403 | A    |
| 48  | LI    | 3407 | C    |
| 48  | LI    | 3413 | U    |
| 48  | LI    | 3419 | U    |
| 48  | LI    | 3430 | C    |
| 48  | LI    | 3431 | A    |
| 48  | LI    | 3433 | A    |
| 48  | LI    | 3437 | A    |
| 48  | LI    | 3446 | PSU  |
| 48  | LI    | 3452 | C    |
| 48  | LI    | 3457 | G    |
| 48  | LI    | 3461 | U    |
| 48  | LI    | 3462 | C    |
| 48  | LI    | 3467 | C    |
| 48  | LI    | 3472 | U    |
| 48  | LI    | 3473 | A    |
| 48  | LI    | 3475 | C    |
| 48  | LI    | 3480 | C    |
| 48  | LI    | 3491 | G    |
| 48  | LI    | 3498 | A    |
| 48  | LI    | 3517 | A    |
| 48  | LI    | 3522 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | LI    | 3523 | A    |
| 48  | LI    | 3528 | A    |
| 48  | LI    | 3529 | C    |
| 48  | LI    | 3534 | G    |
| 48  | LI    | 3539 | G    |
| 48  | LI    | 3558 | A    |
| 48  | LI    | 3563 | G    |
| 48  | LI    | 3565 | U    |
| 48  | LI    | 3566 | U    |
| 48  | LI    | 3570 | C    |
| 48  | LI    | 3577 | G    |
| 48  | LI    | 3584 | A    |
| 49  | LJ    | 3601 | A    |
| 49  | LJ    | 3602 | U    |
| 49  | LJ    | 3612 | G    |
| 49  | LJ    | 3620 | G    |
| 49  | LJ    | 3632 | G    |
| 49  | LJ    | 3639 | C    |
| 49  | LJ    | 3646 | U    |
| 49  | LJ    | 3647 | C    |
| 49  | LJ    | 3649 | A    |
| 49  | LJ    | 3664 | A    |
| 49  | LJ    | 3668 | G    |
| 49  | LJ    | 3669 | U    |
| 49  | LJ    | 3672 | A    |
| 49  | LJ    | 3682 | C    |
| 49  | LJ    | 3683 | C    |
| 49  | LJ    | 3686 | G    |
| 49  | LJ    | 3689 | A    |
| 49  | LJ    | 3697 | PSU  |
| 49  | LJ    | 3705 | C    |
| 49  | LJ    | 3713 | A    |
| 49  | LJ    | 3720 | A    |
| 49  | LJ    | 3721 | A    |
| 49  | LJ    | 3727 | G    |
| 49  | LJ    | 3734 | C    |
| 49  | LJ    | 3738 | C    |
| 49  | LJ    | 3739 | A    |
| 49  | LJ    | 3748 | G    |
| 50  | LK    | 3753 | C    |
| 50  | LK    | 3754 | A    |
| 50  | LK    | 3757 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | LK    | 3761 | C    |
| 50  | LK    | 3762 | A    |
| 50  | LK    | 3764 | A    |
| 50  | LK    | 3770 | A    |
| 50  | LK    | 3774 | U    |
| 50  | LK    | 3776 | C    |
| 50  | LK    | 3783 | U    |
| 50  | LK    | 3786 | G    |
| 50  | LK    | 3795 | A    |
| 50  | LK    | 3805 | G    |
| 50  | LK    | 3808 | C    |
| 50  | LK    | 3809 | U    |
| 50  | LK    | 3810 | G    |
| 51  | LL    | 3814 | G    |
| 51  | LL    | 3818 | U    |
| 51  | LL    | 3838 | G    |
| 51  | LL    | 3840 | U    |
| 51  | LL    | 3853 | G    |
| 51  | LL    | 3858 | G    |
| 51  | LL    | 3859 | G    |
| 51  | LL    | 3877 | G    |
| 51  | LL    | 3879 | U    |
| 51  | LL    | 3880 | G    |
| 51  | LL    | 3902 | A    |
| 51  | LL    | 3906 | A2M  |
| 51  | LL    | 3907 | G    |
| 52  | LM    | 3911 | A    |
| 52  | LM    | 3921 | C    |
| 52  | LM    | 3922 | C    |
| 52  | LM    | 3944 | G    |
| 52  | LM    | 3951 | A    |
| 52  | LM    | 3961 | G    |
| 53  | LN    | 3980 | G    |
| 53  | LN    | 3981 | A    |
| 53  | LN    | 3984 | U    |
| 53  | LN    | 3987 | A    |
| 53  | LN    | 3990 | G    |
| 53  | LN    | 3994 | G    |
| 53  | LN    | 3998 | U    |
| 53  | LN    | 4000 | U    |
| 53  | LN    | 4009 | U    |
| 53  | LN    | 4018 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | LN    | 4023 | C    |
| 53  | LN    | 4030 | G    |
| 53  | LN    | 4031 | G    |
| 53  | LN    | 4042 | C    |
| 53  | LN    | 4043 | A    |
| 53  | LN    | 4044 | G    |
| 54  | LO    | 7    | G    |
| 54  | LO    | 22   | A    |
| 54  | LO    | 25   | A    |
| 54  | LO    | 33   | A    |
| 54  | LO    | 50   | A    |
| 54  | LO    | 53   | U    |
| 54  | LO    | 54   | A    |
| 54  | LO    | 57   | C    |
| 54  | LO    | 64   | A    |
| 54  | LO    | 74   | A    |
| 54  | LO    | 91   | C    |
| 54  | LO    | 110  | G    |
| 54  | LO    | 113  | G    |
| 54  | LO    | 117  | G    |
| 54  | LO    | 120  | U    |

All (43) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S1    | 143  | C    |
| 1   | S1    | 193  | U    |
| 1   | S1    | 267  | U    |
| 1   | S1    | 282  | C    |
| 1   | S1    | 303  | C    |
| 1   | S1    | 1243 | C    |
| 1   | S1    | 1245 | C    |
| 1   | S1    | 1247 | U    |
| 1   | S1    | 1249 | G    |
| 1   | S1    | 1454 | A    |
| 1   | S1    | 1458 | U    |
| 1   | S1    | 1912 | A    |
| 1   | S1    | 1919 | U    |
| 1   | S1    | 1957 | U    |
| 1   | S1    | 1958 | U    |
| 1   | S1    | 1976 | G    |
| 2   | S2    | 13   | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S2    | 34   | G    |
| 3   | S3    | 6    | G    |
| 3   | S3    | 34   | C    |
| 4   | S4    | 13   | C    |
| 4   | S4    | 19   | G    |
| 4   | S4    | 34   | G    |
| 41  | LB    | 278  | U    |
| 42  | LC    | 447  | C    |
| 42  | LC    | 465  | U    |
| 42  | LC    | 466  | A    |
| 42  | LC    | 579  | A    |
| 42  | LC    | 602  | A    |
| 43  | LD    | 726  | C    |
| 44  | LE    | 1075 | PSU  |
| 44  | LE    | 1208 | OMG  |
| 44  | LE    | 1224 | G    |
| 44  | LE    | 1431 | A    |
| 45  | LF    | 1856 | OMG  |
| 47  | LH    | 2342 | G    |
| 47  | LH    | 2656 | C    |
| 47  | LH    | 2768 | A2M  |
| 47  | LH    | 2937 | G    |
| 47  | LH    | 2938 | G    |
| 47  | LH    | 2939 | G    |
| 47  | LH    | 2964 | G    |
| 48  | LI    | 2994 | U    |

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

316 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 | $\# Z  > 2$ |
| 47  | OMG  | LH    | 2879 | 47,48 | 23,26,27     | 1.02 | 2 (8%)      | 33,38,41    | 0.99 | 3 (9%)      |
| 47  | PSU  | LH    | 2617 | 47    | 18,21,22     | 4.15 | 7 (38%)     | 22,30,33    | 1.95 | 5 (22%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 47  | A2M  | LH    | 2768 | 47    | 22,25,26     | 3.43 | 10 (45%) | 31,36,39    | 2.59 | 12 (38%) |
| 40  | PSU  | LA    | 16   | 40,42 | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 48  | A2M  | LI    | 3348 | 48    | 22,25,26     | 3.43 | 10 (45%) | 31,36,39    | 2.53 | 11 (35%) |
| 1   | PSU  | S1    | 2305 | 1     | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.72 | 5 (22%)  |
| 47  | JMH  | LH    | 2636 | 47    | 18,22,23     | 1.11 | 1 (5%)   | 21,32,35    | 1.51 | 5 (23%)  |
| 47  | PSU  | LH    | 2361 | 47    | 18,21,22     | 4.05 | 7 (38%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 48  | OMG  | LI    | 3509 | 48,2  | 23,26,27     | 1.06 | 2 (8%)   | 33,38,41    | 1.00 | 1 (3%)   |
| 41  | A2M  | LB    | 183  | 41    | 22,25,26     | 3.45 | 10 (45%) | 31,36,39    | 2.46 | 9 (29%)  |
| 1   | OMC  | S1    | 393  | 1     | 19,22,23     | 0.86 | 0        | 26,31,34    | 1.05 | 2 (7%)   |
| 44  | 7MG  | LE    | 938  | 44    | 22,26,27     | 1.71 | 2 (9%)   | 29,39,42    | 1.15 | 3 (10%)  |
| 44  | OMC  | LE    | 949  | 44    | 19,22,23     | 0.78 | 0        | 26,31,34    | 1.02 | 2 (7%)   |
| 47  | PSU  | LH    | 2742 | 47    | 18,21,22     | 4.18 | 7 (38%)  | 22,30,33    | 1.79 | 4 (18%)  |
| 45  | OMC  | LF    | 1573 | 45    | 19,22,23     | 1.16 | 1 (5%)   | 26,31,34    | 1.21 | 4 (15%)  |
| 1   | OMG  | S1    | 1705 | 1     | 23,26,27     | 1.07 | 2 (8%)   | 33,38,41    | 1.13 | 2 (6%)   |
| 47  | OMG  | LH    | 2776 | 47    | 23,26,27     | 1.06 | 4 (17%)  | 33,38,41    | 1.05 | 3 (9%)   |
| 48  | PSU  | LI    | 3042 | 48    | 18,21,22     | 4.32 | 7 (38%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 1   | A2M  | S1    | 28   | 1     | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.49 | 9 (29%)  |
| 42  | OMG  | LC    | 541  | 40,42 | 23,26,27     | 1.06 | 3 (13%)  | 33,38,41    | 1.03 | 3 (9%)   |
| 41  | PSU  | LB    | 281  | 41    | 18,21,22     | 4.13 | 7 (38%)  | 22,30,33    | 1.72 | 4 (18%)  |
| 45  | OMU  | LF    | 1504 | 45    | 19,22,23     | 0.57 | 0        | 26,31,34    | 0.98 | 2 (7%)   |
| 47  | OMC  | LH    | 2348 | 47    | 19,22,23     | 0.89 | 1 (5%)   | 26,31,34    | 1.06 | 3 (11%)  |
| 48  | OMC  | LI    | 3546 | 48    | 19,22,23     | 0.82 | 0        | 26,31,34    | 1.21 | 4 (15%)  |
| 45  | OMG  | LF    | 1856 | 45    | 23,26,27     | 1.09 | 3 (13%)  | 33,38,41    | 1.03 | 1 (3%)   |
| 47  | OMC  | LH    | 2825 | 47    | 19,22,23     | 0.79 | 0        | 26,31,34    | 1.07 | 4 (15%)  |
| 45  | OMC  | LF    | 1836 | 47,45 | 19,22,23     | 0.82 | 1 (5%)   | 26,31,34    | 1.17 | 3 (11%)  |
| 1   | OMU  | S1    | 1966 | 29,1  | 19,22,23     | 0.53 | 0        | 26,31,34    | 0.83 | 2 (7%)   |
| 48  | A2M  | LI    | 3500 | 48    | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.43 | 8 (25%)  |
| 1   | PSU  | S1    | 2129 | 1     | 18,21,22     | 4.10 | 7 (38%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 1   | OMU  | S1    | 186  | 1     | 19,22,23     | 0.52 | 0        | 26,31,34    | 1.08 | 2 (7%)   |
| 44  | A2M  | LE    | 1106 | 44    | 22,25,26     | 3.43 | 10 (45%) | 31,36,39    | 2.68 | 14 (45%) |
| 45  | A2M  | LF    | 1929 | 45    | 22,25,26     | 3.44 | 10 (45%) | 31,36,39    | 2.51 | 10 (32%) |
| 45  | OMU  | LF    | 1898 | 47,45 | 19,22,23     | 0.62 | 0        | 26,31,34    | 0.98 | 2 (7%)   |
| 47  | OMU  | LH    | 2909 | 47,48 | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.95 | 2 (7%)   |
| 46  | OMU  | LG    | 2129 | 46    | 19,22,23     | 0.59 | 0        | 26,31,34    | 0.87 | 1 (3%)   |
| 45  | A2M  | LF    | 1502 | 45    | 22,25,26     | 3.50 | 10 (45%) | 31,36,39    | 2.55 | 10 (32%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 44  | OMU  | LE    | 1185 | 44    | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.83 | 1 (3%)   |
| 45  | PSU  | LF    | 1859 | 45    | 18,21,22     | 4.13 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 47  | PSU  | LH    | 2586 | 47    | 18,21,22     | 4.21 | 7 (38%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 42  | PSU  | LC    | 480  | 42    | 18,21,22     | 4.16 | 7 (38%)  | 22,30,33    | 1.97 | 5 (22%)  |
| 47  | OMG  | LH    | 2610 | 47    | 23,26,27     | 1.06 | 3 (13%)  | 33,38,41    | 1.11 | 4 (12%)  |
| 1   | PSU  | S1    | 176  | 1     | 18,21,22     | 4.16 | 7 (38%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 42  | PSU  | LC    | 421  | 42    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.76 | 4 (18%)  |
| 1   | OMU  | S1    | 702  | 1     | 19,22,23     | 0.57 | 0        | 26,31,34    | 0.91 | 2 (7%)   |
| 44  | OMC  | LE    | 1312 | 44    | 19,22,23     | 0.84 | 1 (5%)   | 26,31,34    | 1.07 | 3 (11%)  |
| 47  | OMU  | LH    | 2605 | 47,49 | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.82 | 1 (3%)   |
| 47  | A2M  | LH    | 2812 | 47    | 22,25,26     | 3.42 | 10 (45%) | 31,36,39    | 2.52 | 11 (35%) |
| 45  | OMC  | LF    | 1976 | 45    | 19,22,23     | 0.87 | 1 (5%)   | 26,31,34    | 1.16 | 3 (11%)  |
| 48  | OMG  | LI    | 3504 | 48    | 23,26,27     | 1.02 | 2 (8%)   | 33,38,41    | 1.01 | 2 (6%)   |
| 44  | A2M  | LE    | 1204 | 44    | 22,25,26     | 3.49 | 10 (45%) | 31,36,39    | 2.56 | 10 (32%) |
| 44  | OMG  | LE    | 1104 | 44    | 23,26,27     | 1.01 | 1 (4%)   | 33,38,41    | 1.13 | 3 (9%)   |
| 1   | A2M  | S1    | 533  | 1     | 22,25,26     | 3.47 | 10 (45%) | 31,36,39    | 2.36 | 9 (29%)  |
| 44  | OMC  | LE    | 1218 | 44    | 19,22,23     | 0.84 | 0        | 26,31,34    | 1.15 | 4 (15%)  |
| 45  | PSU  | LF    | 1586 | 45    | 18,21,22     | 4.17 | 7 (38%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 1   | OMU  | S1    | 682  | 1     | 19,22,23     | 0.48 | 0        | 26,31,34    | 1.06 | 2 (7%)   |
| 1   | OMC  | S1    | 621  | 1     | 19,22,23     | 0.90 | 1 (5%)   | 26,31,34    | 1.20 | 4 (15%)  |
| 41  | OMU  | LB    | 206  | 41    | 19,22,23     | 0.57 | 0        | 26,31,34    | 0.83 | 1 (3%)   |
| 1   | PSU  | S1    | 89   | 1     | 18,21,22     | 4.12 | 7 (38%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 45  | PSU  | LF    | 1692 | 45    | 18,21,22     | 4.10 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 45  | OMG  | LF    | 1662 | 45    | 23,26,27     | 1.09 | 4 (17%)  | 33,38,41    | 1.06 | 3 (9%)   |
| 47  | OMU  | LH    | 2835 | 47    | 19,22,23     | 0.69 | 1 (5%)   | 26,31,34    | 0.86 | 1 (3%)   |
| 44  | PSU  | LE    | 1198 | 44    | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 1   | PSU  | S1    | 640  | 1     | 18,21,22     | 4.16 | 7 (38%)  | 22,30,33    | 1.67 | 4 (18%)  |
| 48  | PSU  | LI    | 3446 | 48    | 18,21,22     | 4.27 | 7 (38%)  | 22,30,33    | 1.77 | 4 (18%)  |
| 47  | OMU  | LH    | 2713 | 47    | 19,22,23     | 0.68 | 0        | 26,31,34    | 0.88 | 2 (7%)   |
| 45  | PSU  | LF    | 1876 | 45    | 18,21,22     | 4.17 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 48  | OMG  | LI    | 3379 | 48    | 23,26,27     | 1.02 | 2 (8%)   | 33,38,41    | 1.04 | 3 (9%)   |
| 45  | PSU  | LF    | 1582 | 45    | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 48  | OMC  | LI    | 3208 | 48    | 19,22,23     | 0.85 | 0        | 26,31,34    | 1.17 | 4 (15%)  |
| 45  | OMU  | LF    | 1553 | 45    | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.94 | 2 (7%)   |
| 49  | OMU  | LJ    | 3694 | 49    | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.94 | 2 (7%)   |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 53  | PSU  | LN    | 3969 | 52,53 | 18,21,22     | 4.30 | 7 (38%)  | 22,30,33    | 1.73 | 5 (22%)  |
| 42  | OMC  | LC    | 483  | 42    | 19,22,23     | 0.93 | 1 (5%)   | 26,31,34    | 1.04 | 3 (11%)  |
| 48  | PSU  | LI    | 3440 | 48    | 18,21,22     | 4.12 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 47  | PSU  | LH    | 2837 | 47    | 18,21,22     | 4.16 | 7 (38%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 1   | OMU  | S1    | 2041 | 1     | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.76 | 1 (3%)   |
| 44  | PSU  | LE    | 1126 | 44    | 18,21,22     | 4.09 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 1   | OMG  | S1    | 390  | 1     | 23,26,27     | 1.09 | 3 (13%)  | 33,38,41    | 1.06 | 3 (9%)   |
| 44  | OMU  | LE    | 1452 | 44    | 19,22,23     | 0.65 | 0        | 26,31,34    | 0.88 | 2 (7%)   |
| 47  | OMG  | LH    | 2883 | 47,48 | 23,26,27     | 1.09 | 3 (13%)  | 33,38,41    | 1.03 | 2 (6%)   |
| 41  | OMU  | LB    | 247  | 41    | 19,22,23     | 0.70 | 0        | 26,31,34    | 0.92 | 2 (7%)   |
| 47  | PSU  | LH    | 2621 | 47,44 | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.75 | 5 (22%)  |
| 1   | OMU  | S1    | 704  | 1     | 19,22,23     | 0.52 | 0        | 26,31,34    | 0.93 | 2 (7%)   |
| 1   | OMG  | S1    | 1901 | 1     | 23,26,27     | 1.02 | 2 (8%)   | 33,38,41    | 1.09 | 3 (9%)   |
| 1   | PSU  | S1    | 1592 | 1     | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.91 | 5 (22%)  |
| 47  | PSU  | LH    | 2754 | 47    | 18,21,22     | 4.05 | 7 (38%)  | 22,30,33    | 1.96 | 5 (22%)  |
| 42  | OMG  | LC    | 631  | 44,42 | 23,26,27     | 1.07 | 4 (17%)  | 33,38,41    | 1.06 | 2 (6%)   |
| 41  | PSU  | LB    | 280  | 41    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 40  | A2M  | LA    | 39   | 40    | 22,25,26     | 3.46 | 10 (45%) | 31,36,39    | 2.47 | 9 (29%)  |
| 1   | B8N  | S1    | 1601 | 1     | 24,29,30     | 0.98 | 2 (8%)   | 29,42,45    | 2.20 | 8 (27%)  |
| 1   | PSU  | S1    | 1660 | 1     | 18,21,22     | 4.25 | 7 (38%)  | 22,30,33    | 1.90 | 5 (22%)  |
| 47  | PSU  | LH    | 2679 | 47    | 18,21,22     | 4.08 | 7 (38%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 46  | PSU  | LG    | 2154 | 46    | 18,21,22     | 4.09 | 7 (38%)  | 22,30,33    | 1.85 | 6 (27%)  |
| 44  | OMU  | LE    | 1189 | 44    | 19,22,23     | 0.47 | 0        | 26,31,34    | 0.94 | 2 (7%)   |
| 1   | A2M  | S1    | 1063 | 1     | 22,25,26     | 3.45 | 9 (40%)  | 31,36,39    | 2.49 | 11 (35%) |
| 48  | PSU  | LI    | 3542 | 47,48 | 18,21,22     | 4.16 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 47  | PSU  | LH    | 2623 | 47    | 18,21,22     | 4.09 | 7 (38%)  | 22,30,33    | 1.95 | 5 (22%)  |
| 1   | A2M  | S1    | 723  | 1     | 22,25,26     | 3.46 | 10 (45%) | 31,36,39    | 2.54 | 11 (35%) |
| 47  | PSU  | LH    | 2591 | 47    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 1   | PSU  | S1    | 465  | 1     | 18,21,22     | 4.12 | 7 (38%)  | 22,30,33    | 1.94 | 5 (22%)  |
| 1   | OMC  | S1    | 1625 | 1     | 19,22,23     | 0.77 | 0        | 26,31,34    | 0.98 | 3 (11%)  |
| 47  | A2M  | LH    | 2349 | 47    | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.58 | 11 (35%) |
| 47  | PSU  | LH    | 2624 | 47    | 18,21,22     | 4.10 | 8 (44%)  | 22,30,33    | 1.75 | 4 (18%)  |
| 42  | OMU  | LC    | 491  | 42    | 19,22,23     | 0.66 | 0        | 26,31,34    | 0.94 | 2 (7%)   |
| 1   | OMU  | S1    | 8    | 1     | 19,22,23     | 0.43 | 0        | 26,31,34    | 1.02 | 2 (7%)   |
| 40  | A2M  | LA    | 97   | 40    | 22,25,26     | 3.45 | 9 (40%)  | 31,36,39    | 2.62 | 12 (38%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 47  | PSU  | LH    | 2642 | 47    | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 47  | OMG  | LH    | 2870 | 47    | 23,26,27     | 1.02 | 2 (8%)   | 33,38,41    | 1.01 | 3 (9%)   |
| 48  | PSU  | LI    | 3510 | 48,2  | 18,21,22     | 4.19 | 7 (38%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 42  | PSU  | LC    | 567  | 42    | 18,21,22     | 4.06 | 7 (38%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 52  | PSU  | LM    | 3963 | 53,52 | 18,21,22     | 4.24 | 7 (38%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 44  | A2M  | LE    | 1121 | 44    | 22,25,26     | 3.45 | 10 (45%) | 31,36,39    | 2.51 | 9 (29%)  |
| 48  | OMC  | LI    | 3374 | 48    | 19,22,23     | 0.85 | 1 (5%)   | 26,31,34    | 1.09 | 3 (11%)  |
| 45  | A2M  | LF    | 1888 | 45    | 22,25,26     | 3.47 | 9 (40%)  | 31,36,39    | 2.47 | 10 (32%) |
| 1   | PSU  | S1    | 121  | 1     | 18,21,22     | 1.41 | 4 (22%)  | 22,30,33    | 1.92 | 4 (18%)  |
| 47  | OMC  | LH    | 2602 | 47    | 19,22,23     | 0.84 | 0        | 26,31,34    | 1.15 | 2 (7%)   |
| 44  | OMG  | LE    | 1201 | 44    | 23,26,27     | 1.06 | 3 (13%)  | 33,38,41    | 1.02 | 0        |
| 46  | A2M  | LG    | 2022 | 46,45 | 22,25,26     | 3.46 | 10 (45%) | 31,36,39    | 2.52 | 11 (35%) |
| 1   | PSU  | S1    | 32   | 1     | 18,21,22     | 4.12 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 1   | A2M  | S1    | 1900 | 1     | 22,25,26     | 3.43 | 9 (40%)  | 31,36,39    | 2.48 | 10 (32%) |
| 48  | OMC  | LI    | 3222 | 48    | 19,22,23     | 0.91 | 1 (5%)   | 26,31,34    | 1.17 | 4 (15%)  |
| 44  | PSU  | LE    | 1075 | 48,44 | 18,21,22     | 4.07 | 8 (44%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 48  | OMU  | LI    | 3159 | 48    | 19,22,23     | 0.60 | 0        | 26,31,34    | 0.97 | 2 (7%)   |
| 48  | PSU  | LI    | 2999 | 47,48 | 18,21,22     | 4.33 | 7 (38%)  | 22,30,33    | 1.96 | 5 (22%)  |
| 47  | PSU  | LH    | 2842 | 47,45 | 18,21,22     | 4.02 | 8 (44%)  | 22,30,33    | 1.80 | 6 (27%)  |
| 48  | A2M  | LI    | 3367 | 48,42 | 22,25,26     | 3.43 | 10 (45%) | 31,36,39    | 2.52 | 10 (32%) |
| 44  | OMU  | LE    | 1081 | 44    | 19,22,23     | 0.51 | 0        | 26,31,34    | 0.88 | 2 (7%)   |
| 44  | OMU  | LE    | 1222 | 44    | 19,22,23     | 1.37 | 4 (21%)  | 26,31,34    | 1.93 | 7 (26%)  |
| 48  | UR3  | LI    | 3540 | 48    | 19,22,23     | 0.73 | 0        | 26,32,35    | 0.60 | 0        |
| 1   | PSU  | S1    | 2116 | 1     | 18,21,22     | 4.10 | 7 (38%)  | 22,30,33    | 1.71 | 4 (18%)  |
| 45  | OMU  | LF    | 1957 | 45    | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.99 | 2 (7%)   |
| 48  | OMG  | LI    | 3434 | 48    | 23,26,27     | 1.04 | 2 (8%)   | 33,38,41    | 1.05 | 4 (12%)  |
| 48  | PSU  | LI    | 3167 | 48    | 18,21,22     | 4.22 | 7 (38%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 1   | A2M  | S1    | 1096 | 1     | 22,25,26     | 3.45 | 9 (40%)  | 31,36,39    | 2.51 | 10 (32%) |
| 1   | MA6  | S1    | 2288 | 1     | 23,26,27     | 1.43 | 4 (17%)  | 34,38,41    | 3.45 | 12 (35%) |
| 45  | OMU  | LF    | 1681 | 45    | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.99 | 2 (7%)   |
| 47  | OMG  | LH    | 2897 | 47,48 | 23,26,27     | 1.03 | 2 (8%)   | 33,38,41    | 1.14 | 3 (9%)   |
| 1   | OMU  | S1    | 1641 | 1     | 19,22,23     | 0.65 | 0        | 26,31,34    | 0.99 | 2 (7%)   |
| 42  | OMC  | LC    | 537  | 40,42 | 19,22,23     | 0.98 | 1 (5%)   | 26,31,34    | 1.11 | 4 (15%)  |
| 44  | A2M  | LE    | 935  | 44    | 22,25,26     | 3.46 | 10 (45%) | 31,36,39    | 2.54 | 9 (29%)  |
| 1   | A2M  | S1    | 2046 | 1     | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.59 | 10 (32%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | OMG  | LI    | 3401 | 47,48 | 23,26,27     | 0.97 | 2 (8%)   | 33,38,41    | 1.08 | 4 (12%)  |
| 48  | PSU  | LI    | 3451 | 48    | 18,21,22     | 4.16 | 8 (44%)  | 22,30,33    | 1.96 | 6 (27%)  |
| 48  | OMC  | LI    | 3465 | 48    | 19,22,23     | 0.88 | 1 (5%)   | 26,31,34    | 1.04 | 3 (11%)  |
| 1   | OMG  | S1    | 180  | 1     | 23,26,27     | 1.09 | 4 (17%)  | 33,38,41    | 1.13 | 3 (9%)   |
| 46  | OMU  | LG    | 1999 | 46,45 | 19,22,23     | 0.60 | 0        | 26,31,34    | 0.89 | 2 (7%)   |
| 48  | OMG  | LI    | 3377 | 48    | 23,26,27     | 1.03 | 2 (8%)   | 33,38,41    | 1.08 | 3 (9%)   |
| 47  | A2M  | LH    | 2920 | 47,48 | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.52 | 10 (32%) |
| 1   | A2M  | S1    | 649  | 1     | 22,25,26     | 3.43 | 10 (45%) | 31,36,39    | 2.53 | 11 (35%) |
| 51  | A2M  | LL    | 3906 | 51    | 22,25,26     | 3.44 | 9 (40%)  | 31,36,39    | 2.48 | 11 (35%) |
| 1   | PSU  | S1    | 1554 | 1     | 18,21,22     | 3.97 | 7 (38%)  | 22,30,33    | 1.76 | 4 (18%)  |
| 48  | OMC  | LI    | 3355 | 48,44 | 19,22,23     | 0.97 | 1 (5%)   | 26,31,34    | 1.08 | 3 (11%)  |
| 47  | PSU  | LH    | 2915 | 47,48 | 18,21,22     | 4.13 | 7 (38%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 44  | PSU  | LE    | 1171 | 44    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 47  | OMC  | LH    | 2313 | 47,45 | 19,22,23     | 0.83 | 1 (5%)   | 26,31,34    | 1.09 | 4 (15%)  |
| 46  | PSU  | LG    | 2119 | 46    | 18,21,22     | 4.20 | 7 (38%)  | 22,30,33    | 1.97 | 5 (22%)  |
| 47  | A2M  | LH    | 2814 | 47    | 22,25,26     | 3.47 | 10 (45%) | 31,36,39    | 2.47 | 10 (32%) |
| 44  | OMG  | LE    | 1324 | 44    | 23,26,27     | 1.12 | 4 (17%)  | 33,38,41    | 0.97 | 1 (3%)   |
| 44  | PSU  | LE    | 1365 | 44    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 48  | A2M  | LI    | 3521 | 48    | 22,25,26     | 3.47 | 9 (40%)  | 31,36,39    | 2.47 | 9 (29%)  |
| 1   | PSU  | S1    | 1393 | 1     | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.94 | 5 (22%)  |
| 49  | OMU  | LJ    | 3636 | 49    | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.87 | 1 (3%)   |
| 44  | OMC  | LE    | 936  | 44    | 19,22,23     | 0.81 | 0        | 26,31,34    | 1.09 | 3 (11%)  |
| 48  | PSU  | LI    | 3503 | 48    | 18,21,22     | 4.10 | 7 (38%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 45  | OMU  | LF    | 1828 | 47,45 | 19,22,23     | 0.50 | 0        | 26,31,34    | 0.87 | 0        |
| 1   | A2M  | S1    | 645  | 1     | 22,25,26     | 3.37 | 9 (40%)  | 31,36,39    | 2.65 | 11 (35%) |
| 44  | 1MA  | LE    | 931  | 44    | 21,25,26     | 1.36 | 3 (14%)  | 31,37,40    | 1.69 | 5 (16%)  |
| 47  | PSU  | LH    | 2752 | 47    | 18,21,22     | 4.14 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 40  | OMG  | LA    | 74   | 40    | 23,26,27     | 1.07 | 3 (13%)  | 33,38,41    | 1.00 | 1 (3%)   |
| 1   | MA6  | S1    | 2287 | 1     | 23,26,27     | 1.45 | 4 (17%)  | 34,38,41    | 3.34 | 11 (32%) |
| 1   | PSU  | S1    | 403  | 1     | 18,21,22     | 4.20 | 7 (38%)  | 22,30,33    | 1.69 | 4 (18%)  |
| 1   | PSU  | S1    | 2081 | 1     | 18,21,22     | 4.17 | 7 (38%)  | 22,30,33    | 1.95 | 5 (22%)  |
| 1   | A2M  | S1    | 110  | 1     | 22,25,26     | 3.45 | 10 (45%) | 31,36,39    | 2.55 | 11 (35%) |
| 1   | OMG  | S1    | 42   | 1     | 23,26,27     | 1.08 | 4 (17%)  | 33,38,41    | 1.10 | 3 (9%)   |
| 1   | OMC  | S1    | 1037 | 1     | 19,22,23     | 0.92 | 1 (5%)   | 26,31,34    | 1.14 | 3 (11%)  |
| 45  | OMC  | LF    | 1822 | 44,45 | 19,22,23     | 0.87 | 1 (5%)   | 26,31,34    | 1.06 | 2 (7%)   |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | S1    | 1681 | 1     | 23,26,27     | 1.05 | 3 (13%)  | 33,38,41    | 1.01 | 2 (6%)   |
| 1   | PSU  | S1    | 105  | 1     | 18,21,22     | 4.21 | 7 (38%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 1   | OMC  | S1    | 2142 | 1     | 19,22,23     | 0.78 | 0        | 26,31,34    | 1.06 | 3 (11%)  |
| 48  | 5MC  | LI    | 3518 | 48    | 18,22,23     | 1.53 | 4 (22%)  | 26,32,35    | 1.31 | 5 (19%)  |
| 1   | A2M  | S1    | 565  | 1     | 22,25,26     | 3.47 | 10 (45%) | 31,36,39    | 2.52 | 10 (32%) |
| 1   | OMC  | S1    | 99   | 1     | 19,22,23     | 0.85 | 1 (5%)   | 26,31,34    | 1.12 | 4 (15%)  |
| 44  | PSU  | LE    | 1235 | 44    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 48  | OMG  | LI    | 3187 | 48    | 23,26,27     | 1.04 | 2 (8%)   | 33,38,41    | 1.02 | 3 (9%)   |
| 1   | OMG  | S1    | 2075 | 1     | 23,26,27     | 1.11 | 3 (13%)  | 33,38,41    | 1.04 | 2 (6%)   |
| 47  | A2M  | LH    | 2849 | 47    | 22,25,26     | 3.49 | 10 (45%) | 31,36,39    | 2.48 | 9 (29%)  |
| 1   | OMG  | S1    | 57   | 1     | 23,26,27     | 1.01 | 3 (13%)  | 33,38,41    | 1.11 | 3 (9%)   |
| 52  | OMC  | LM    | 3957 | 53,52 | 19,22,23     | 0.95 | 2 (10%)  | 26,31,34    | 1.02 | 2 (7%)   |
| 45  | A2M  | LF    | 1815 | 45    | 22,25,26     | 3.47 | 10 (45%) | 31,36,39    | 2.50 | 11 (35%) |
| 1   | OMG  | S1    | 1536 | 94,1  | 23,26,27     | 1.04 | 2 (8%)   | 33,38,41    | 1.12 | 3 (9%)   |
| 51  | PSU  | LL    | 3865 | 51    | 18,21,22     | 4.23 | 7 (38%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 1   | PSU  | S1    | 1591 | 1     | 18,21,22     | 3.97 | 7 (38%)  | 22,30,33    | 1.83 | 6 (27%)  |
| 44  | OMU  | LE    | 1270 | 44,45 | 19,22,23     | 0.60 | 0        | 26,31,34    | 1.06 | 2 (7%)   |
| 1   | PSU  | S1    | 2101 | 1     | 18,21,22     | 4.12 | 8 (44%)  | 22,30,33    | 1.75 | 4 (18%)  |
| 48  | OMC  | LI    | 3535 | 48    | 19,22,23     | 0.91 | 1 (5%)   | 26,31,34    | 0.98 | 3 (11%)  |
| 1   | PSU  | S1    | 2065 | 1     | 18,21,22     | 4.16 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 48  | PSU  | LI    | 3175 | 47,48 | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.95 | 5 (22%)  |
| 45  | OMG  | LF    | 1819 | 44,45 | 23,26,27     | 1.04 | 3 (13%)  | 33,38,41    | 1.07 | 3 (9%)   |
| 47  | OMU  | LH    | 2806 | 47    | 19,22,23     | 0.63 | 0        | 26,31,34    | 0.89 | 2 (7%)   |
| 47  | OMC  | LH    | 2853 | 47    | 19,22,23     | 0.88 | 1 (5%)   | 26,31,34    | 1.12 | 3 (11%)  |
| 1   | UR3  | S1    | 1597 | 1     | 19,22,23     | 0.78 | 1 (5%)   | 26,32,35    | 0.58 | 0        |
| 44  | OMC  | LE    | 1165 | 44    | 19,22,23     | 1.08 | 1 (5%)   | 26,31,34    | 1.28 | 4 (15%)  |
| 48  | PSU  | LI    | 3444 | 48    | 18,21,22     | 4.14 | 8 (44%)  | 22,30,33    | 1.97 | 6 (27%)  |
| 45  | A2M  | LF    | 1738 | 45    | 22,25,26     | 3.45 | 10 (45%) | 31,36,39    | 2.54 | 9 (29%)  |
| 47  | A2M  | LH    | 2809 | 47    | 22,25,26     | 3.46 | 10 (45%) | 31,36,39    | 2.53 | 11 (35%) |
| 48  | A2M  | LI    | 3315 | 48    | 22,25,26     | 3.46 | 10 (45%) | 31,36,39    | 2.53 | 11 (35%) |
| 47  | OMU  | LH    | 2346 | 47    | 19,22,23     | 0.63 | 0        | 26,31,34    | 1.06 | 2 (7%)   |
| 45  | OMG  | LF    | 1826 | 44,45 | 23,26,27     | 1.04 | 2 (8%)   | 33,38,41    | 1.04 | 2 (6%)   |
| 42  | OMG  | LC    | 628  | 42    | 23,26,27     | 1.07 | 3 (13%)  | 33,38,41    | 1.03 | 3 (9%)   |
| 49  | PSU  | LJ    | 3701 | 49    | 18,21,22     | 4.10 | 7 (38%)  | 22,30,33    | 1.90 | 5 (22%)  |
| 2   | MIA  | S2    | 37   | 2     | 28,31,32     | 2.55 | 7 (25%)  | 40,44,47    | 2.85 | 17 (42%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 45  | OMG  | LF    | 1683 | 45    | 23,26,27     | 1.03 | 3 (13%)  | 33,38,41    | 0.99 | 2 (6%)   |
| 44  | A2M  | LE    | 1039 | 44    | 22,25,26     | 3.48 | 9 (40%)  | 31,36,39    | 2.48 | 9 (29%)  |
| 47  | A2M  | LH    | 2744 | 47    | 22,25,26     | 3.46 | 11 (50%) | 31,36,39    | 2.58 | 11 (35%) |
| 1   | PSU  | S1    | 27   | 1     | 18,21,22     | 4.08 | 7 (38%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 1   | PSU  | S1    | 1396 | 1     | 18,21,22     | 4.17 | 7 (38%)  | 22,30,33    | 1.95 | 5 (22%)  |
| 1   | PSU  | S1    | 1378 | 1     | 18,21,22     | 4.04 | 7 (38%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 48  | A2M  | LI    | 3533 | 47,48 | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.47 | 10 (32%) |
| 44  | PSU  | LE    | 1184 | 44    | 18,21,22     | 4.13 | 7 (38%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 1   | A2M  | S1    | 407  | 1     | 22,25,26     | 3.42 | 10 (45%) | 31,36,39    | 2.66 | 10 (32%) |
| 48  | OMU  | LI    | 3300 | 48    | 19,22,23     | 0.53 | 0        | 26,31,34    | 1.00 | 2 (7%)   |
| 41  | PSU  | LB    | 234  | 41    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 44  | PSU  | LE    | 1023 | 44    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.90 | 5 (22%)  |
| 48  | PSU  | LI    | 3204 | 48    | 18,21,22     | 4.09 | 7 (38%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 49  | PSU  | LJ    | 3680 | 49    | 18,21,22     | 4.13 | 8 (44%)  | 22,30,33    | 2.11 | 6 (27%)  |
| 45  | OMG  | LF    | 1956 | 45    | 23,26,27     | 1.02 | 2 (8%)   | 33,38,41    | 1.08 | 2 (6%)   |
| 1   | OMU  | S1    | 179  | 1     | 19,22,23     | 0.64 | 0        | 26,31,34    | 0.93 | 2 (7%)   |
| 1   | OMU  | S1    | 1616 | 1     | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.85 | 2 (7%)   |
| 48  | PSU  | LI    | 3206 | 48    | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.96 | 6 (27%)  |
| 47  | OMG  | LH    | 2925 | 47,48 | 23,26,27     | 1.09 | 3 (13%)  | 33,38,41    | 1.03 | 1 (3%)   |
| 48  | 5MC  | LI    | 3456 | 47,48 | 18,22,23     | 1.62 | 4 (22%)  | 26,32,35    | 1.23 | 3 (11%)  |
| 48  | PSU  | LI    | 3145 | 48    | 18,21,22     | 4.31 | 8 (44%)  | 22,30,33    | 1.95 | 5 (22%)  |
| 49  | PSU  | LJ    | 3591 | 49    | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.90 | 5 (22%)  |
| 47  | PSU  | LH    | 2330 | 47,45 | 18,21,22     | 4.05 | 7 (38%)  | 22,30,33    | 1.77 | 5 (22%)  |
| 48  | PSU  | LI    | 3562 | 48    | 18,21,22     | 4.05 | 7 (38%)  | 22,30,33    | 1.97 | 5 (22%)  |
| 48  | PSU  | LI    | 3531 | 48    | 18,21,22     | 4.19 | 7 (38%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 42  | PSU  | LC    | 498  | 42    | 18,21,22     | 4.14 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 47  | PSU  | LH    | 2874 | 47,48 | 18,21,22     | 4.19 | 7 (38%)  | 22,30,33    | 1.98 | 5 (22%)  |
| 48  | OMG  | LI    | 3191 | 3,48  | 23,26,27     | 1.01 | 2 (8%)   | 33,38,41    | 1.01 | 2 (6%)   |
| 42  | A2M  | LC    | 594  | 42    | 22,25,26     | 3.52 | 10 (45%) | 31,36,39    | 2.40 | 10 (32%) |
| 1   | PSU  | S1    | 1960 | 1     | 18,21,22     | 4.08 | 7 (38%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 46  | A2M  | LG    | 2005 | 46,45 | 22,25,26     | 3.43 | 10 (45%) | 31,36,39    | 2.59 | 10 (32%) |
| 1   | A2M  | S1    | 2180 | 1     | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.26 | 9 (29%)  |
| 1   | A2M  | S1    | 1371 | 1     | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.74 | 13 (41%) |
| 49  | OMG  | LJ    | 3688 | 49    | 23,26,27     | 1.07 | 3 (13%)  | 33,38,41    | 1.12 | 1 (3%)   |
| 1   | PSU  | S1    | 2131 | 1     | 18,21,22     | 4.14 | 7 (38%)  | 22,30,33    | 1.91 | 5 (22%)  |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 47  | A2M  | LH    | 2708 | 47       | 22,25,26     | 3.47 | 9 (40%)  | 31,36,39    | 2.49 | 11 (35%) |
| 47  | OMC  | LH    | 2832 | 47       | 19,22,23     | 0.81 | 0        | 26,31,34    | 1.10 | 3 (11%)  |
| 47  | OMC  | LH    | 2242 | 46,47    | 19,22,23     | 0.83 | 0        | 26,31,34    | 0.99 | 3 (11%)  |
| 48  | PSU  | LI    | 3185 | 48       | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 49  | OMU  | LJ    | 3718 | 49       | 19,22,23     | 0.59 | 0        | 26,31,34    | 0.75 | 1 (3%)   |
| 48  | OMG  | LI    | 3223 | 48       | 23,26,27     | 1.07 | 3 (13%)  | 33,38,41    | 1.06 | 2 (6%)   |
| 48  | PSU  | LI    | 3568 | 47,48    | 18,21,22     | 4.05 | 7 (38%)  | 22,30,33    | 1.83 | 6 (27%)  |
| 46  | PSU  | LG    | 2125 | 46       | 18,21,22     | 4.12 | 7 (38%)  | 22,30,33    | 1.89 | 6 (27%)  |
| 45  | OMG  | LF    | 1835 | 47,45    | 23,26,27     | 1.04 | 3 (13%)  | 33,38,41    | 1.08 | 3 (9%)   |
| 47  | PSU  | LH    | 2914 | 47,48    | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 1   | PSU  | S1    | 280  | 1        | 18,21,22     | 4.19 | 7 (38%)  | 22,30,33    | 1.90 | 5 (22%)  |
| 44  | PSU  | LE    | 1407 | 44       | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 47  | B8H  | LH    | 2904 | 47,48    | 19,22,23     | 1.35 | 3 (15%)  | 22,32,35    | 1.97 | 3 (13%)  |
| 48  | OMU  | LI    | 3508 | 48       | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.95 | 2 (7%)   |
| 49  | PSU  | LJ    | 3644 | 49       | 18,21,22     | 3.97 | 7 (38%)  | 22,30,33    | 1.97 | 6 (27%)  |
| 1   | A2M  | S1    | 1549 | 1        | 22,25,26     | 3.49 | 10 (45%) | 31,36,39    | 2.62 | 14 (45%) |
| 1   | OMC  | S1    | 38   | 1        | 19,22,23     | 1.01 | 1 (5%)   | 26,31,34    | 1.13 | 3 (11%)  |
| 49  | PSU  | LJ    | 3697 | 49       | 18,21,22     | 4.15 | 7 (38%)  | 22,30,33    | 1.90 | 5 (22%)  |
| 45  | PSU  | LF    | 1568 | 54,45    | 18,21,22     | 4.34 | 7 (38%)  | 22,30,33    | 1.74 | 5 (22%)  |
| 47  | A2M  | LH    | 2358 | 47       | 22,25,26     | 3.44 | 10 (45%) | 31,36,39    | 2.59 | 11 (35%) |
| 1   | PSU  | S1    | 1624 | 1        | 18,21,22     | 4.14 | 7 (38%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 47  | A2M  | LH    | 2887 | 47,48    | 22,25,26     | 3.55 | 10 (45%) | 31,36,39    | 2.53 | 10 (32%) |
| 42  | PSU  | LC    | 302  | 42       | 18,21,22     | 4.20 | 7 (38%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 1   | A2M  | S1    | 40   | 1        | 22,25,26     | 3.45 | 10 (45%) | 31,36,39    | 2.50 | 10 (32%) |
| 48  | 6MZ  | LI    | 3214 | 48,45    | 22,25,26     | 1.42 | 4 (18%)  | 30,36,39    | 2.27 | 9 (30%)  |
| 41  | OMG  | LB    | 215  | 41       | 23,26,27     | 1.05 | 2 (8%)   | 33,38,41    | 1.07 | 1 (3%)   |
| 1   | PSU  | S1    | 1068 | 1        | 18,21,22     | 4.20 | 7 (38%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 40  | OMG  | LA    | 41   | 40       | 23,26,27     | 1.04 | 2 (8%)   | 33,38,41    | 0.96 | 1 (3%)   |
| 47  | PSU  | LH    | 2802 | 47       | 18,21,22     | 4.17 | 7 (38%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 47  | PSU  | LH    | 2899 | 47,48    | 18,21,22     | 4.11 | 7 (38%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 1   | 5MC  | S1    | 2144 | 1        | 18,22,23     | 1.57 | 4 (22%)  | 26,32,35    | 1.20 | 4 (15%)  |
| 45  | OMG  | LF    | 1667 | 45       | 23,26,27     | 1.03 | 3 (13%)  | 33,38,41    | 1.10 | 2 (6%)   |
| 45  | OMU  | LF    | 1824 | 44,45,42 | 19,22,23     | 0.50 | 0        | 26,31,34    | 1.01 | 2 (7%)   |
| 45  | A2M  | LF    | 1891 | 47,45    | 22,25,26     | 3.47 | 10 (45%) | 31,36,39    | 2.59 | 11 (35%) |
| 42  | PSU  | LC    | 308  | 42       | 18,21,22     | 4.22 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 44  | PSU  | LE    | 1363 | 44    | 18,21,22     | 4.14 | 7 (38%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 1   | OMG  | S1    | 485  | 1     | 23,26,27     | 1.07 | 3 (13%)  | 33,38,41    | 1.03 | 1 (3%)   |
| 44  | PSU  | LE    | 1118 | 44    | 18,21,22     | 4.12 | 7 (38%)  | 22,30,33    | 1.86 | 4 (18%)  |
| 46  | PSU  | LG    | 2171 | 46    | 18,21,22     | 4.23 | 8 (44%)  | 22,30,33    | 1.78 | 4 (18%)  |
| 47  | A2M  | LH    | 2769 | 47    | 22,25,26     | 3.42 | 10 (45%) | 31,36,39    | 2.76 | 13 (41%) |
| 45  | OMG  | LF    | 1883 | 45    | 23,26,27     | 1.07 | 4 (17%)  | 33,38,41    | 1.03 | 2 (6%)   |
| 44  | OMG  | LE    | 1217 | 44    | 23,26,27     | 1.04 | 2 (8%)   | 33,38,41    | 1.12 | 3 (9%)   |
| 1   | OMU  | S1    | 1679 | 1     | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.96 | 2 (7%)   |
| 47  | OMC  | LH    | 2685 | 47    | 19,22,23     | 1.26 | 1 (5%)   | 26,31,34    | 1.42 | 4 (15%)  |
| 1   | OMC  | S1    | 2123 | 1     | 19,22,23     | 0.87 | 1 (5%)   | 26,31,34    | 1.01 | 3 (11%)  |
| 45  | PSU  | LF    | 1926 | 45    | 18,21,22     | 4.19 | 8 (44%)  | 22,30,33    | 1.72 | 4 (18%)  |
| 1   | PSU  | S1    | 544  | 1     | 18,21,22     | 4.09 | 7 (38%)  | 22,30,33    | 1.95 | 5 (22%)  |
| 47  | PSU  | LH    | 2746 | 47    | 18,21,22     | 4.09 | 7 (38%)  | 22,30,33    | 2.14 | 5 (22%)  |
| 44  | OMG  | LE    | 1208 | 44    | 23,26,27     | 1.27 | 3 (13%)  | 33,38,41    | 1.99 | 8 (24%)  |
| 48  | PSU  | LI    | 3332 | 48    | 18,21,22     | 4.10 | 7 (38%)  | 22,30,33    | 1.91 | 5 (22%)  |
| 46  | OMG  | LG    | 2146 | 46    | 23,26,27     | 1.04 | 3 (13%)  | 33,38,41    | 1.02 | 1 (3%)   |
| 52  | PSU  | LM    | 3953 | 53,52 | 18,21,22     | 4.18 | 7 (38%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 42  | OMC  | LC    | 577  | 42    | 19,22,23     | 0.90 | 1 (5%)   | 26,31,34    | 1.00 | 2 (7%)   |
| 44  | PSU  | LE    | 1266 | 44    | 18,21,22     | 4.07 | 7 (38%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 1   | 7MG  | S1    | 2078 | 3,1   | 22,26,27     | 1.73 | 2 (9%)   | 29,39,42    | 1.23 | 5 (17%)  |
| 1   | OMU  | S1    | 1744 | 1     | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.85 | 1 (3%)   |
| 1   | PSU  | S1    | 1715 | 1     | 18,21,22     | 4.14 | 7 (38%)  | 22,30,33    | 1.77 | 5 (22%)  |
| 46  | OMG  | LG    | 2009 | 46    | 23,26,27     | 1.03 | 2 (8%)   | 33,38,41    | 1.08 | 3 (9%)   |
| 40  | PSU  | LA    | 68   | 40    | 18,21,22     | 4.13 | 8 (44%)  | 22,30,33    | 2.07 | 6 (27%)  |
| 48  | OMU  | LI    | 3171 | 47,48 | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.90 | 2 (7%)   |
| 48  | OMC  | LI    | 3347 | 48    | 19,22,23     | 0.94 | 1 (5%)   | 26,31,34    | 1.03 | 3 (11%)  |
| 44  | PSU  | LE    | 1260 | 48,44 | 18,21,22     | 4.28 | 8 (44%)  | 22,30,33    | 2.09 | 6 (27%)  |
| 47  | 5MC  | LH    | 2766 | 47    | 18,22,23     | 1.58 | 3 (16%)  | 26,32,35    | 1.21 | 3 (11%)  |
| 1   | PSU  | S1    | 1711 | 1     | 18,21,22     | 4.00 | 7 (38%)  | 22,30,33    | 1.95 | 5 (22%)  |
| 44  | OMU  | LE    | 1315 | 44    | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.89 | 2 (7%)   |
| 1   | OMC  | S1    | 103  | 1     | 19,22,23     | 1.05 | 1 (5%)   | 26,31,34    | 1.13 | 3 (11%)  |
| 47  | OMU  | LH    | 2625 | 47    | 19,22,23     | 0.56 | 0        | 26,31,34    | 1.10 | 2 (7%)   |
| 48  | PSU  | LI    | 3412 | 48    | 18,21,22     | 4.08 | 8 (44%)  | 22,30,33    | 1.99 | 6 (27%)  |
| 1   | OMG  | S1    | 641  | 1     | 23,26,27     | 1.10 | 4 (17%)  | 33,38,41    | 1.10 | 2 (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   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 47  | OMG  | LH    | 2879 | 47,48 | -       | 1/9/27/28 | 0/3/3/3 |
| 47  | PSU  | LH    | 2617 | 47    | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | A2M  | LH    | 2768 | 47    | -       | 2/9/27/28 | 0/3/3/3 |
| 40  | PSU  | LA    | 16   | 40,42 | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | A2M  | LI    | 3348 | 48    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | S1    | 2305 | 1     | -       | 3/7/25/26 | 0/2/2/2 |
| 47  | JMH  | LH    | 2636 | 47    | -       | 2/7/25/26 | 0/2/2/2 |
| 47  | PSU  | LH    | 2361 | 47    | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMG  | LI    | 3509 | 48,2  | -       | 0/9/27/28 | 0/3/3/3 |
| 41  | A2M  | LB    | 183  | 41    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMC  | S1    | 393  | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 44  | 7MG  | LE    | 938  | 44    | -       | 0/7/37/38 | 0/3/3/3 |
| 44  | OMC  | LE    | 949  | 44    | -       | 1/9/27/28 | 0/2/2/2 |
| 47  | PSU  | LH    | 2742 | 47    | -       | 2/7/25/26 | 0/2/2/2 |
| 45  | OMC  | LF    | 1573 | 45    | -       | 5/9/27/28 | 0/2/2/2 |
| 1   | OMG  | S1    | 1705 | 1     | -       | 2/9/27/28 | 0/3/3/3 |
| 47  | OMG  | LH    | 2776 | 47    | -       | 3/9/27/28 | 0/3/3/3 |
| 48  | PSU  | LI    | 3042 | 48    | -       | 3/7/25/26 | 0/2/2/2 |
| 1   | A2M  | S1    | 28   | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 42  | OMG  | LC    | 541  | 40,42 | -       | 1/9/27/28 | 0/3/3/3 |
| 41  | PSU  | LB    | 281  | 41    | -       | 3/7/25/26 | 0/2/2/2 |
| 45  | OMU  | LF    | 1504 | 45    | -       | 2/9/27/28 | 0/2/2/2 |
| 47  | OMC  | LH    | 2348 | 47    | -       | 0/9/27/28 | 0/2/2/2 |
| 48  | OMC  | LI    | 3546 | 48    | -       | 0/9/27/28 | 0/2/2/2 |
| 45  | OMG  | LF    | 1856 | 45    | -       | 2/9/27/28 | 0/3/3/3 |
| 47  | OMC  | LH    | 2825 | 47    | -       | 0/9/27/28 | 0/2/2/2 |
| 45  | OMC  | LF    | 1836 | 47,45 | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | S1    | 1966 | 29,1  | -       | 1/9/27/28 | 0/2/2/2 |
| 48  | A2M  | LI    | 3500 | 48    | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | PSU  | S1    | 2129 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMU  | S1    | 186  | 1     | -       | 1/9/27/28 | 0/2/2/2 |
| 44  | A2M  | LE    | 1106 | 44    | -       | 2/9/27/28 | 0/3/3/3 |
| 45  | A2M  | LF    | 1929 | 45    | -       | 2/9/27/28 | 0/3/3/3 |
| 45  | OMU  | LF    | 1898 | 47,45 | -       | 0/9/27/28 | 0/2/2/2 |
| 47  | OMU  | LH    | 2909 | 47,48 | -       | 0/9/27/28 | 0/2/2/2 |
| 46  | OMU  | LG    | 2129 | 46    | -       | 1/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 45  | A2M  | LF    | 1502 | 45    | -       | 0/9/27/28 | 0/3/3/3 |
| 44  | OMU  | LE    | 1185 | 44    | -       | 1/9/27/28 | 0/2/2/2 |
| 45  | PSU  | LF    | 1859 | 45    | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | PSU  | LH    | 2586 | 47    | -       | 1/7/25/26 | 0/2/2/2 |
| 42  | PSU  | LC    | 480  | 42    | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | OMG  | LH    | 2610 | 47    | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | PSU  | S1    | 176  | 1     | -       | 2/7/25/26 | 0/2/2/2 |
| 42  | PSU  | LC    | 421  | 42    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMU  | S1    | 702  | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 44  | OMC  | LE    | 1312 | 44    | -       | 0/9/27/28 | 0/2/2/2 |
| 47  | OMU  | LH    | 2605 | 47,49 | -       | 0/9/27/28 | 0/2/2/2 |
| 47  | A2M  | LH    | 2812 | 47    | -       | 4/9/27/28 | 0/3/3/3 |
| 45  | OMC  | LF    | 1976 | 45    | -       | 2/9/27/28 | 0/2/2/2 |
| 48  | OMG  | LI    | 3504 | 48    | -       | 1/9/27/28 | 0/3/3/3 |
| 44  | A2M  | LE    | 1204 | 44    | -       | 0/9/27/28 | 0/3/3/3 |
| 44  | OMG  | LE    | 1104 | 44    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | A2M  | S1    | 533  | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 44  | OMC  | LE    | 1218 | 44    | -       | 0/9/27/28 | 0/2/2/2 |
| 45  | PSU  | LF    | 1586 | 45    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMU  | S1    | 682  | 1     | -       | 2/9/27/28 | 0/2/2/2 |
| 1   | OMC  | S1    | 621  | 1     | -       | 2/9/27/28 | 0/2/2/2 |
| 41  | OMU  | LB    | 206  | 41    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | PSU  | S1    | 89   | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 45  | PSU  | LF    | 1692 | 45    | -       | 0/7/25/26 | 0/2/2/2 |
| 45  | OMG  | LF    | 1662 | 45    | -       | 2/9/27/28 | 0/3/3/3 |
| 47  | OMU  | LH    | 2835 | 47    | -       | 3/9/27/28 | 0/2/2/2 |
| 44  | PSU  | LE    | 1198 | 44    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | S1    | 640  | 1     | -       | 3/7/25/26 | 0/2/2/2 |
| 48  | PSU  | LI    | 3446 | 48    | -       | 3/7/25/26 | 0/2/2/2 |
| 47  | OMU  | LH    | 2713 | 47    | -       | 3/9/27/28 | 0/2/2/2 |
| 45  | PSU  | LF    | 1876 | 45    | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMG  | LI    | 3379 | 48    | -       | 0/9/27/28 | 0/3/3/3 |
| 45  | PSU  | LF    | 1582 | 45    | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMC  | LI    | 3208 | 48    | -       | 4/9/27/28 | 0/2/2/2 |
| 45  | OMU  | LF    | 1553 | 45    | -       | 0/9/27/28 | 0/2/2/2 |
| 49  | OMU  | LJ    | 3694 | 49    | -       | 2/9/27/28 | 0/2/2/2 |
| 53  | PSU  | LN    | 3969 | 52,53 | -       | 0/7/25/26 | 0/2/2/2 |
| 42  | OMC  | LC    | 483  | 42    | -       | 3/9/27/28 | 0/2/2/2 |
| 48  | PSU  | LI    | 3440 | 48    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 47  | PSU  | LH    | 2837 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | S1    | 2041 | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 44  | PSU  | LE    | 1126 | 44    | -       | 3/7/25/26  | 0/2/2/2 |
| 1   | OMG  | S1    | 390  | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 44  | OMU  | LE    | 1452 | 44    | -       | 0/9/27/28  | 0/2/2/2 |
| 47  | OMG  | LH    | 2883 | 47,48 | -       | 0/9/27/28  | 0/3/3/3 |
| 41  | OMU  | LB    | 247  | 41    | -       | 5/9/27/28  | 0/2/2/2 |
| 47  | PSU  | LH    | 2621 | 47,44 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | S1    | 704  | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | OMG  | S1    | 1901 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | S1    | 1592 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 47  | PSU  | LH    | 2754 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 42  | OMG  | LC    | 631  | 44,42 | -       | 0/9/27/28  | 0/3/3/3 |
| 41  | PSU  | LB    | 280  | 41    | -       | 2/7/25/26  | 0/2/2/2 |
| 40  | A2M  | LA    | 39   | 40    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | B8N  | S1    | 1601 | 1     | 1/1/7/7 | 3/16/34/35 | 0/2/2/2 |
| 1   | PSU  | S1    | 1660 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 47  | PSU  | LH    | 2679 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | LG    | 2154 | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 44  | OMU  | LE    | 1189 | 44    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | A2M  | S1    | 1063 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | PSU  | LI    | 3542 | 47,48 | -       | 0/7/25/26  | 0/2/2/2 |
| 47  | PSU  | LH    | 2623 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | S1    | 723  | 1     | -       | 5/9/27/28  | 0/3/3/3 |
| 47  | PSU  | LH    | 2591 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | S1    | 465  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | S1    | 1625 | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 47  | A2M  | LH    | 2349 | 47    | -       | 2/9/27/28  | 0/3/3/3 |
| 47  | PSU  | LH    | 2624 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 42  | OMU  | LC    | 491  | 42    | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMU  | S1    | 8    | 1     | -       | 6/9/27/28  | 0/2/2/2 |
| 40  | A2M  | LA    | 97   | 40    | -       | 2/9/27/28  | 0/3/3/3 |
| 47  | PSU  | LH    | 2642 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 47  | OMG  | LH    | 2870 | 47    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | LI    | 3510 | 48,2  | -       | 1/7/25/26  | 0/2/2/2 |
| 42  | PSU  | LC    | 567  | 42    | -       | 1/7/25/26  | 0/2/2/2 |
| 52  | PSU  | LM    | 3963 | 53,52 | -       | 0/7/25/26  | 0/2/2/2 |
| 44  | A2M  | LE    | 1121 | 44    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMC  | LI    | 3374 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 45  | A2M  | LF    | 1888 | 45    | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | PSU  | S1    | 121  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 47  | OMC  | LH    | 2602 | 47    | -       | 5/9/27/28  | 0/2/2/2 |
| 44  | OMG  | LE    | 1201 | 44    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | A2M  | LG    | 2022 | 46,45 | -       | 3/9/27/28  | 0/3/3/3 |
| 1   | PSU  | S1    | 32   | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | S1    | 1900 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | OMC  | LI    | 3222 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 44  | PSU  | LE    | 1075 | 48,44 | -       | 4/7/25/26  | 0/2/2/2 |
| 48  | OMU  | LI    | 3159 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | PSU  | LI    | 2999 | 47,48 | -       | 1/7/25/26  | 0/2/2/2 |
| 47  | PSU  | LH    | 2842 | 47,45 | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | A2M  | LI    | 3367 | 48,42 | -       | 1/9/27/28  | 0/3/3/3 |
| 44  | OMU  | LE    | 1081 | 44    | -       | 1/9/27/28  | 0/2/2/2 |
| 44  | OMU  | LE    | 1222 | 44    | -       | 4/9/27/28  | 0/2/2/2 |
| 48  | UR3  | LI    | 3540 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | S1    | 2116 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 45  | OMU  | LF    | 1957 | 45    | -       | 2/9/27/28  | 0/2/2/2 |
| 48  | OMG  | LI    | 3434 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | LI    | 3167 | 48    | -       | 5/7/25/26  | 0/2/2/2 |
| 1   | A2M  | S1    | 1096 | 1     | -       | 3/9/27/28  | 0/3/3/3 |
| 1   | MA6  | S1    | 2288 | 1     | -       | 2/11/29/30 | 0/3/3/3 |
| 45  | OMU  | LF    | 1681 | 45    | -       | 2/9/27/28  | 0/2/2/2 |
| 47  | OMG  | LH    | 2897 | 47,48 | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMU  | S1    | 1641 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 42  | OMC  | LC    | 537  | 40,42 | -       | 2/9/27/28  | 0/2/2/2 |
| 44  | A2M  | LE    | 935  | 44    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | A2M  | S1    | 2046 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMG  | LI    | 3401 | 47,48 | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | LI    | 3451 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMC  | LI    | 3465 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | S1    | 180  | 1     | -       | 3/9/27/28  | 0/3/3/3 |
| 46  | OMU  | LG    | 1999 | 46,45 | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | OMG  | LI    | 3377 | 48    | -       | 2/9/27/28  | 0/3/3/3 |
| 47  | A2M  | LH    | 2920 | 47,48 | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | A2M  | S1    | 649  | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 51  | A2M  | LL    | 3906 | 51    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | S1    | 1554 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 48  | OMC  | LI    | 3355 | 48,44 | -       | 1/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 47  | PSU  | LH    | 2915 | 47,48 | -       | 0/7/25/26  | 0/2/2/2 |
| 44  | PSU  | LE    | 1171 | 44    | -       | 0/7/25/26  | 0/2/2/2 |
| 47  | OMC  | LH    | 2313 | 47,45 | -       | 0/9/27/28  | 0/2/2/2 |
| 46  | PSU  | LG    | 2119 | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 47  | A2M  | LH    | 2814 | 47    | -       | 0/9/27/28  | 0/3/3/3 |
| 44  | OMG  | LE    | 1324 | 44    | -       | 0/9/27/28  | 0/3/3/3 |
| 44  | PSU  | LE    | 1365 | 44    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | A2M  | LI    | 3521 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | S1    | 1393 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 49  | OMU  | LJ    | 3636 | 49    | -       | 1/9/27/28  | 0/2/2/2 |
| 44  | OMC  | LE    | 936  | 44    | -       | 2/9/27/28  | 0/2/2/2 |
| 48  | PSU  | LI    | 3503 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 45  | OMU  | LF    | 1828 | 47,45 | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | A2M  | S1    | 645  | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 44  | 1MA  | LE    | 931  | 44    | -       | 2/7/25/26  | 0/3/3/3 |
| 47  | PSU  | LH    | 2752 | 47    | -       | 0/7/25/26  | 0/2/2/2 |
| 40  | OMG  | LA    | 74   | 40    | -       | 3/9/27/28  | 0/3/3/3 |
| 1   | MA6  | S1    | 2287 | 1     | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | PSU  | S1    | 403  | 1     | -       | 3/7/25/26  | 0/2/2/2 |
| 1   | PSU  | S1    | 2081 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | S1    | 110  | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | OMG  | S1    | 42   | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | S1    | 1037 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 45  | OMC  | LF    | 1822 | 44,45 | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMG  | S1    | 1681 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | S1    | 105  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | S1    | 2142 | 1     | -       | 2/9/27/28  | 0/2/2/2 |
| 48  | 5MC  | LI    | 3518 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | S1    | 565  | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | OMC  | S1    | 99   | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 44  | PSU  | LE    | 1235 | 44    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMG  | LI    | 3187 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | S1    | 2075 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 47  | A2M  | LH    | 2849 | 47    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | OMG  | S1    | 57   | 1     | -       | 3/9/27/28  | 0/3/3/3 |
| 52  | OMC  | LM    | 3957 | 53,52 | -       | 2/9/27/28  | 0/2/2/2 |
| 45  | A2M  | LF    | 1815 | 45    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | S1    | 1536 | 94,1  | -       | 2/9/27/28  | 0/3/3/3 |
| 51  | PSU  | LL    | 3865 | 51    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | PSU  | S1    | 1591 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 44  | OMU  | LE    | 1270 | 44,45 | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | S1    | 2101 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 48  | OMC  | LI    | 3535 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | S1    | 2065 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | LI    | 3175 | 47,48 | -       | 0/7/25/26  | 0/2/2/2 |
| 45  | OMG  | LF    | 1819 | 44,45 | -       | 5/9/27/28  | 0/3/3/3 |
| 47  | OMU  | LH    | 2806 | 47    | -       | 0/9/27/28  | 0/2/2/2 |
| 47  | OMC  | LH    | 2853 | 47    | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | UR3  | S1    | 1597 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 44  | OMC  | LE    | 1165 | 44    | -       | 2/9/27/28  | 0/2/2/2 |
| 48  | PSU  | LI    | 3444 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 45  | A2M  | LF    | 1738 | 45    | -       | 0/9/27/28  | 0/3/3/3 |
| 47  | A2M  | LH    | 2809 | 47    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | A2M  | LI    | 3315 | 48    | -       | 2/9/27/28  | 0/3/3/3 |
| 47  | OMU  | LH    | 2346 | 47    | -       | 0/9/27/28  | 0/2/2/2 |
| 45  | OMG  | LF    | 1826 | 44,45 | -       | 0/9/27/28  | 0/3/3/3 |
| 42  | OMG  | LC    | 628  | 42    | -       | 0/9/27/28  | 0/3/3/3 |
| 49  | PSU  | LJ    | 3701 | 49    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | MIA  | S2    | 37   | 2     | -       | 4/15/33/34 | 0/3/3/3 |
| 45  | OMG  | LF    | 1683 | 45    | -       | 0/9/27/28  | 0/3/3/3 |
| 44  | A2M  | LE    | 1039 | 44    | -       | 0/9/27/28  | 0/3/3/3 |
| 47  | A2M  | LH    | 2744 | 47    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | S1    | 27   | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | S1    | 1396 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | S1    | 1378 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | A2M  | LI    | 3533 | 47,48 | -       | 0/9/27/28  | 0/3/3/3 |
| 44  | PSU  | LE    | 1184 | 44    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | S1    | 407  | 1     | -       | 3/9/27/28  | 0/3/3/3 |
| 48  | OMU  | LI    | 3300 | 48    | -       | 0/9/27/28  | 0/2/2/2 |
| 41  | PSU  | LB    | 234  | 41    | -       | 1/7/25/26  | 0/2/2/2 |
| 44  | PSU  | LE    | 1023 | 44    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | LI    | 3204 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 49  | PSU  | LJ    | 3680 | 49    | -       | 1/7/25/26  | 0/2/2/2 |
| 45  | OMG  | LF    | 1956 | 45    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMU  | S1    | 179  | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMU  | S1    | 1616 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | PSU  | LI    | 3206 | 48    | -       | 1/7/25/26  | 0/2/2/2 |
| 47  | OMG  | LH    | 2925 | 47,48 | -       | 3/9/27/28  | 0/3/3/3 |
| 48  | 5MC  | LI    | 3456 | 47,48 | -       | 4/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 48  | PSU  | LI    | 3145 | 48    | -       | 0/7/25/26 | 0/2/2/2 |
| 49  | PSU  | LJ    | 3591 | 49    | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | PSU  | LH    | 2330 | 47,45 | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | PSU  | LI    | 3562 | 48    | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | PSU  | LI    | 3531 | 48    | -       | 1/7/25/26 | 0/2/2/2 |
| 42  | PSU  | LC    | 498  | 42    | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | PSU  | LH    | 2874 | 47,48 | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMG  | LI    | 3191 | 3,48  | -       | 3/9/27/28 | 0/3/3/3 |
| 42  | A2M  | LC    | 594  | 42    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | S1    | 1960 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | A2M  | LG    | 2005 | 46,45 | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | A2M  | S1    | 2180 | 1     | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | A2M  | S1    | 1371 | 1     | -       | 3/9/27/28 | 0/3/3/3 |
| 49  | OMG  | LJ    | 3688 | 49    | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | PSU  | S1    | 2131 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | A2M  | LH    | 2708 | 47    | -       | 0/9/27/28 | 0/3/3/3 |
| 47  | OMC  | LH    | 2832 | 47    | -       | 0/9/27/28 | 0/2/2/2 |
| 47  | OMC  | LH    | 2242 | 46,47 | -       | 3/9/27/28 | 0/2/2/2 |
| 48  | PSU  | LI    | 3185 | 48    | -       | 0/7/25/26 | 0/2/2/2 |
| 49  | OMU  | LJ    | 3718 | 49    | -       | 1/9/27/28 | 0/2/2/2 |
| 48  | OMG  | LI    | 3223 | 48    | -       | 1/9/27/28 | 0/3/3/3 |
| 48  | PSU  | LI    | 3568 | 47,48 | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | PSU  | LG    | 2125 | 46    | -       | 1/7/25/26 | 0/2/2/2 |
| 45  | OMG  | LF    | 1835 | 47,45 | -       | 2/9/27/28 | 0/3/3/3 |
| 47  | PSU  | LH    | 2914 | 47,48 | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | S1    | 280  | 1     | -       | 4/7/25/26 | 0/2/2/2 |
| 44  | PSU  | LE    | 1407 | 44    | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | B8H  | LH    | 2904 | 47,48 | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMU  | LI    | 3508 | 48    | -       | 0/9/27/28 | 0/2/2/2 |
| 49  | PSU  | LJ    | 3644 | 49    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | A2M  | S1    | 1549 | 1     | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | OMC  | S1    | 38   | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 49  | PSU  | LJ    | 3697 | 49    | -       | 2/7/25/26 | 0/2/2/2 |
| 45  | PSU  | LF    | 1568 | 54,45 | -       | 1/7/25/26 | 0/2/2/2 |
| 47  | A2M  | LH    | 2358 | 47    | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | PSU  | S1    | 1624 | 1     | -       | 2/7/25/26 | 0/2/2/2 |
| 47  | A2M  | LH    | 2887 | 47,48 | -       | 1/9/27/28 | 0/3/3/3 |
| 42  | PSU  | LC    | 302  | 42    | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | A2M  | S1    | 40   | 1     | -       | 0/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions  | Rings   |
|-----|------|-------|------|----------|---------|-----------|---------|
| 48  | 6MZ  | LI    | 3214 | 48,45    | -       | 4/9/27/28 | 0/3/3/3 |
| 41  | OMG  | LB    | 215  | 41       | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | PSU  | S1    | 1068 | 1        | -       | 3/7/25/26 | 0/2/2/2 |
| 40  | OMG  | LA    | 41   | 40       | -       | 0/9/27/28 | 0/3/3/3 |
| 47  | PSU  | LH    | 2802 | 47       | -       | 4/7/25/26 | 0/2/2/2 |
| 47  | PSU  | LH    | 2899 | 47,48    | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 5MC  | S1    | 2144 | 1        | -       | 0/7/25/26 | 0/2/2/2 |
| 45  | OMG  | LF    | 1667 | 45       | -       | 3/9/27/28 | 0/3/3/3 |
| 45  | OMU  | LF    | 1824 | 44,45,42 | -       | 0/9/27/28 | 0/2/2/2 |
| 45  | A2M  | LF    | 1891 | 47,45    | -       | 0/9/27/28 | 0/3/3/3 |
| 42  | PSU  | LC    | 308  | 42       | -       | 2/7/25/26 | 0/2/2/2 |
| 44  | PSU  | LE    | 1363 | 44       | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMG  | S1    | 485  | 1        | -       | 2/9/27/28 | 0/3/3/3 |
| 44  | PSU  | LE    | 1118 | 44       | -       | 2/7/25/26 | 0/2/2/2 |
| 46  | PSU  | LG    | 2171 | 46       | -       | 2/7/25/26 | 0/2/2/2 |
| 47  | A2M  | LH    | 2769 | 47       | -       | 3/9/27/28 | 0/3/3/3 |
| 45  | OMG  | LF    | 1883 | 45       | -       | 0/9/27/28 | 0/3/3/3 |
| 44  | OMG  | LE    | 1217 | 44       | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMU  | S1    | 1679 | 1        | -       | 0/9/27/28 | 0/2/2/2 |
| 47  | OMC  | LH    | 2685 | 47       | -       | 5/9/27/28 | 0/2/2/2 |
| 1   | OMC  | S1    | 2123 | 1        | -       | 0/9/27/28 | 0/2/2/2 |
| 45  | PSU  | LF    | 1926 | 45       | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | PSU  | S1    | 544  | 1        | -       | 0/7/25/26 | 0/2/2/2 |
| 47  | PSU  | LH    | 2746 | 47       | -       | 3/7/25/26 | 0/2/2/2 |
| 44  | OMG  | LE    | 1208 | 44       | -       | 0/9/27/28 | 0/3/3/3 |
| 48  | PSU  | LI    | 3332 | 48       | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | OMG  | LG    | 2146 | 46       | -       | 2/9/27/28 | 0/3/3/3 |
| 52  | PSU  | LM    | 3953 | 53,52    | -       | 0/7/25/26 | 0/2/2/2 |
| 42  | OMC  | LC    | 577  | 42       | -       | 3/9/27/28 | 0/2/2/2 |
| 44  | PSU  | LE    | 1266 | 44       | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 7MG  | S1    | 2078 | 3,1      | -       | 2/7/37/38 | 0/3/3/3 |
| 1   | OMU  | S1    | 1744 | 1        | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | PSU  | S1    | 1715 | 1        | -       | 1/7/25/26 | 0/2/2/2 |
| 46  | OMG  | LG    | 2009 | 46       | -       | 1/9/27/28 | 0/3/3/3 |
| 40  | PSU  | LA    | 68   | 40       | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMU  | LI    | 3171 | 47,48    | -       | 2/9/27/28 | 0/2/2/2 |
| 48  | OMC  | LI    | 3347 | 48       | -       | 0/9/27/28 | 0/2/2/2 |
| 44  | PSU  | LE    | 1260 | 48,44    | -       | 3/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 47  | 5MC  | LH    | 2766 | 47   | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | PSU  | S1    | 1711 | 1    | -       | 2/7/25/26 | 0/2/2/2 |
| 44  | OMU  | LE    | 1315 | 44   | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMC  | S1    | 103  | 1    | -       | 3/9/27/28 | 0/2/2/2 |
| 47  | OMU  | LH    | 2625 | 47   | -       | 0/9/27/28 | 0/2/2/2 |
| 48  | PSU  | LI    | 3412 | 48   | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMG  | S1    | 641  | 1    | -       | 2/9/27/28 | 0/3/3/3 |

All (1536) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 48  | LI    | 2999 | PSU  | C6-C5 | 11.41 | 1.48        | 1.35     |
| 45  | LF    | 1568 | PSU  | C6-C5 | 11.40 | 1.48        | 1.35     |
| 48  | LI    | 3042 | PSU  | C6-C5 | 11.34 | 1.48        | 1.35     |
| 53  | LN    | 3969 | PSU  | C6-C5 | 11.24 | 1.48        | 1.35     |
| 1   | S1    | 1660 | PSU  | C6-C5 | 11.24 | 1.48        | 1.35     |
| 44  | LE    | 1260 | PSU  | C6-C5 | 11.19 | 1.48        | 1.35     |
| 48  | LI    | 3446 | PSU  | C6-C5 | 11.15 | 1.48        | 1.35     |
| 48  | LI    | 3145 | PSU  | C6-C5 | 11.13 | 1.48        | 1.35     |
| 46  | LG    | 2171 | PSU  | C6-C5 | 11.07 | 1.48        | 1.35     |
| 42  | LC    | 308  | PSU  | C6-C5 | 11.07 | 1.48        | 1.35     |
| 47  | LH    | 2874 | PSU  | C6-C5 | 11.02 | 1.48        | 1.35     |
| 1   | S1    | 105  | PSU  | C6-C5 | 11.00 | 1.48        | 1.35     |
| 46  | LG    | 2119 | PSU  | C6-C5 | 10.99 | 1.48        | 1.35     |
| 48  | LI    | 3167 | PSU  | C6-C5 | 10.99 | 1.48        | 1.35     |
| 48  | LI    | 3510 | PSU  | C6-C5 | 10.98 | 1.48        | 1.35     |
| 51  | LL    | 3865 | PSU  | C6-C5 | 10.96 | 1.48        | 1.35     |
| 52  | LM    | 3963 | PSU  | C6-C5 | 10.95 | 1.48        | 1.35     |
| 1   | S1    | 1068 | PSU  | C6-C5 | 10.93 | 1.48        | 1.35     |
| 1   | S1    | 2065 | PSU  | C6-C5 | 10.92 | 1.48        | 1.35     |
| 42  | LC    | 302  | PSU  | C6-C5 | 10.91 | 1.48        | 1.35     |
| 42  | LC    | 480  | PSU  | C6-C5 | 10.90 | 1.48        | 1.35     |
| 45  | LF    | 1926 | PSU  | C6-C5 | 10.90 | 1.48        | 1.35     |
| 40  | LA    | 68   | PSU  | C6-C5 | 10.88 | 1.48        | 1.35     |
| 44  | LE    | 1023 | PSU  | C6-C5 | 10.88 | 1.48        | 1.35     |
| 48  | LI    | 3531 | PSU  | C6-C5 | 10.88 | 1.48        | 1.35     |
| 1   | S1    | 2081 | PSU  | C6-C5 | 10.88 | 1.48        | 1.35     |
| 47  | LH    | 2586 | PSU  | C6-C5 | 10.87 | 1.48        | 1.35     |
| 41  | LB    | 281  | PSU  | C6-C5 | 10.87 | 1.48        | 1.35     |
| 52  | LM    | 3953 | PSU  | C6-C5 | 10.86 | 1.48        | 1.35     |
| 47  | LH    | 2746 | PSU  | C6-C5 | 10.86 | 1.48        | 1.35     |
| 47  | LH    | 2752 | PSU  | C6-C5 | 10.86 | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 47  | LH    | 2915 | PSU  | C6-C5 | 10.85 | 1.47        | 1.35     |
| 1   | S1    | 1715 | PSU  | C6-C5 | 10.85 | 1.47        | 1.35     |
| 1   | S1    | 176  | PSU  | C6-C5 | 10.83 | 1.47        | 1.35     |
| 1   | S1    | 403  | PSU  | C6-C5 | 10.83 | 1.47        | 1.35     |
| 49  | LJ    | 3697 | PSU  | C6-C5 | 10.83 | 1.47        | 1.35     |
| 44  | LE    | 1365 | PSU  | C6-C5 | 10.83 | 1.47        | 1.35     |
| 1   | S1    | 640  | PSU  | C6-C5 | 10.82 | 1.47        | 1.35     |
| 1   | S1    | 280  | PSU  | C6-C5 | 10.82 | 1.47        | 1.35     |
| 1   | S1    | 89   | PSU  | C6-C5 | 10.82 | 1.47        | 1.35     |
| 47  | LH    | 2742 | PSU  | C6-C5 | 10.81 | 1.47        | 1.35     |
| 47  | LH    | 2914 | PSU  | C6-C5 | 10.80 | 1.47        | 1.35     |
| 46  | LG    | 2125 | PSU  | C6-C5 | 10.80 | 1.47        | 1.35     |
| 47  | LH    | 2591 | PSU  | C6-C5 | 10.80 | 1.47        | 1.35     |
| 44  | LE    | 1184 | PSU  | C6-C5 | 10.80 | 1.47        | 1.35     |
| 1   | S1    | 2131 | PSU  | C6-C5 | 10.80 | 1.47        | 1.35     |
| 41  | LB    | 234  | PSU  | C6-C5 | 10.79 | 1.47        | 1.35     |
| 41  | LB    | 280  | PSU  | C6-C5 | 10.79 | 1.47        | 1.35     |
| 1   | S1    | 2305 | PSU  | C6-C5 | 10.79 | 1.47        | 1.35     |
| 45  | LF    | 1586 | PSU  | C6-C5 | 10.78 | 1.47        | 1.35     |
| 47  | LH    | 2617 | PSU  | C6-C5 | 10.78 | 1.47        | 1.35     |
| 47  | LH    | 2837 | PSU  | C6-C5 | 10.78 | 1.47        | 1.35     |
| 40  | LA    | 16   | PSU  | C6-C5 | 10.78 | 1.47        | 1.35     |
| 44  | LE    | 1171 | PSU  | C6-C5 | 10.76 | 1.47        | 1.35     |
| 44  | LE    | 1118 | PSU  | C6-C5 | 10.76 | 1.47        | 1.35     |
| 49  | LJ    | 3680 | PSU  | C6-C5 | 10.76 | 1.47        | 1.35     |
| 45  | LF    | 1582 | PSU  | C6-C5 | 10.75 | 1.47        | 1.35     |
| 1   | S1    | 27   | PSU  | C6-C5 | 10.75 | 1.47        | 1.35     |
| 44  | LE    | 1198 | PSU  | C6-C5 | 10.75 | 1.47        | 1.35     |
| 48  | LI    | 3542 | PSU  | C6-C5 | 10.74 | 1.47        | 1.35     |
| 44  | LE    | 1126 | PSU  | C6-C5 | 10.74 | 1.47        | 1.35     |
| 1   | S1    | 465  | PSU  | C6-C5 | 10.73 | 1.47        | 1.35     |
| 1   | S1    | 1393 | PSU  | C6-C5 | 10.73 | 1.47        | 1.35     |
| 1   | S1    | 1396 | PSU  | C6-C5 | 10.70 | 1.47        | 1.35     |
| 1   | S1    | 32   | PSU  | C6-C5 | 10.70 | 1.47        | 1.35     |
| 1   | S1    | 544  | PSU  | C6-C5 | 10.69 | 1.47        | 1.35     |
| 1   | S1    | 2116 | PSU  | C6-C5 | 10.69 | 1.47        | 1.35     |
| 48  | LI    | 3444 | PSU  | C6-C5 | 10.69 | 1.47        | 1.35     |
| 1   | S1    | 1624 | PSU  | C6-C5 | 10.69 | 1.47        | 1.35     |
| 48  | LI    | 3175 | PSU  | C6-C5 | 10.68 | 1.47        | 1.35     |
| 44  | LE    | 1363 | PSU  | C6-C5 | 10.67 | 1.47        | 1.35     |
| 49  | LJ    | 3701 | PSU  | C6-C5 | 10.66 | 1.47        | 1.35     |
| 47  | LH    | 2361 | PSU  | C6-C5 | 10.66 | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | S1    | 1592 | PSU  | C6-C5 | 10.66 | 1.47        | 1.35     |
| 44  | LE    | 1235 | PSU  | C6-C5 | 10.66 | 1.47        | 1.35     |
| 48  | LI    | 3412 | PSU  | C6-C5 | 10.66 | 1.47        | 1.35     |
| 45  | LF    | 1876 | PSU  | C6-C5 | 10.66 | 1.47        | 1.35     |
| 42  | LC    | 421  | PSU  | C6-C5 | 10.66 | 1.47        | 1.35     |
| 47  | LH    | 2623 | PSU  | C6-C5 | 10.65 | 1.47        | 1.35     |
| 49  | LJ    | 3591 | PSU  | C6-C5 | 10.65 | 1.47        | 1.35     |
| 45  | LF    | 1859 | PSU  | C6-C5 | 10.65 | 1.47        | 1.35     |
| 47  | LH    | 2802 | PSU  | C6-C5 | 10.65 | 1.47        | 1.35     |
| 1   | S1    | 2101 | PSU  | C6-C5 | 10.65 | 1.47        | 1.35     |
| 47  | LH    | 2621 | PSU  | C6-C5 | 10.65 | 1.47        | 1.35     |
| 48  | LI    | 3185 | PSU  | C6-C5 | 10.64 | 1.47        | 1.35     |
| 48  | LI    | 3204 | PSU  | C6-C5 | 10.64 | 1.47        | 1.35     |
| 48  | LI    | 3451 | PSU  | C6-C5 | 10.63 | 1.47        | 1.35     |
| 44  | LE    | 1075 | PSU  | C6-C5 | 10.63 | 1.47        | 1.35     |
| 46  | LG    | 2154 | PSU  | C6-C5 | 10.63 | 1.47        | 1.35     |
| 42  | LC    | 498  | PSU  | C6-C5 | 10.63 | 1.47        | 1.35     |
| 48  | LI    | 3562 | PSU  | C6-C5 | 10.62 | 1.47        | 1.35     |
| 48  | LI    | 3503 | PSU  | C6-C5 | 10.61 | 1.47        | 1.35     |
| 47  | LH    | 2899 | PSU  | C6-C5 | 10.61 | 1.47        | 1.35     |
| 48  | LI    | 3440 | PSU  | C6-C5 | 10.61 | 1.47        | 1.35     |
| 44  | LE    | 1407 | PSU  | C6-C5 | 10.61 | 1.47        | 1.35     |
| 48  | LI    | 3332 | PSU  | C6-C5 | 10.60 | 1.47        | 1.35     |
| 47  | LH    | 2679 | PSU  | C6-C5 | 10.60 | 1.47        | 1.35     |
| 42  | LC    | 567  | PSU  | C6-C5 | 10.59 | 1.47        | 1.35     |
| 1   | S1    | 2129 | PSU  | C6-C5 | 10.59 | 1.47        | 1.35     |
| 1   | S1    | 1960 | PSU  | C6-C5 | 10.58 | 1.47        | 1.35     |
| 47  | LH    | 2642 | PSU  | C6-C5 | 10.55 | 1.47        | 1.35     |
| 48  | LI    | 3206 | PSU  | C6-C5 | 10.55 | 1.47        | 1.35     |
| 47  | LH    | 2330 | PSU  | C6-C5 | 10.53 | 1.47        | 1.35     |
| 45  | LF    | 1692 | PSU  | C6-C5 | 10.51 | 1.47        | 1.35     |
| 47  | LH    | 2624 | PSU  | C6-C5 | 10.47 | 1.47        | 1.35     |
| 44  | LE    | 1266 | PSU  | C6-C5 | 10.46 | 1.47        | 1.35     |
| 47  | LH    | 2754 | PSU  | C6-C5 | 10.45 | 1.47        | 1.35     |
| 47  | LH    | 2842 | PSU  | C6-C5 | 10.43 | 1.47        | 1.35     |
| 48  | LI    | 3568 | PSU  | C6-C5 | 10.40 | 1.47        | 1.35     |
| 1   | S1    | 1378 | PSU  | C6-C5 | 10.38 | 1.47        | 1.35     |
| 1   | S1    | 1711 | PSU  | C6-C5 | 10.28 | 1.47        | 1.35     |
| 49  | LJ    | 3644 | PSU  | C6-C5 | 10.25 | 1.47        | 1.35     |
| 1   | S1    | 1591 | PSU  | C6-C5 | 10.25 | 1.47        | 1.35     |
| 1   | S1    | 1554 | PSU  | C6-C5 | 10.08 | 1.47        | 1.35     |
| 48  | LI    | 2999 | PSU  | C2-N1 | 9.61  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 48  | LI    | 3145 | PSU  | C2-N1 | 9.60 | 1.49        | 1.36     |
| 45  | LF    | 1568 | PSU  | C2-N1 | 9.59 | 1.49        | 1.36     |
| 48  | LI    | 3446 | PSU  | C2-N1 | 9.58 | 1.49        | 1.36     |
| 48  | LI    | 3042 | PSU  | C2-N1 | 9.56 | 1.49        | 1.36     |
| 47  | LH    | 2742 | PSU  | C2-N1 | 9.55 | 1.49        | 1.36     |
| 47  | LH    | 2621 | PSU  | C2-N1 | 9.52 | 1.49        | 1.36     |
| 53  | LN    | 3969 | PSU  | C2-N1 | 9.50 | 1.49        | 1.36     |
| 52  | LM    | 3963 | PSU  | C2-N1 | 9.49 | 1.49        | 1.36     |
| 44  | LE    | 1260 | PSU  | C2-N1 | 9.45 | 1.49        | 1.36     |
| 51  | LL    | 3865 | PSU  | C2-N1 | 9.45 | 1.49        | 1.36     |
| 48  | LI    | 3531 | PSU  | C2-N1 | 9.43 | 1.49        | 1.36     |
| 1   | S1    | 403  | PSU  | C2-N1 | 9.43 | 1.49        | 1.36     |
| 48  | LI    | 3451 | PSU  | C2-N1 | 9.42 | 1.49        | 1.36     |
| 1   | S1    | 105  | PSU  | C2-N1 | 9.41 | 1.49        | 1.36     |
| 47  | LH    | 2586 | PSU  | C2-N1 | 9.41 | 1.49        | 1.36     |
| 45  | LF    | 1876 | PSU  | C2-N1 | 9.40 | 1.49        | 1.36     |
| 46  | LG    | 2119 | PSU  | C2-N1 | 9.40 | 1.49        | 1.36     |
| 1   | S1    | 1396 | PSU  | C2-N1 | 9.39 | 1.49        | 1.36     |
| 48  | LI    | 3542 | PSU  | C2-N1 | 9.38 | 1.49        | 1.36     |
| 52  | LM    | 3953 | PSU  | C2-N1 | 9.38 | 1.49        | 1.36     |
| 47  | LH    | 2802 | PSU  | C2-N1 | 9.38 | 1.49        | 1.36     |
| 44  | LE    | 1118 | PSU  | C2-N1 | 9.37 | 1.49        | 1.36     |
| 1   | S1    | 1660 | PSU  | C2-N1 | 9.37 | 1.49        | 1.36     |
| 47  | LH    | 2617 | PSU  | C2-N1 | 9.35 | 1.49        | 1.36     |
| 1   | S1    | 1068 | PSU  | C2-N1 | 9.34 | 1.49        | 1.36     |
| 42  | LC    | 302  | PSU  | C2-N1 | 9.34 | 1.49        | 1.36     |
| 48  | LI    | 3175 | PSU  | C2-N1 | 9.34 | 1.49        | 1.36     |
| 1   | S1    | 2081 | PSU  | C2-N1 | 9.33 | 1.49        | 1.36     |
| 44  | LE    | 1171 | PSU  | C2-N1 | 9.33 | 1.49        | 1.36     |
| 47  | LH    | 2837 | PSU  | C2-N1 | 9.32 | 1.49        | 1.36     |
| 47  | LH    | 2874 | PSU  | C2-N1 | 9.32 | 1.49        | 1.36     |
| 44  | LE    | 1235 | PSU  | C2-N1 | 9.32 | 1.49        | 1.36     |
| 47  | LH    | 2642 | PSU  | C2-N1 | 9.32 | 1.49        | 1.36     |
| 47  | LH    | 2914 | PSU  | C2-N1 | 9.31 | 1.49        | 1.36     |
| 46  | LG    | 2171 | PSU  | C2-N1 | 9.30 | 1.49        | 1.36     |
| 1   | S1    | 2065 | PSU  | C2-N1 | 9.30 | 1.49        | 1.36     |
| 48  | LI    | 3167 | PSU  | C2-N1 | 9.30 | 1.49        | 1.36     |
| 1   | S1    | 32   | PSU  | C2-N1 | 9.30 | 1.49        | 1.36     |
| 1   | S1    | 280  | PSU  | C2-N1 | 9.30 | 1.49        | 1.36     |
| 41  | LB    | 280  | PSU  | C2-N1 | 9.29 | 1.49        | 1.36     |
| 42  | LC    | 308  | PSU  | C2-N1 | 9.29 | 1.49        | 1.36     |
| 47  | LH    | 2624 | PSU  | C2-N1 | 9.28 | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 1592 | PSU  | C2-N1   | 9.27  | 1.49        | 1.36     |
| 1   | S1    | 640  | PSU  | C2-N1   | 9.26  | 1.49        | 1.36     |
| 45  | LF    | 1586 | PSU  | C2-N1   | 9.26  | 1.49        | 1.36     |
| 45  | LF    | 1692 | PSU  | C2-N1   | 9.25  | 1.49        | 1.36     |
| 42  | LC    | 498  | PSU  | C2-N1   | 9.24  | 1.49        | 1.36     |
| 45  | LF    | 1926 | PSU  | C2-N1   | 9.24  | 1.49        | 1.36     |
| 47  | LH    | 2591 | PSU  | C2-N1   | 9.24  | 1.49        | 1.36     |
| 1   | S1    | 176  | PSU  | C2-N1   | 9.24  | 1.49        | 1.36     |
| 48  | LI    | 3510 | PSU  | C2-N1   | 9.23  | 1.49        | 1.36     |
| 1   | S1    | 2129 | PSU  | C2-N1   | 9.22  | 1.49        | 1.36     |
| 48  | LI    | 3440 | PSU  | C2-N1   | 9.22  | 1.49        | 1.36     |
| 48  | LI    | 3185 | PSU  | C2-N1   | 9.21  | 1.49        | 1.36     |
| 44  | LE    | 1407 | PSU  | C2-N1   | 9.21  | 1.49        | 1.36     |
| 47  | LH    | 2887 | A2M  | C2'-C1' | -9.21 | 1.29        | 1.53     |
| 49  | LJ    | 3591 | PSU  | C2-N1   | 9.20  | 1.49        | 1.36     |
| 44  | LE    | 1198 | PSU  | C2-N1   | 9.19  | 1.49        | 1.36     |
| 45  | LF    | 1859 | PSU  | C2-N1   | 9.19  | 1.49        | 1.36     |
| 42  | LC    | 480  | PSU  | C2-N1   | 9.19  | 1.49        | 1.36     |
| 48  | LI    | 3332 | PSU  | C2-N1   | 9.19  | 1.49        | 1.36     |
| 44  | LE    | 1363 | PSU  | C2-N1   | 9.18  | 1.49        | 1.36     |
| 49  | LJ    | 3680 | PSU  | C2-N1   | 9.18  | 1.49        | 1.36     |
| 1   | S1    | 2131 | PSU  | C2-N1   | 9.18  | 1.49        | 1.36     |
| 44  | LE    | 1365 | PSU  | C2-N1   | 9.17  | 1.49        | 1.36     |
| 48  | LI    | 3444 | PSU  | C2-N1   | 9.17  | 1.49        | 1.36     |
| 47  | LH    | 2915 | PSU  | C2-N1   | 9.17  | 1.49        | 1.36     |
| 49  | LJ    | 3697 | PSU  | C2-N1   | 9.16  | 1.49        | 1.36     |
| 41  | LB    | 234  | PSU  | C2-N1   | 9.16  | 1.49        | 1.36     |
| 1   | S1    | 2305 | PSU  | C2-N1   | 9.15  | 1.49        | 1.36     |
| 1   | S1    | 1624 | PSU  | C2-N1   | 9.15  | 1.49        | 1.36     |
| 47  | LH    | 2899 | PSU  | C2-N1   | 9.15  | 1.49        | 1.36     |
| 1   | S1    | 465  | PSU  | C2-N1   | 9.14  | 1.49        | 1.36     |
| 48  | LI    | 3206 | PSU  | C2-N1   | 9.14  | 1.49        | 1.36     |
| 47  | LH    | 2623 | PSU  | C2-N1   | 9.13  | 1.49        | 1.36     |
| 47  | LH    | 2746 | PSU  | C2-N1   | 9.13  | 1.49        | 1.36     |
| 40  | LA    | 16   | PSU  | C2-N1   | 9.12  | 1.49        | 1.36     |
| 1   | S1    | 544  | PSU  | C2-N1   | 9.11  | 1.49        | 1.36     |
| 1   | S1    | 89   | PSU  | C2-N1   | 9.10  | 1.49        | 1.36     |
| 47  | LH    | 2679 | PSU  | C2-N1   | 9.10  | 1.49        | 1.36     |
| 47  | LH    | 2752 | PSU  | C2-N1   | 9.10  | 1.49        | 1.36     |
| 44  | LE    | 1266 | PSU  | C2-N1   | 9.10  | 1.49        | 1.36     |
| 48  | LI    | 3503 | PSU  | C2-N1   | 9.09  | 1.49        | 1.36     |
| 1   | S1    | 1715 | PSU  | C2-N1   | 9.09  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 41  | LB    | 281  | PSU  | C2-N1   | 9.09  | 1.49        | 1.36     |
| 47  | LH    | 2330 | PSU  | C2-N1   | 9.09  | 1.49        | 1.36     |
| 1   | S1    | 1554 | PSU  | C2-N1   | 9.09  | 1.49        | 1.36     |
| 44  | LE    | 1126 | PSU  | C2-N1   | 9.08  | 1.49        | 1.36     |
| 49  | LJ    | 3701 | PSU  | C2-N1   | 9.08  | 1.49        | 1.36     |
| 44  | LE    | 1023 | PSU  | C2-N1   | 9.07  | 1.49        | 1.36     |
| 46  | LG    | 2154 | PSU  | C2-N1   | 9.07  | 1.49        | 1.36     |
| 48  | LI    | 3412 | PSU  | C2-N1   | 9.06  | 1.49        | 1.36     |
| 48  | LI    | 3562 | PSU  | C2-N1   | 9.05  | 1.49        | 1.36     |
| 40  | LA    | 68   | PSU  | C2-N1   | 9.05  | 1.49        | 1.36     |
| 1   | S1    | 2116 | PSU  | C2-N1   | 9.04  | 1.49        | 1.36     |
| 42  | LC    | 421  | PSU  | C2-N1   | 9.04  | 1.49        | 1.36     |
| 44  | LE    | 1184 | PSU  | C2-N1   | 9.03  | 1.48        | 1.36     |
| 1   | S1    | 1393 | PSU  | C2-N1   | 9.02  | 1.48        | 1.36     |
| 1   | S1    | 27   | PSU  | C2-N1   | 9.02  | 1.48        | 1.36     |
| 1   | S1    | 1378 | PSU  | C2-N1   | 9.01  | 1.48        | 1.36     |
| 48  | LI    | 3568 | PSU  | C2-N1   | 9.00  | 1.48        | 1.36     |
| 1   | S1    | 1960 | PSU  | C2-N1   | 8.99  | 1.48        | 1.36     |
| 42  | LC    | 567  | PSU  | C2-N1   | 8.99  | 1.48        | 1.36     |
| 48  | LI    | 3204 | PSU  | C2-N1   | 8.99  | 1.48        | 1.36     |
| 44  | LE    | 1039 | A2M  | C2'-C1' | -8.98 | 1.30        | 1.53     |
| 47  | LH    | 2361 | PSU  | C2-N1   | 8.98  | 1.48        | 1.36     |
| 46  | LG    | 2125 | PSU  | C2-N1   | 8.97  | 1.48        | 1.36     |
| 42  | LC    | 594  | A2M  | C2'-C1' | -8.97 | 1.30        | 1.53     |
| 45  | LF    | 1582 | PSU  | C2-N1   | 8.95  | 1.48        | 1.36     |
| 45  | LF    | 1502 | A2M  | C2'-C1' | -8.95 | 1.30        | 1.53     |
| 44  | LE    | 1075 | PSU  | C2-N1   | 8.94  | 1.48        | 1.36     |
| 1   | S1    | 1549 | A2M  | C2'-C1' | -8.94 | 1.30        | 1.53     |
| 48  | LI    | 3500 | A2M  | C2'-C1' | -8.93 | 1.30        | 1.53     |
| 47  | LH    | 2754 | PSU  | C2-N1   | 8.93  | 1.48        | 1.36     |
| 44  | LE    | 935  | A2M  | C2'-C1' | -8.92 | 1.30        | 1.53     |
| 1   | S1    | 2101 | PSU  | C2-N1   | 8.91  | 1.48        | 1.36     |
| 1   | S1    | 565  | A2M  | C2'-C1' | -8.91 | 1.30        | 1.53     |
| 1   | S1    | 28   | A2M  | C2'-C1' | -8.90 | 1.30        | 1.53     |
| 47  | LH    | 2849 | A2M  | C2'-C1' | -8.90 | 1.30        | 1.53     |
| 47  | LH    | 2769 | A2M  | C2'-C1' | -8.90 | 1.30        | 1.53     |
| 41  | LB    | 183  | A2M  | C2'-C1' | -8.87 | 1.30        | 1.53     |
| 47  | LH    | 2349 | A2M  | C2'-C1' | -8.86 | 1.30        | 1.53     |
| 1   | S1    | 1591 | PSU  | C2-N1   | 8.85  | 1.48        | 1.36     |
| 1   | S1    | 533  | A2M  | C2'-C1' | -8.84 | 1.30        | 1.53     |
| 1   | S1    | 2046 | A2M  | C2'-C1' | -8.84 | 1.30        | 1.53     |
| 45  | LF    | 1738 | A2M  | C2'-C1' | -8.84 | 1.30        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | LA    | 97   | A2M  | C2'-C1' | -8.82 | 1.30        | 1.53     |
| 45  | LF    | 1929 | A2M  | C2'-C1' | -8.81 | 1.30        | 1.53     |
| 45  | LF    | 1891 | A2M  | C2'-C1' | -8.81 | 1.30        | 1.53     |
| 45  | LF    | 1888 | A2M  | C2'-C1' | -8.80 | 1.30        | 1.53     |
| 48  | LI    | 3521 | A2M  | C2'-C1' | -8.80 | 1.30        | 1.53     |
| 51  | LL    | 3906 | A2M  | C2'-C1' | -8.79 | 1.30        | 1.53     |
| 1   | S1    | 40   | A2M  | C2'-C1' | -8.79 | 1.30        | 1.53     |
| 49  | LJ    | 3644 | PSU  | C2-N1   | 8.79  | 1.48        | 1.36     |
| 46  | LG    | 2005 | A2M  | C2'-C1' | -8.79 | 1.30        | 1.53     |
| 48  | LI    | 3533 | A2M  | C2'-C1' | -8.79 | 1.30        | 1.53     |
| 40  | LA    | 39   | A2M  | C2'-C1' | -8.78 | 1.30        | 1.53     |
| 47  | LH    | 2842 | PSU  | C2-N1   | 8.77  | 1.48        | 1.36     |
| 44  | LE    | 1204 | A2M  | C2'-C1' | -8.77 | 1.30        | 1.53     |
| 47  | LH    | 2708 | A2M  | C2'-C1' | -8.77 | 1.30        | 1.53     |
| 47  | LH    | 2809 | A2M  | C2'-C1' | -8.76 | 1.30        | 1.53     |
| 1   | S1    | 1900 | A2M  | C2'-C1' | -8.74 | 1.30        | 1.53     |
| 47  | LH    | 2768 | A2M  | C2'-C1' | -8.72 | 1.30        | 1.53     |
| 47  | LH    | 2814 | A2M  | C2'-C1' | -8.72 | 1.30        | 1.53     |
| 1   | S1    | 649  | A2M  | C2'-C1' | -8.72 | 1.30        | 1.53     |
| 1   | S1    | 1096 | A2M  | C2'-C1' | -8.70 | 1.30        | 1.53     |
| 45  | LF    | 1815 | A2M  | C2'-C1' | -8.69 | 1.30        | 1.53     |
| 1   | S1    | 1371 | A2M  | O4'-C1' | 8.69  | 1.62        | 1.42     |
| 48  | LI    | 3315 | A2M  | C2'-C1' | -8.66 | 1.30        | 1.53     |
| 47  | LH    | 2744 | A2M  | C2'-C1' | -8.66 | 1.30        | 1.53     |
| 47  | LH    | 2708 | A2M  | O4'-C1' | 8.66  | 1.62        | 1.42     |
| 40  | LA    | 39   | A2M  | O4'-C1' | 8.66  | 1.62        | 1.42     |
| 48  | LI    | 3348 | A2M  | C2'-C1' | -8.64 | 1.30        | 1.53     |
| 44  | LE    | 1121 | A2M  | C2'-C1' | -8.64 | 1.30        | 1.53     |
| 51  | LL    | 3906 | A2M  | O4'-C1' | 8.62  | 1.62        | 1.42     |
| 48  | LI    | 3315 | A2M  | O4'-C1' | 8.62  | 1.62        | 1.42     |
| 1   | S1    | 1711 | PSU  | C2-N1   | 8.62  | 1.48        | 1.36     |
| 1   | S1    | 723  | A2M  | C2'-C1' | -8.60 | 1.30        | 1.53     |
| 1   | S1    | 110  | A2M  | C2'-C1' | -8.60 | 1.30        | 1.53     |
| 44  | LE    | 1106 | A2M  | C2'-C1' | -8.60 | 1.30        | 1.53     |
| 46  | LG    | 2022 | A2M  | C2'-C1' | -8.59 | 1.31        | 1.53     |
| 47  | LH    | 2920 | A2M  | C2'-C1' | -8.58 | 1.31        | 1.53     |
| 44  | LE    | 1204 | A2M  | O4'-C1' | 8.57  | 1.62        | 1.42     |
| 44  | LE    | 1121 | A2M  | O4'-C1' | 8.57  | 1.62        | 1.42     |
| 48  | LI    | 3500 | A2M  | O4'-C1' | 8.56  | 1.62        | 1.42     |
| 45  | LF    | 1888 | A2M  | O4'-C1' | 8.55  | 1.62        | 1.42     |
| 47  | LH    | 2887 | A2M  | O4'-C1' | 8.55  | 1.62        | 1.42     |
| 1   | S1    | 1063 | A2M  | C2'-C1' | -8.55 | 1.31        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 47  | LH    | 2358 | A2M  | C2'-C1' | -8.55 | 1.31        | 1.53     |
| 44  | LE    | 1039 | A2M  | O4'-C1' | 8.55  | 1.62        | 1.42     |
| 48  | LI    | 3367 | A2M  | O4'-C1' | 8.52  | 1.62        | 1.42     |
| 47  | LH    | 2920 | A2M  | O4'-C1' | 8.52  | 1.62        | 1.42     |
| 47  | LH    | 2349 | A2M  | O4'-C1' | 8.52  | 1.62        | 1.42     |
| 1   | S1    | 1549 | A2M  | O4'-C1' | 8.52  | 1.62        | 1.42     |
| 48  | LI    | 3348 | A2M  | O4'-C1' | 8.51  | 1.62        | 1.42     |
| 48  | LI    | 3367 | A2M  | C2'-C1' | -8.50 | 1.31        | 1.53     |
| 1   | S1    | 1096 | A2M  | O4'-C1' | 8.50  | 1.62        | 1.42     |
| 1   | S1    | 407  | A2M  | O4'-C1' | 8.49  | 1.62        | 1.42     |
| 46  | LG    | 2022 | A2M  | O4'-C1' | 8.48  | 1.62        | 1.42     |
| 47  | LH    | 2814 | A2M  | O4'-C1' | 8.47  | 1.62        | 1.42     |
| 47  | LH    | 2812 | A2M  | O4'-C1' | 8.47  | 1.62        | 1.42     |
| 1   | S1    | 28   | A2M  | O4'-C1' | 8.46  | 1.62        | 1.42     |
| 1   | S1    | 565  | A2M  | O4'-C1' | 8.46  | 1.62        | 1.42     |
| 1   | S1    | 1371 | A2M  | C2'-C1' | -8.45 | 1.31        | 1.53     |
| 1   | S1    | 533  | A2M  | O4'-C1' | 8.43  | 1.62        | 1.42     |
| 1   | S1    | 1900 | A2M  | O4'-C1' | 8.42  | 1.62        | 1.42     |
| 42  | LC    | 594  | A2M  | O4'-C1' | 8.42  | 1.61        | 1.42     |
| 45  | LF    | 1891 | A2M  | O4'-C1' | 8.42  | 1.61        | 1.42     |
| 1   | S1    | 407  | A2M  | C2'-C1' | -8.41 | 1.31        | 1.53     |
| 1   | S1    | 1063 | A2M  | O4'-C1' | 8.41  | 1.61        | 1.42     |
| 47  | LH    | 2812 | A2M  | C2'-C1' | -8.40 | 1.31        | 1.53     |
| 47  | LH    | 2809 | A2M  | O4'-C1' | 8.40  | 1.61        | 1.42     |
| 45  | LF    | 1502 | A2M  | O4'-C1' | 8.40  | 1.61        | 1.42     |
| 45  | LF    | 1815 | A2M  | O4'-C1' | 8.40  | 1.61        | 1.42     |
| 47  | LH    | 2768 | A2M  | O4'-C1' | 8.36  | 1.61        | 1.42     |
| 45  | LF    | 1929 | A2M  | O4'-C1' | 8.36  | 1.61        | 1.42     |
| 48  | LI    | 3533 | A2M  | O4'-C1' | 8.35  | 1.61        | 1.42     |
| 1   | S1    | 2046 | A2M  | O4'-C1' | 8.35  | 1.61        | 1.42     |
| 44  | LE    | 935  | A2M  | O4'-C1' | 8.34  | 1.61        | 1.42     |
| 44  | LE    | 1106 | A2M  | O4'-C1' | 8.33  | 1.61        | 1.42     |
| 46  | LG    | 2005 | A2M  | O4'-C1' | 8.33  | 1.61        | 1.42     |
| 1   | S1    | 645  | A2M  | C2'-C1' | -8.32 | 1.31        | 1.53     |
| 1   | S1    | 110  | A2M  | O4'-C1' | 8.32  | 1.61        | 1.42     |
| 1   | S1    | 645  | A2M  | O4'-C1' | 8.31  | 1.61        | 1.42     |
| 1   | S1    | 40   | A2M  | O4'-C1' | 8.30  | 1.61        | 1.42     |
| 48  | LI    | 3521 | A2M  | O4'-C1' | 8.30  | 1.61        | 1.42     |
| 41  | LB    | 183  | A2M  | O4'-C1' | 8.29  | 1.61        | 1.42     |
| 45  | LF    | 1738 | A2M  | O4'-C1' | 8.28  | 1.61        | 1.42     |
| 40  | LA    | 97   | A2M  | O4'-C1' | 8.24  | 1.61        | 1.42     |
| 47  | LH    | 2849 | A2M  | O4'-C1' | 8.20  | 1.61        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 47  | LH    | 2744 | A2M  | O4'-C1' | 8.16 | 1.61        | 1.42     |
| 1   | S1    | 649  | A2M  | O4'-C1' | 8.12 | 1.61        | 1.42     |
| 47  | LH    | 2358 | A2M  | O4'-C1' | 8.09 | 1.61        | 1.42     |
| 47  | LH    | 2769 | A2M  | O4'-C1' | 8.04 | 1.61        | 1.42     |
| 1   | S1    | 723  | A2M  | O4'-C1' | 7.92 | 1.60        | 1.42     |
| 48  | LI    | 3042 | PSU  | C2-N3   | 7.50 | 1.50        | 1.37     |
| 48  | LI    | 2999 | PSU  | C2-N3   | 7.47 | 1.50        | 1.37     |
| 53  | LN    | 3969 | PSU  | C2-N3   | 7.46 | 1.50        | 1.37     |
| 48  | LI    | 3167 | PSU  | C2-N3   | 7.37 | 1.50        | 1.37     |
| 42  | LC    | 308  | PSU  | C2-N3   | 7.36 | 1.50        | 1.37     |
| 52  | LM    | 3963 | PSU  | C2-N3   | 7.35 | 1.50        | 1.37     |
| 48  | LI    | 3510 | PSU  | C2-N3   | 7.33 | 1.50        | 1.37     |
| 51  | LL    | 3865 | PSU  | C2-N3   | 7.32 | 1.50        | 1.37     |
| 1   | S1    | 280  | PSU  | C2-N3   | 7.32 | 1.50        | 1.37     |
| 45  | LF    | 1568 | PSU  | C2-N3   | 7.32 | 1.50        | 1.37     |
| 2   | S2    | 37   | MIA  | C13-C14 | 7.28 | 1.53        | 1.32     |
| 1   | S1    | 1624 | PSU  | C2-N3   | 7.27 | 1.50        | 1.37     |
| 42  | LC    | 421  | PSU  | C2-N3   | 7.27 | 1.50        | 1.37     |
| 45  | LF    | 1586 | PSU  | C2-N3   | 7.26 | 1.49        | 1.37     |
| 44  | LE    | 1235 | PSU  | C2-N3   | 7.26 | 1.49        | 1.37     |
| 47  | LH    | 2586 | PSU  | C2-N3   | 7.25 | 1.49        | 1.37     |
| 48  | LI    | 3145 | PSU  | C2-N3   | 7.25 | 1.49        | 1.37     |
| 46  | LG    | 2171 | PSU  | C2-N3   | 7.23 | 1.49        | 1.37     |
| 42  | LC    | 498  | PSU  | C2-N3   | 7.23 | 1.49        | 1.37     |
| 1   | S1    | 2081 | PSU  | C2-N3   | 7.22 | 1.49        | 1.37     |
| 1   | S1    | 1396 | PSU  | C2-N3   | 7.22 | 1.49        | 1.37     |
| 47  | LH    | 2802 | PSU  | C2-N3   | 7.21 | 1.49        | 1.37     |
| 44  | LE    | 1363 | PSU  | C2-N3   | 7.21 | 1.49        | 1.37     |
| 46  | LG    | 2125 | PSU  | C2-N3   | 7.21 | 1.49        | 1.37     |
| 1   | S1    | 1068 | PSU  | C2-N3   | 7.21 | 1.49        | 1.37     |
| 48  | LI    | 3206 | PSU  | C2-N3   | 7.20 | 1.49        | 1.37     |
| 42  | LC    | 302  | PSU  | C2-N3   | 7.20 | 1.49        | 1.37     |
| 48  | LI    | 3440 | PSU  | C2-N3   | 7.20 | 1.49        | 1.37     |
| 48  | LI    | 3175 | PSU  | C2-N3   | 7.20 | 1.49        | 1.37     |
| 1   | S1    | 2101 | PSU  | C2-N3   | 7.18 | 1.49        | 1.37     |
| 45  | LF    | 1859 | PSU  | C2-N3   | 7.18 | 1.49        | 1.37     |
| 1   | S1    | 1660 | PSU  | C2-N3   | 7.18 | 1.49        | 1.37     |
| 1   | S1    | 1393 | PSU  | C2-N3   | 7.18 | 1.49        | 1.37     |
| 47  | LH    | 2842 | PSU  | C2-N3   | 7.17 | 1.49        | 1.37     |
| 49  | LJ    | 3697 | PSU  | C2-N3   | 7.17 | 1.49        | 1.37     |
| 44  | LE    | 1260 | PSU  | C2-N3   | 7.17 | 1.49        | 1.37     |
| 44  | LE    | 1023 | PSU  | C2-N3   | 7.16 | 1.49        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | LI    | 3568 | PSU  | C2-N3   | 7.16  | 1.49        | 1.37     |
| 47  | LH    | 2591 | PSU  | C2-N3   | 7.16  | 1.49        | 1.37     |
| 48  | LI    | 3444 | PSU  | C2-N3   | 7.15  | 1.49        | 1.37     |
| 1   | S1    | 176  | PSU  | C2-N3   | 7.14  | 1.49        | 1.37     |
| 48  | LI    | 3446 | PSU  | C2-N3   | 7.14  | 1.49        | 1.37     |
| 47  | LH    | 2874 | PSU  | C2-N3   | 7.14  | 1.49        | 1.37     |
| 42  | LC    | 480  | PSU  | C2-N3   | 7.14  | 1.49        | 1.37     |
| 49  | LJ    | 3680 | PSU  | C2-N3   | 7.14  | 1.49        | 1.37     |
| 44  | LE    | 1171 | PSU  | C2-N3   | 7.13  | 1.49        | 1.37     |
| 47  | LH    | 2617 | PSU  | C2-N3   | 7.13  | 1.49        | 1.37     |
| 1   | S1    | 1711 | PSU  | C2-N3   | 7.13  | 1.49        | 1.37     |
| 47  | LH    | 2899 | PSU  | C2-N3   | 7.12  | 1.49        | 1.37     |
| 1   | S1    | 2065 | PSU  | C2-N3   | 7.12  | 1.49        | 1.37     |
| 44  | LE    | 1266 | PSU  | C2-N3   | 7.12  | 1.49        | 1.37     |
| 47  | LH    | 2752 | PSU  | C2-N3   | 7.11  | 1.49        | 1.37     |
| 45  | LF    | 1876 | PSU  | C2-N3   | 7.10  | 1.49        | 1.37     |
| 52  | LM    | 3953 | PSU  | C2-N3   | 7.10  | 1.49        | 1.37     |
| 1   | S1    | 2305 | PSU  | C2-N3   | 7.10  | 1.49        | 1.37     |
| 46  | LG    | 2154 | PSU  | C2-N3   | 7.10  | 1.49        | 1.37     |
| 1   | S1    | 105  | PSU  | C2-N3   | 7.10  | 1.49        | 1.37     |
| 1   | S1    | 1960 | PSU  | C2-N3   | 7.09  | 1.49        | 1.37     |
| 44  | LE    | 1365 | PSU  | C2-N3   | 7.09  | 1.49        | 1.37     |
| 44  | LE    | 1184 | PSU  | C2-N3   | 7.09  | 1.49        | 1.37     |
| 45  | LF    | 1582 | PSU  | C2-N3   | 7.09  | 1.49        | 1.37     |
| 48  | LI    | 3531 | PSU  | C2-N3   | 7.08  | 1.49        | 1.37     |
| 1   | S1    | 1715 | PSU  | C2-N3   | 7.08  | 1.49        | 1.37     |
| 47  | LH    | 2837 | PSU  | C2-N3   | 7.08  | 1.49        | 1.37     |
| 48  | LI    | 3451 | PSU  | C2-N3   | 7.08  | 1.49        | 1.37     |
| 1   | S1    | 2131 | PSU  | C2-N3   | 7.08  | 1.49        | 1.37     |
| 48  | LI    | 3503 | PSU  | C2-N3   | 7.08  | 1.49        | 1.37     |
| 46  | LG    | 2119 | PSU  | C2-N3   | 7.08  | 1.49        | 1.37     |
| 44  | LE    | 1407 | PSU  | C2-N3   | 7.07  | 1.49        | 1.37     |
| 47  | LH    | 2754 | PSU  | C2-N3   | 7.07  | 1.49        | 1.37     |
| 45  | LF    | 1692 | PSU  | C2-N3   | 7.06  | 1.49        | 1.37     |
| 1   | S1    | 465  | PSU  | C2-N3   | 7.05  | 1.49        | 1.37     |
| 41  | LB    | 234  | PSU  | C2-N3   | 7.05  | 1.49        | 1.37     |
| 1   | S1    | 403  | PSU  | C2-N3   | 7.05  | 1.49        | 1.37     |
| 1   | S1    | 723  | A2M  | O4'-C4' | -7.04 | 1.29        | 1.45     |
| 49  | LJ    | 3701 | PSU  | C2-N3   | 7.04  | 1.49        | 1.37     |
| 1   | S1    | 640  | PSU  | C2-N3   | 7.03  | 1.49        | 1.37     |
| 1   | S1    | 2129 | PSU  | C2-N3   | 7.03  | 1.49        | 1.37     |
| 47  | LH    | 2914 | PSU  | C2-N3   | 7.03  | 1.49        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 1378 | PSU  | C2-N3   | 7.03  | 1.49        | 1.37     |
| 41  | LB    | 281  | PSU  | C2-N3   | 7.03  | 1.49        | 1.37     |
| 45  | LF    | 1926 | PSU  | C2-N3   | 7.02  | 1.49        | 1.37     |
| 47  | LH    | 2624 | PSU  | C2-N3   | 7.01  | 1.49        | 1.37     |
| 48  | LI    | 3542 | PSU  | C2-N3   | 7.01  | 1.49        | 1.37     |
| 49  | LJ    | 3591 | PSU  | C2-N3   | 7.01  | 1.49        | 1.37     |
| 48  | LI    | 3204 | PSU  | C2-N3   | 7.00  | 1.49        | 1.37     |
| 41  | LB    | 280  | PSU  | C2-N3   | 6.99  | 1.49        | 1.37     |
| 40  | LA    | 68   | PSU  | C2-N3   | 6.99  | 1.49        | 1.37     |
| 47  | LH    | 2642 | PSU  | C2-N3   | 6.99  | 1.49        | 1.37     |
| 48  | LI    | 3332 | PSU  | C2-N3   | 6.98  | 1.49        | 1.37     |
| 1   | S1    | 89   | PSU  | C2-N3   | 6.97  | 1.49        | 1.37     |
| 47  | LH    | 2621 | PSU  | C2-N3   | 6.97  | 1.49        | 1.37     |
| 47  | LH    | 2330 | PSU  | C2-N3   | 6.96  | 1.49        | 1.37     |
| 47  | LH    | 2742 | PSU  | C2-N3   | 6.95  | 1.49        | 1.37     |
| 47  | LH    | 2915 | PSU  | C2-N3   | 6.94  | 1.49        | 1.37     |
| 1   | S1    | 32   | PSU  | C2-N3   | 6.94  | 1.49        | 1.37     |
| 1   | S1    | 544  | PSU  | C2-N3   | 6.93  | 1.49        | 1.37     |
| 44  | LE    | 1198 | PSU  | C2-N3   | 6.92  | 1.49        | 1.37     |
| 1   | S1    | 27   | PSU  | C2-N3   | 6.92  | 1.49        | 1.37     |
| 40  | LA    | 16   | PSU  | C2-N3   | 6.91  | 1.49        | 1.37     |
| 47  | LH    | 2623 | PSU  | C2-N3   | 6.90  | 1.49        | 1.37     |
| 1   | S1    | 2116 | PSU  | C2-N3   | 6.89  | 1.49        | 1.37     |
| 44  | LE    | 1126 | PSU  | C2-N3   | 6.89  | 1.49        | 1.37     |
| 47  | LH    | 2679 | PSU  | C2-N3   | 6.88  | 1.49        | 1.37     |
| 42  | LC    | 567  | PSU  | C2-N3   | 6.87  | 1.49        | 1.37     |
| 48  | LI    | 3412 | PSU  | C2-N3   | 6.87  | 1.49        | 1.37     |
| 48  | LI    | 3185 | PSU  | C2-N3   | 6.86  | 1.49        | 1.37     |
| 48  | LI    | 3562 | PSU  | C2-N3   | 6.86  | 1.49        | 1.37     |
| 2   | S2    | 37   | MIA  | C6-N6   | 6.85  | 1.45        | 1.34     |
| 47  | LH    | 2361 | PSU  | C2-N3   | 6.83  | 1.49        | 1.37     |
| 44  | LE    | 1075 | PSU  | C2-N3   | 6.81  | 1.49        | 1.37     |
| 49  | LJ    | 3644 | PSU  | C2-N3   | 6.78  | 1.49        | 1.37     |
| 1   | S1    | 1592 | PSU  | C2-N3   | 6.78  | 1.49        | 1.37     |
| 1   | S1    | 1591 | PSU  | C2-N3   | 6.74  | 1.49        | 1.37     |
| 47  | LH    | 2849 | A2M  | O4'-C4' | -6.74 | 1.29        | 1.45     |
| 47  | LH    | 2920 | A2M  | O4'-C4' | -6.72 | 1.30        | 1.45     |
| 45  | LF    | 1502 | A2M  | O4'-C4' | -6.70 | 1.30        | 1.45     |
| 42  | LC    | 594  | A2M  | O4'-C4' | -6.68 | 1.30        | 1.45     |
| 1   | S1    | 1554 | PSU  | C2-N3   | 6.68  | 1.48        | 1.37     |
| 47  | LH    | 2887 | A2M  | O4'-C4' | -6.66 | 1.30        | 1.45     |
| 1   | S1    | 2046 | A2M  | O4'-C4' | -6.65 | 1.30        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | LI    | 3533 | A2M  | O4'-C4' | -6.63 | 1.30        | 1.45     |
| 1   | S1    | 1063 | A2M  | O4'-C4' | -6.61 | 1.30        | 1.45     |
| 1   | S1    | 40   | A2M  | O4'-C4' | -6.60 | 1.30        | 1.45     |
| 1   | S1    | 110  | A2M  | O4'-C4' | -6.59 | 1.30        | 1.45     |
| 44  | LE    | 1106 | A2M  | O4'-C4' | -6.59 | 1.30        | 1.45     |
| 48  | LI    | 3521 | A2M  | O4'-C4' | -6.59 | 1.30        | 1.45     |
| 47  | LH    | 2744 | A2M  | O4'-C4' | -6.56 | 1.30        | 1.45     |
| 1   | S1    | 1096 | A2M  | O4'-C4' | -6.55 | 1.30        | 1.45     |
| 44  | LE    | 1204 | A2M  | O4'-C4' | -6.55 | 1.30        | 1.45     |
| 1   | S1    | 1371 | A2M  | O4'-C4' | -6.55 | 1.30        | 1.45     |
| 46  | LG    | 2022 | A2M  | O4'-C4' | -6.55 | 1.30        | 1.45     |
| 1   | S1    | 645  | A2M  | O4'-C4' | -6.54 | 1.30        | 1.45     |
| 47  | LH    | 2768 | A2M  | O4'-C4' | -6.54 | 1.30        | 1.45     |
| 47  | LH    | 2358 | A2M  | O4'-C4' | -6.54 | 1.30        | 1.45     |
| 1   | S1    | 407  | A2M  | O4'-C4' | -6.53 | 1.30        | 1.45     |
| 44  | LE    | 1118 | PSU  | C2-N3   | 6.50  | 1.48        | 1.37     |
| 47  | LH    | 2809 | A2M  | O4'-C4' | -6.50 | 1.30        | 1.45     |
| 45  | LF    | 1891 | A2M  | O4'-C4' | -6.49 | 1.30        | 1.45     |
| 41  | LB    | 183  | A2M  | O4'-C4' | -6.48 | 1.30        | 1.45     |
| 1   | S1    | 649  | A2M  | O4'-C4' | -6.48 | 1.30        | 1.45     |
| 1   | S1    | 28   | A2M  | O4'-C4' | -6.48 | 1.30        | 1.45     |
| 48  | LI    | 3315 | A2M  | O4'-C4' | -6.48 | 1.30        | 1.45     |
| 45  | LF    | 1815 | A2M  | O4'-C4' | -6.47 | 1.30        | 1.45     |
| 47  | LH    | 2814 | A2M  | O4'-C4' | -6.47 | 1.30        | 1.45     |
| 1   | S1    | 1549 | A2M  | O4'-C4' | -6.47 | 1.30        | 1.45     |
| 48  | LI    | 3367 | A2M  | O4'-C4' | -6.45 | 1.30        | 1.45     |
| 47  | LH    | 2812 | A2M  | O4'-C4' | -6.45 | 1.30        | 1.45     |
| 44  | LE    | 1121 | A2M  | O4'-C4' | -6.42 | 1.30        | 1.45     |
| 45  | LF    | 1888 | A2M  | O4'-C4' | -6.41 | 1.30        | 1.45     |
| 1   | S1    | 533  | A2M  | O4'-C4' | -6.41 | 1.30        | 1.45     |
| 46  | LG    | 2005 | A2M  | O4'-C4' | -6.41 | 1.30        | 1.45     |
| 40  | LA    | 39   | A2M  | O4'-C4' | -6.39 | 1.30        | 1.45     |
| 44  | LE    | 1039 | A2M  | O4'-C4' | -6.39 | 1.30        | 1.45     |
| 47  | LH    | 2746 | PSU  | C2-N3   | 6.38  | 1.48        | 1.37     |
| 45  | LF    | 1929 | A2M  | O4'-C4' | -6.35 | 1.30        | 1.45     |
| 1   | S1    | 1900 | A2M  | O4'-C4' | -6.35 | 1.30        | 1.45     |
| 44  | LE    | 935  | A2M  | O4'-C4' | -6.35 | 1.30        | 1.45     |
| 45  | LF    | 1738 | A2M  | O4'-C4' | -6.34 | 1.30        | 1.45     |
| 47  | LH    | 2349 | A2M  | O4'-C4' | -6.34 | 1.30        | 1.45     |
| 1   | S1    | 565  | A2M  | O4'-C4' | -6.33 | 1.30        | 1.45     |
| 47  | LH    | 2769 | A2M  | O4'-C4' | -6.33 | 1.30        | 1.45     |
| 47  | LH    | 2708 | A2M  | O4'-C4' | -6.32 | 1.30        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | LI    | 3348 | A2M  | O4'-C4' | -6.31 | 1.30        | 1.45     |
| 48  | LI    | 3500 | A2M  | O4'-C4' | -6.26 | 1.31        | 1.45     |
| 40  | LA    | 97   | A2M  | O4'-C4' | -6.22 | 1.31        | 1.45     |
| 2   | S2    | 37   | MIA  | C2-S10  | 6.15  | 1.80        | 1.75     |
| 51  | LL    | 3906 | A2M  | O4'-C4' | -6.15 | 1.31        | 1.45     |
| 1   | S1    | 2078 | 7MG  | C8-N9   | 5.53  | 1.49        | 1.46     |
| 53  | LN    | 3969 | PSU  | C6-N1   | 5.31  | 1.45        | 1.36     |
| 48  | LI    | 3042 | PSU  | C6-N1   | 5.30  | 1.45        | 1.36     |
| 45  | LF    | 1568 | PSU  | C6-N1   | 5.27  | 1.45        | 1.36     |
| 47  | LH    | 2802 | PSU  | C6-N1   | 5.22  | 1.44        | 1.36     |
| 48  | LI    | 3446 | PSU  | C6-N1   | 5.22  | 1.44        | 1.36     |
| 44  | LE    | 938  | 7MG  | C8-N9   | 5.21  | 1.48        | 1.46     |
| 1   | S1    | 403  | PSU  | C6-N1   | 5.19  | 1.44        | 1.36     |
| 48  | LI    | 2999 | PSU  | C6-N1   | 5.17  | 1.44        | 1.36     |
| 45  | LF    | 1876 | PSU  | C6-N1   | 5.17  | 1.44        | 1.36     |
| 1   | S1    | 105  | PSU  | C6-N1   | 5.17  | 1.44        | 1.36     |
| 48  | LI    | 3185 | PSU  | C6-N1   | 5.16  | 1.44        | 1.36     |
| 1   | S1    | 280  | PSU  | C6-N1   | 5.15  | 1.44        | 1.36     |
| 48  | LI    | 3145 | PSU  | C6-N1   | 5.15  | 1.44        | 1.36     |
| 1   | S1    | 1660 | PSU  | C6-N1   | 5.14  | 1.44        | 1.36     |
| 47  | LH    | 2586 | PSU  | C6-N1   | 5.14  | 1.44        | 1.36     |
| 52  | LM    | 3953 | PSU  | C6-N1   | 5.13  | 1.44        | 1.36     |
| 52  | LM    | 3963 | PSU  | C6-N1   | 5.12  | 1.44        | 1.36     |
| 45  | LF    | 1926 | PSU  | C6-N1   | 5.12  | 1.44        | 1.36     |
| 1   | S1    | 2305 | PSU  | C6-N1   | 5.11  | 1.44        | 1.36     |
| 41  | LB    | 280  | PSU  | C6-N1   | 5.11  | 1.44        | 1.36     |
| 51  | LL    | 3865 | PSU  | C6-N1   | 5.10  | 1.44        | 1.36     |
| 42  | LC    | 302  | PSU  | C6-N1   | 5.10  | 1.44        | 1.36     |
| 1   | S1    | 2101 | PSU  | C6-N1   | 5.09  | 1.44        | 1.36     |
| 44  | LE    | 1260 | PSU  | C6-N1   | 5.09  | 1.44        | 1.36     |
| 1   | S1    | 640  | PSU  | C6-N1   | 5.08  | 1.44        | 1.36     |
| 47  | LH    | 2742 | PSU  | C6-N1   | 5.07  | 1.44        | 1.36     |
| 1   | S1    | 1592 | PSU  | C6-N1   | 5.06  | 1.44        | 1.36     |
| 1   | S1    | 1068 | PSU  | C6-N1   | 5.06  | 1.44        | 1.36     |
| 48  | LI    | 3542 | PSU  | C6-N1   | 5.05  | 1.44        | 1.36     |
| 44  | LE    | 1363 | PSU  | C6-N1   | 5.05  | 1.44        | 1.36     |
| 45  | LF    | 1586 | PSU  | C6-N1   | 5.04  | 1.44        | 1.36     |
| 44  | LE    | 1118 | PSU  | C6-N1   | 5.03  | 1.44        | 1.36     |
| 47  | LH    | 2591 | PSU  | C6-N1   | 5.03  | 1.44        | 1.36     |
| 47  | LH    | 2899 | PSU  | C6-N1   | 5.03  | 1.44        | 1.36     |
| 47  | LH    | 2621 | PSU  | C6-N1   | 5.03  | 1.44        | 1.36     |
| 47  | LH    | 2837 | PSU  | C6-N1   | 5.03  | 1.44        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 48  | LI    | 3451 | PSU  | C6-N1 | 5.03 | 1.44        | 1.36     |
| 46  | LG    | 2119 | PSU  | C6-N1 | 5.02 | 1.44        | 1.36     |
| 1   | S1    | 32   | PSU  | C6-N1 | 5.02 | 1.44        | 1.36     |
| 47  | LH    | 2874 | PSU  | C6-N1 | 5.02 | 1.44        | 1.36     |
| 49  | LJ    | 3591 | PSU  | C6-N1 | 5.02 | 1.44        | 1.36     |
| 41  | LB    | 234  | PSU  | C6-N1 | 5.01 | 1.44        | 1.36     |
| 44  | LE    | 1184 | PSU  | C6-N1 | 5.01 | 1.44        | 1.36     |
| 42  | LC    | 421  | PSU  | C6-N1 | 5.01 | 1.44        | 1.36     |
| 48  | LI    | 3167 | PSU  | C6-N1 | 5.01 | 1.44        | 1.36     |
| 48  | LI    | 3204 | PSU  | C6-N1 | 5.00 | 1.44        | 1.36     |
| 48  | LI    | 3531 | PSU  | C6-N1 | 5.00 | 1.44        | 1.36     |
| 44  | LE    | 1365 | PSU  | C6-N1 | 4.99 | 1.44        | 1.36     |
| 42  | LC    | 308  | PSU  | C6-N1 | 4.99 | 1.44        | 1.36     |
| 44  | LE    | 1171 | PSU  | C6-N1 | 4.99 | 1.44        | 1.36     |
| 48  | LI    | 3440 | PSU  | C6-N1 | 4.99 | 1.44        | 1.36     |
| 1   | S1    | 1715 | PSU  | C6-N1 | 4.99 | 1.44        | 1.36     |
| 44  | LE    | 1407 | PSU  | C6-N1 | 4.99 | 1.44        | 1.36     |
| 47  | LH    | 2915 | PSU  | C6-N1 | 4.98 | 1.44        | 1.36     |
| 1   | S1    | 1624 | PSU  | C6-N1 | 4.98 | 1.44        | 1.36     |
| 45  | LF    | 1859 | PSU  | C6-N1 | 4.98 | 1.44        | 1.36     |
| 40  | LA    | 16   | PSU  | C6-N1 | 4.97 | 1.44        | 1.36     |
| 47  | LH    | 2624 | PSU  | C6-N1 | 4.97 | 1.44        | 1.36     |
| 47  | LH    | 2914 | PSU  | C6-N1 | 4.97 | 1.44        | 1.36     |
| 42  | LC    | 480  | PSU  | C6-N1 | 4.97 | 1.44        | 1.36     |
| 1   | S1    | 2116 | PSU  | C6-N1 | 4.97 | 1.44        | 1.36     |
| 48  | LI    | 3332 | PSU  | C6-N1 | 4.97 | 1.44        | 1.36     |
| 45  | LF    | 1582 | PSU  | C6-N1 | 4.97 | 1.44        | 1.36     |
| 1   | S1    | 2131 | PSU  | C6-N1 | 4.96 | 1.44        | 1.36     |
| 1   | S1    | 1396 | PSU  | C6-N1 | 4.96 | 1.44        | 1.36     |
| 1   | S1    | 2065 | PSU  | C6-N1 | 4.96 | 1.44        | 1.36     |
| 46  | LG    | 2171 | PSU  | C6-N1 | 4.96 | 1.44        | 1.36     |
| 48  | LI    | 3503 | PSU  | C6-N1 | 4.95 | 1.44        | 1.36     |
| 1   | S1    | 89   | PSU  | C6-N1 | 4.95 | 1.44        | 1.36     |
| 48  | LI    | 3510 | PSU  | C6-N1 | 4.95 | 1.44        | 1.36     |
| 1   | S1    | 176  | PSU  | C6-N1 | 4.94 | 1.44        | 1.36     |
| 49  | LJ    | 3697 | PSU  | C6-N1 | 4.94 | 1.44        | 1.36     |
| 42  | LC    | 498  | PSU  | C6-N1 | 4.93 | 1.44        | 1.36     |
| 44  | LE    | 1198 | PSU  | C6-N1 | 4.93 | 1.44        | 1.36     |
| 1   | S1    | 27   | PSU  | C6-N1 | 4.93 | 1.44        | 1.36     |
| 1   | S1    | 2129 | PSU  | C6-N1 | 4.93 | 1.44        | 1.36     |
| 49  | LJ    | 3680 | PSU  | C6-N1 | 4.92 | 1.44        | 1.36     |
| 40  | LA    | 68   | PSU  | C6-N1 | 4.92 | 1.44        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 44  | LE    | 938  | 7MG  | C5-N7 | 4.91 | 1.41        | 1.35     |
| 46  | LG    | 2154 | PSU  | C6-N1 | 4.90 | 1.44        | 1.36     |
| 41  | LB    | 281  | PSU  | C6-N1 | 4.90 | 1.44        | 1.36     |
| 1   | S1    | 1711 | PSU  | C6-N1 | 4.90 | 1.44        | 1.36     |
| 44  | LE    | 1235 | PSU  | C6-N1 | 4.90 | 1.44        | 1.36     |
| 45  | LF    | 1692 | PSU  | C6-N1 | 4.90 | 1.44        | 1.36     |
| 48  | LI    | 3206 | PSU  | C6-N1 | 4.89 | 1.44        | 1.36     |
| 1   | S1    | 2081 | PSU  | C6-N1 | 4.89 | 1.44        | 1.36     |
| 48  | LI    | 3444 | PSU  | C6-N1 | 4.89 | 1.44        | 1.36     |
| 44  | LE    | 1126 | PSU  | C6-N1 | 4.88 | 1.44        | 1.36     |
| 47  | LH    | 2679 | PSU  | C6-N1 | 4.88 | 1.44        | 1.36     |
| 46  | LG    | 2125 | PSU  | C6-N1 | 4.87 | 1.44        | 1.36     |
| 48  | LI    | 3175 | PSU  | C6-N1 | 4.87 | 1.44        | 1.36     |
| 47  | LH    | 2617 | PSU  | C6-N1 | 4.86 | 1.44        | 1.36     |
| 1   | S1    | 465  | PSU  | C6-N1 | 4.86 | 1.44        | 1.36     |
| 47  | LH    | 2642 | PSU  | C6-N1 | 4.86 | 1.44        | 1.36     |
| 42  | LC    | 567  | PSU  | C6-N1 | 4.84 | 1.44        | 1.36     |
| 47  | LH    | 2752 | PSU  | C6-N1 | 4.84 | 1.44        | 1.36     |
| 1   | S1    | 544  | PSU  | C6-N1 | 4.84 | 1.44        | 1.36     |
| 1   | S1    | 1960 | PSU  | C6-N1 | 4.84 | 1.44        | 1.36     |
| 47  | LH    | 2623 | PSU  | C6-N1 | 4.82 | 1.44        | 1.36     |
| 1   | S1    | 1554 | PSU  | C6-N1 | 4.82 | 1.44        | 1.36     |
| 49  | LJ    | 3701 | PSU  | C6-N1 | 4.81 | 1.44        | 1.36     |
| 1   | S1    | 1591 | PSU  | C6-N1 | 4.81 | 1.44        | 1.36     |
| 48  | LI    | 3568 | PSU  | C6-N1 | 4.81 | 1.44        | 1.36     |
| 1   | S1    | 1393 | PSU  | C6-N1 | 4.81 | 1.44        | 1.36     |
| 44  | LE    | 1023 | PSU  | C6-N1 | 4.80 | 1.44        | 1.36     |
| 44  | LE    | 1266 | PSU  | C6-N1 | 4.79 | 1.44        | 1.36     |
| 47  | LH    | 2330 | PSU  | C6-N1 | 4.79 | 1.44        | 1.36     |
| 1   | S1    | 1378 | PSU  | C6-N1 | 4.78 | 1.44        | 1.36     |
| 47  | LH    | 2746 | PSU  | C6-N1 | 4.77 | 1.44        | 1.36     |
| 47  | LH    | 2754 | PSU  | C6-N1 | 4.77 | 1.44        | 1.36     |
| 44  | LE    | 1075 | PSU  | C6-N1 | 4.75 | 1.44        | 1.36     |
| 48  | LI    | 3562 | PSU  | C6-N1 | 4.70 | 1.44        | 1.36     |
| 49  | LJ    | 3644 | PSU  | C6-N1 | 4.66 | 1.44        | 1.36     |
| 48  | LI    | 3412 | PSU  | C6-N1 | 4.65 | 1.43        | 1.36     |
| 47  | LH    | 2361 | PSU  | C6-N1 | 4.63 | 1.43        | 1.36     |
| 47  | LH    | 2842 | PSU  | C6-N1 | 4.62 | 1.43        | 1.36     |
| 1   | S1    | 2078 | 7MG  | C5-N7 | 4.58 | 1.40        | 1.35     |
| 40  | LA    | 97   | A2M  | C6-N6 | 4.49 | 1.45        | 1.34     |
| 45  | LF    | 1929 | A2M  | C6-N6 | 4.48 | 1.45        | 1.34     |
| 48  | LI    | 3315 | A2M  | C6-N6 | 4.47 | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 48  | LI    | 3500 | A2M  | C6-N6 | 4.46 | 1.45        | 1.34     |
| 1   | S1    | 1063 | A2M  | C6-N6 | 4.46 | 1.45        | 1.34     |
| 1   | S1    | 1096 | A2M  | C6-N6 | 4.45 | 1.45        | 1.34     |
| 47  | LH    | 2685 | OMC  | C2-N1 | 4.44 | 1.49        | 1.40     |
| 1   | S1    | 2180 | A2M  | C5-C4 | 4.43 | 1.47        | 1.39     |
| 47  | LH    | 2920 | A2M  | C6-N6 | 4.43 | 1.45        | 1.34     |
| 1   | S1    | 407  | A2M  | C6-N6 | 4.43 | 1.45        | 1.34     |
| 1   | S1    | 645  | A2M  | C6-N6 | 4.42 | 1.45        | 1.34     |
| 1   | S1    | 1549 | A2M  | C6-N6 | 4.42 | 1.45        | 1.34     |
| 46  | LG    | 2022 | A2M  | C6-N6 | 4.41 | 1.45        | 1.34     |
| 41  | LB    | 183  | A2M  | C6-N6 | 4.41 | 1.45        | 1.34     |
| 44  | LE    | 1106 | A2M  | C6-N6 | 4.41 | 1.45        | 1.34     |
| 44  | LE    | 1121 | A2M  | C6-N6 | 4.41 | 1.45        | 1.34     |
| 45  | LF    | 1891 | A2M  | C6-N6 | 4.40 | 1.45        | 1.34     |
| 1   | S1    | 533  | A2M  | C6-N6 | 4.40 | 1.45        | 1.34     |
| 46  | LG    | 2005 | A2M  | C6-N6 | 4.40 | 1.45        | 1.34     |
| 1   | S1    | 649  | A2M  | C6-N6 | 4.40 | 1.45        | 1.34     |
| 42  | LC    | 594  | A2M  | C6-N6 | 4.40 | 1.45        | 1.34     |
| 1   | S1    | 565  | A2M  | C6-N6 | 4.40 | 1.45        | 1.34     |
| 47  | LH    | 2349 | A2M  | C6-N6 | 4.40 | 1.45        | 1.34     |
| 48  | LI    | 3348 | A2M  | C6-N6 | 4.39 | 1.45        | 1.34     |
| 45  | LF    | 1815 | A2M  | C6-N6 | 4.38 | 1.45        | 1.34     |
| 48  | LI    | 3521 | A2M  | C6-N6 | 4.38 | 1.45        | 1.34     |
| 1   | S1    | 110  | A2M  | C6-N6 | 4.37 | 1.45        | 1.34     |
| 1   | S1    | 2046 | A2M  | C6-N6 | 4.37 | 1.45        | 1.34     |
| 1   | S1    | 1900 | A2M  | C6-N6 | 4.37 | 1.45        | 1.34     |
| 47  | LH    | 2708 | A2M  | C6-N6 | 4.37 | 1.45        | 1.34     |
| 45  | LF    | 1502 | A2M  | C6-N6 | 4.37 | 1.45        | 1.34     |
| 45  | LF    | 1738 | A2M  | C6-N6 | 4.36 | 1.45        | 1.34     |
| 1   | S1    | 723  | A2M  | C6-N6 | 4.36 | 1.45        | 1.34     |
| 51  | LL    | 3906 | A2M  | C6-N6 | 4.36 | 1.45        | 1.34     |
| 47  | LH    | 2809 | A2M  | C6-N6 | 4.35 | 1.45        | 1.34     |
| 47  | LH    | 2887 | A2M  | C6-N6 | 4.35 | 1.45        | 1.34     |
| 47  | LH    | 2744 | A2M  | C6-N6 | 4.35 | 1.45        | 1.34     |
| 48  | LI    | 3533 | A2M  | C6-N6 | 4.34 | 1.45        | 1.34     |
| 44  | LE    | 1204 | A2M  | C6-N6 | 4.34 | 1.45        | 1.34     |
| 47  | LH    | 2814 | A2M  | C6-N6 | 4.34 | 1.45        | 1.34     |
| 45  | LF    | 1888 | A2M  | C6-N6 | 4.34 | 1.45        | 1.34     |
| 47  | LH    | 2812 | A2M  | C6-N6 | 4.33 | 1.45        | 1.34     |
| 1   | S1    | 1371 | A2M  | C6-N6 | 4.33 | 1.45        | 1.34     |
| 47  | LH    | 2849 | A2M  | C6-N6 | 4.33 | 1.45        | 1.34     |
| 1   | S1    | 28   | A2M  | C6-N6 | 4.31 | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 47  | LH    | 2768 | A2M  | C6-N6 | 4.31 | 1.45        | 1.34     |
| 48  | LI    | 3367 | A2M  | C6-N6 | 4.30 | 1.44        | 1.34     |
| 44  | LE    | 1039 | A2M  | C6-N6 | 4.30 | 1.44        | 1.34     |
| 47  | LH    | 2358 | A2M  | C6-N6 | 4.30 | 1.44        | 1.34     |
| 1   | S1    | 40   | A2M  | C6-N6 | 4.27 | 1.44        | 1.34     |
| 44  | LE    | 935  | A2M  | C6-N6 | 4.26 | 1.44        | 1.34     |
| 40  | LA    | 39   | A2M  | C6-N6 | 4.26 | 1.44        | 1.34     |
| 48  | LI    | 3214 | 6MZ  | C5-C4 | 4.25 | 1.47        | 1.39     |
| 47  | LH    | 2769 | A2M  | C6-N6 | 4.23 | 1.44        | 1.34     |
| 48  | LI    | 3042 | PSU  | C4-N3 | 4.01 | 1.46        | 1.38     |
| 45  | LF    | 1573 | OMC  | C2-N1 | 3.93 | 1.48        | 1.40     |
| 45  | LF    | 1568 | PSU  | C4-N3 | 3.87 | 1.46        | 1.38     |
| 48  | LI    | 2999 | PSU  | C4-N3 | 3.83 | 1.45        | 1.38     |
| 48  | LI    | 3446 | PSU  | C4-N3 | 3.82 | 1.45        | 1.38     |
| 53  | LN    | 3969 | PSU  | C4-N3 | 3.80 | 1.45        | 1.38     |
| 52  | LM    | 3963 | PSU  | C4-N3 | 3.80 | 1.45        | 1.38     |
| 1   | S1    | 280  | PSU  | C4-N3 | 3.80 | 1.45        | 1.38     |
| 42  | LC    | 421  | PSU  | C4-N3 | 3.78 | 1.45        | 1.38     |
| 47  | LH    | 2766 | 5MC  | C2-N1 | 3.78 | 1.48        | 1.40     |
| 48  | LI    | 3145 | PSU  | C4-N3 | 3.77 | 1.45        | 1.38     |
| 46  | LG    | 2125 | PSU  | C4-N3 | 3.76 | 1.45        | 1.38     |
| 42  | LC    | 308  | PSU  | C4-N3 | 3.75 | 1.45        | 1.38     |
| 41  | LB    | 281  | PSU  | C4-N3 | 3.74 | 1.45        | 1.38     |
| 47  | LH    | 2586 | PSU  | C4-N3 | 3.74 | 1.45        | 1.38     |
| 51  | LL    | 3865 | PSU  | C4-N3 | 3.73 | 1.45        | 1.38     |
| 44  | LE    | 1023 | PSU  | C4-N3 | 3.71 | 1.45        | 1.38     |
| 48  | LI    | 3510 | PSU  | C4-N3 | 3.71 | 1.45        | 1.38     |
| 48  | LI    | 3542 | PSU  | C4-N3 | 3.70 | 1.45        | 1.38     |
| 45  | LF    | 1586 | PSU  | C4-N3 | 3.70 | 1.45        | 1.38     |
| 1   | S1    | 1660 | PSU  | C4-N3 | 3.68 | 1.45        | 1.38     |
| 42  | LC    | 302  | PSU  | C4-N3 | 3.68 | 1.45        | 1.38     |
| 45  | LF    | 1926 | PSU  | C4-N3 | 3.67 | 1.45        | 1.38     |
| 1   | S1    | 640  | PSU  | C4-N3 | 3.67 | 1.45        | 1.38     |
| 1   | S1    | 1068 | PSU  | C4-N3 | 3.66 | 1.45        | 1.38     |
| 1   | S1    | 1715 | PSU  | C4-N3 | 3.66 | 1.45        | 1.38     |
| 1   | S1    | 176  | PSU  | C4-N3 | 3.66 | 1.45        | 1.38     |
| 48  | LI    | 3175 | PSU  | C4-N3 | 3.66 | 1.45        | 1.38     |
| 48  | LI    | 3444 | PSU  | C4-N3 | 3.65 | 1.45        | 1.38     |
| 47  | LH    | 2802 | PSU  | C4-N3 | 3.65 | 1.45        | 1.38     |
| 1   | S1    | 465  | PSU  | C4-N3 | 3.65 | 1.45        | 1.38     |
| 45  | LF    | 1859 | PSU  | C4-N3 | 3.65 | 1.45        | 1.38     |
| 1   | S1    | 1393 | PSU  | C4-N3 | 3.64 | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 48  | LI    | 3440 | PSU  | C4-N3 | 3.64 | 1.45        | 1.38     |
| 49  | LJ    | 3701 | PSU  | C4-N3 | 3.64 | 1.45        | 1.38     |
| 47  | LH    | 2842 | PSU  | C4-N3 | 3.64 | 1.45        | 1.38     |
| 47  | LH    | 2752 | PSU  | C4-N3 | 3.64 | 1.45        | 1.38     |
| 48  | LI    | 3332 | PSU  | C4-N3 | 3.64 | 1.45        | 1.38     |
| 41  | LB    | 234  | PSU  | C4-N3 | 3.64 | 1.45        | 1.38     |
| 52  | LM    | 3953 | PSU  | C4-N3 | 3.63 | 1.45        | 1.38     |
| 1   | S1    | 1624 | PSU  | C4-N3 | 3.63 | 1.45        | 1.38     |
| 1   | S1    | 2101 | PSU  | C4-N3 | 3.63 | 1.45        | 1.38     |
| 41  | LB    | 280  | PSU  | C4-N3 | 3.63 | 1.45        | 1.38     |
| 1   | S1    | 1960 | PSU  | C4-N3 | 3.63 | 1.45        | 1.38     |
| 42  | LC    | 498  | PSU  | C4-N3 | 3.63 | 1.45        | 1.38     |
| 47  | LH    | 2642 | PSU  | C4-N3 | 3.62 | 1.45        | 1.38     |
| 44  | LE    | 1365 | PSU  | C4-N3 | 3.62 | 1.45        | 1.38     |
| 1   | S1    | 2305 | PSU  | C4-N3 | 3.62 | 1.45        | 1.38     |
| 1   | S1    | 1378 | PSU  | C4-N3 | 3.62 | 1.45        | 1.38     |
| 45  | LF    | 1876 | PSU  | C4-N3 | 3.62 | 1.45        | 1.38     |
| 44  | LE    | 1363 | PSU  | C4-N3 | 3.61 | 1.45        | 1.38     |
| 48  | LI    | 3167 | PSU  | C4-N3 | 3.61 | 1.45        | 1.38     |
| 45  | LF    | 1582 | PSU  | C4-N3 | 3.60 | 1.45        | 1.38     |
| 44  | LE    | 1407 | PSU  | C4-N3 | 3.60 | 1.45        | 1.38     |
| 45  | LF    | 1692 | PSU  | C4-N3 | 3.59 | 1.45        | 1.38     |
| 44  | LE    | 1184 | PSU  | C4-N3 | 3.58 | 1.45        | 1.38     |
| 1   | S1    | 2081 | PSU  | C4-N3 | 3.58 | 1.45        | 1.38     |
| 47  | LH    | 2679 | PSU  | C4-N3 | 3.58 | 1.45        | 1.38     |
| 44  | LE    | 1235 | PSU  | C4-N3 | 3.58 | 1.45        | 1.38     |
| 47  | LH    | 2621 | PSU  | C4-N3 | 3.57 | 1.45        | 1.38     |
| 47  | LH    | 2617 | PSU  | C4-N3 | 3.57 | 1.45        | 1.38     |
| 47  | LH    | 2837 | PSU  | C4-N3 | 3.56 | 1.45        | 1.38     |
| 1   | S1    | 403  | PSU  | C4-N3 | 3.55 | 1.45        | 1.38     |
| 1   | S1    | 2288 | MA6  | C6-N6 | 3.55 | 1.47        | 1.36     |
| 46  | LG    | 2154 | PSU  | C4-N3 | 3.54 | 1.45        | 1.38     |
| 1   | S1    | 105  | PSU  | C4-N3 | 3.54 | 1.45        | 1.38     |
| 49  | LJ    | 3697 | PSU  | C4-N3 | 3.54 | 1.45        | 1.38     |
| 47  | LH    | 2914 | PSU  | C4-N3 | 3.54 | 1.45        | 1.38     |
| 47  | LH    | 2915 | PSU  | C4-N3 | 3.54 | 1.45        | 1.38     |
| 48  | LI    | 3185 | PSU  | C4-N3 | 3.53 | 1.45        | 1.38     |
| 1   | S1    | 27   | PSU  | C4-N3 | 3.53 | 1.45        | 1.38     |
| 47  | LH    | 2874 | PSU  | C4-N3 | 3.52 | 1.45        | 1.38     |
| 1   | S1    | 1396 | PSU  | C4-N3 | 3.51 | 1.45        | 1.38     |
| 46  | LG    | 2171 | PSU  | C4-N3 | 3.51 | 1.45        | 1.38     |
| 40  | LA    | 68   | PSU  | C4-N3 | 3.51 | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 44  | LE    | 1260 | PSU  | C4-N3   | 3.51  | 1.45        | 1.38     |
| 48  | LI    | 3451 | PSU  | C4-N3   | 3.51  | 1.45        | 1.38     |
| 44  | LE    | 1266 | PSU  | C4-N3   | 3.51  | 1.45        | 1.38     |
| 1   | S1    | 2131 | PSU  | C4-N3   | 3.50  | 1.45        | 1.38     |
| 48  | LI    | 3206 | PSU  | C4-N3   | 3.50  | 1.45        | 1.38     |
| 47  | LH    | 2754 | PSU  | C4-N3   | 3.50  | 1.45        | 1.38     |
| 48  | LI    | 3503 | PSU  | C4-N3   | 3.50  | 1.45        | 1.38     |
| 1   | S1    | 2065 | PSU  | C4-N3   | 3.49  | 1.45        | 1.38     |
| 49  | LJ    | 3644 | PSU  | C4-N3   | 3.49  | 1.45        | 1.38     |
| 49  | LJ    | 3591 | PSU  | C4-N3   | 3.49  | 1.45        | 1.38     |
| 48  | LI    | 3412 | PSU  | C4-N3   | 3.49  | 1.45        | 1.38     |
| 47  | LH    | 2744 | A2M  | C5-C4   | -3.49 | 1.32        | 1.39     |
| 44  | LE    | 1198 | PSU  | C4-N3   | 3.49  | 1.45        | 1.38     |
| 42  | LC    | 480  | PSU  | C4-N3   | 3.49  | 1.45        | 1.38     |
| 44  | LE    | 1075 | PSU  | C4-N3   | 3.48  | 1.45        | 1.38     |
| 47  | LH    | 2591 | PSU  | C4-N3   | 3.48  | 1.45        | 1.38     |
| 47  | LH    | 2330 | PSU  | C4-N3   | 3.48  | 1.45        | 1.38     |
| 46  | LG    | 2119 | PSU  | C4-N3   | 3.48  | 1.45        | 1.38     |
| 48  | LI    | 3204 | PSU  | C4-N3   | 3.47  | 1.45        | 1.38     |
| 42  | LC    | 567  | PSU  | C4-N3   | 3.47  | 1.45        | 1.38     |
| 48  | LI    | 3456 | 5MC  | C2-N1   | 3.47  | 1.47        | 1.40     |
| 48  | LI    | 3568 | PSU  | C4-N3   | 3.47  | 1.45        | 1.38     |
| 47  | LH    | 2623 | PSU  | C4-N3   | 3.47  | 1.45        | 1.38     |
| 44  | LE    | 1171 | PSU  | C4-N3   | 3.47  | 1.45        | 1.38     |
| 47  | LH    | 2899 | PSU  | C4-N3   | 3.46  | 1.45        | 1.38     |
| 1   | S1    | 2116 | PSU  | C4-N3   | 3.46  | 1.45        | 1.38     |
| 1   | S1    | 1711 | PSU  | C4-N3   | 3.46  | 1.45        | 1.38     |
| 1   | S1    | 2129 | PSU  | C4-N3   | 3.44  | 1.45        | 1.38     |
| 45  | LF    | 1891 | A2M  | C5-C4   | -3.44 | 1.32        | 1.39     |
| 44  | LE    | 1165 | OMC  | C2-N1   | 3.43  | 1.47        | 1.40     |
| 48  | LI    | 3531 | PSU  | C4-N3   | 3.41  | 1.45        | 1.38     |
| 47  | LH    | 2624 | PSU  | C4-N3   | 3.40  | 1.45        | 1.38     |
| 1   | S1    | 544  | PSU  | C4-N3   | 3.39  | 1.45        | 1.38     |
| 1   | S1    | 1591 | PSU  | C4-N3   | 3.38  | 1.45        | 1.38     |
| 40  | LA    | 16   | PSU  | C4-N3   | 3.38  | 1.45        | 1.38     |
| 40  | LA    | 97   | A2M  | O3'-C3' | -3.38 | 1.35        | 1.43     |
| 1   | S1    | 2287 | MA6  | C6-N6   | 3.37  | 1.46        | 1.36     |
| 1   | S1    | 103  | OMC  | C2-N1   | 3.35  | 1.47        | 1.40     |
| 48  | LI    | 3518 | 5MC  | C2-N1   | 3.35  | 1.47        | 1.40     |
| 1   | S1    | 89   | PSU  | C4-N3   | 3.34  | 1.45        | 1.38     |
| 1   | S1    | 32   | PSU  | C4-N3   | 3.34  | 1.45        | 1.38     |
| 47  | LH    | 2742 | PSU  | C4-N3   | 3.34  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | LI    | 3533 | A2M  | C5-C4   | -3.33 | 1.32        | 1.39     |
| 1   | S1    | 2287 | MA6  | C5-C4   | -3.32 | 1.32        | 1.39     |
| 49  | LJ    | 3680 | PSU  | C4-N3   | 3.32  | 1.45        | 1.38     |
| 1   | S1    | 1371 | A2M  | O3'-C3' | -3.31 | 1.35        | 1.43     |
| 47  | LH    | 2358 | A2M  | O2'-C2' | 3.30  | 1.51        | 1.42     |
| 47  | LH    | 2809 | A2M  | C5-C4   | -3.30 | 1.32        | 1.39     |
| 1   | S1    | 1592 | PSU  | C4-N3   | 3.30  | 1.45        | 1.38     |
| 47  | LH    | 2769 | A2M  | C5-C4   | -3.29 | 1.32        | 1.39     |
| 44  | LE    | 1126 | PSU  | C4-N3   | 3.29  | 1.44        | 1.38     |
| 47  | LH    | 2361 | PSU  | C4-N3   | 3.29  | 1.44        | 1.38     |
| 2   | S2    | 37   | MIA  | C5-C4   | -3.29 | 1.32        | 1.39     |
| 45  | LF    | 1815 | A2M  | O3'-C3' | -3.27 | 1.35        | 1.43     |
| 47  | LH    | 2358 | A2M  | C5-C4   | -3.25 | 1.32        | 1.39     |
| 1   | S1    | 407  | A2M  | O3'-C3' | -3.24 | 1.35        | 1.43     |
| 1   | S1    | 1554 | PSU  | C4-N3   | 3.24  | 1.44        | 1.38     |
| 44  | LE    | 1118 | PSU  | C4-N3   | 3.23  | 1.44        | 1.38     |
| 1   | S1    | 565  | A2M  | O3'-C3' | -3.23 | 1.35        | 1.43     |
| 47  | LH    | 2349 | A2M  | C5-C4   | -3.23 | 1.33        | 1.39     |
| 44  | LE    | 935  | A2M  | C5-C4   | -3.23 | 1.33        | 1.39     |
| 44  | LE    | 1121 | A2M  | O3'-C3' | -3.23 | 1.35        | 1.43     |
| 48  | LI    | 3562 | PSU  | C4-N3   | 3.23  | 1.44        | 1.38     |
| 1   | S1    | 28   | A2M  | C5-C4   | -3.21 | 1.33        | 1.39     |
| 1   | S1    | 2288 | MA6  | C5-C4   | -3.21 | 1.33        | 1.39     |
| 47  | LH    | 2887 | A2M  | C5-C4   | -3.21 | 1.33        | 1.39     |
| 1   | S1    | 2144 | 5MC  | C2-N1   | 3.21  | 1.47        | 1.40     |
| 48  | LI    | 3315 | A2M  | O3'-C3' | -3.21 | 1.35        | 1.43     |
| 48  | LI    | 3367 | A2M  | C5-C4   | -3.21 | 1.33        | 1.39     |
| 47  | LH    | 2887 | A2M  | O3'-C3' | -3.21 | 1.35        | 1.43     |
| 48  | LI    | 3533 | A2M  | O3'-C3' | -3.20 | 1.35        | 1.43     |
| 42  | LC    | 594  | A2M  | O3'-C3' | -3.20 | 1.35        | 1.43     |
| 1   | S1    | 110  | A2M  | C5-C4   | -3.20 | 1.33        | 1.39     |
| 51  | LL    | 3906 | A2M  | O3'-C3' | -3.19 | 1.35        | 1.43     |
| 47  | LH    | 2814 | A2M  | O3'-C3' | -3.19 | 1.35        | 1.43     |
| 45  | LF    | 1502 | A2M  | C5-C4   | -3.19 | 1.33        | 1.39     |
| 1   | S1    | 2046 | A2M  | C5-C4   | -3.18 | 1.33        | 1.39     |
| 45  | LF    | 1888 | A2M  | O3'-C3' | -3.18 | 1.35        | 1.43     |
| 45  | LF    | 1738 | A2M  | C5-C4   | -3.18 | 1.33        | 1.39     |
| 1   | S1    | 1549 | A2M  | O3'-C3' | -3.17 | 1.35        | 1.43     |
| 45  | LF    | 1502 | A2M  | O3'-C3' | -3.17 | 1.35        | 1.43     |
| 47  | LH    | 2746 | PSU  | O4-C4   | -3.17 | 1.17        | 1.23     |
| 1   | S1    | 28   | A2M  | O3'-C3' | -3.16 | 1.35        | 1.43     |
| 44  | LE    | 1204 | A2M  | O3'-C3' | -3.15 | 1.35        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 723  | A2M  | C5-C4   | -3.15 | 1.33        | 1.39     |
| 44  | LE    | 1118 | PSU  | O4-C4   | -3.15 | 1.17        | 1.23     |
| 48  | LI    | 3521 | A2M  | C5-C4   | -3.15 | 1.33        | 1.39     |
| 47  | LH    | 2349 | A2M  | O3'-C3' | -3.15 | 1.35        | 1.43     |
| 1   | S1    | 1371 | A2M  | C5-C4   | -3.14 | 1.33        | 1.39     |
| 47  | LH    | 2849 | A2M  | O2'-C2' | 3.13  | 1.50        | 1.42     |
| 47  | LH    | 2920 | A2M  | C5-C4   | -3.13 | 1.33        | 1.39     |
| 40  | LA    | 39   | A2M  | O3'-C3' | -3.13 | 1.35        | 1.43     |
| 1   | S1    | 1592 | PSU  | O4-C4   | -3.13 | 1.17        | 1.23     |
| 1   | S1    | 723  | A2M  | O3'-C3' | -3.11 | 1.35        | 1.43     |
| 1   | S1    | 40   | A2M  | C5-C4   | -3.11 | 1.33        | 1.39     |
| 45  | LF    | 1929 | A2M  | O3'-C3' | -3.11 | 1.35        | 1.43     |
| 40  | LA    | 97   | A2M  | C5-C4   | -3.10 | 1.33        | 1.39     |
| 48  | LI    | 3348 | A2M  | C5-C4   | -3.10 | 1.33        | 1.39     |
| 48  | LI    | 3500 | A2M  | C5-C4   | -3.10 | 1.33        | 1.39     |
| 1   | S1    | 649  | A2M  | C5-C4   | -3.10 | 1.33        | 1.39     |
| 47  | LH    | 2708 | A2M  | O3'-C3' | -3.09 | 1.35        | 1.43     |
| 45  | LF    | 1738 | A2M  | O3'-C3' | -3.09 | 1.35        | 1.43     |
| 47  | LH    | 2746 | PSU  | C4-N3   | 3.09  | 1.44        | 1.38     |
| 44  | LE    | 1039 | A2M  | O3'-C3' | -3.08 | 1.35        | 1.43     |
| 1   | S1    | 40   | A2M  | O3'-C3' | -3.08 | 1.35        | 1.43     |
| 1   | S1    | 1063 | A2M  | O3'-C3' | -3.08 | 1.35        | 1.43     |
| 1   | S1    | 1549 | A2M  | C5-C4   | -3.08 | 1.33        | 1.39     |
| 45  | LF    | 1888 | A2M  | C5-C4   | -3.07 | 1.33        | 1.39     |
| 47  | LH    | 2358 | A2M  | O3'-C3' | -3.07 | 1.35        | 1.43     |
| 44  | LE    | 935  | A2M  | O3'-C3' | -3.07 | 1.35        | 1.43     |
| 44  | LE    | 1106 | A2M  | C5-C4   | -3.06 | 1.33        | 1.39     |
| 1   | S1    | 1063 | A2M  | O2'-C2' | 3.06  | 1.50        | 1.42     |
| 41  | LB    | 183  | A2M  | O3'-C3' | -3.06 | 1.35        | 1.43     |
| 47  | LH    | 2812 | A2M  | C5-C4   | -3.06 | 1.33        | 1.39     |
| 42  | LC    | 594  | A2M  | C5-C4   | -3.06 | 1.33        | 1.39     |
| 48  | LI    | 3500 | A2M  | O3'-C3' | -3.06 | 1.35        | 1.43     |
| 47  | LH    | 2849 | A2M  | C5-C4   | -3.06 | 1.33        | 1.39     |
| 44  | LE    | 1204 | A2M  | C5-C4   | -3.05 | 1.33        | 1.39     |
| 40  | LA    | 39   | A2M  | C5-C4   | -3.05 | 1.33        | 1.39     |
| 48  | LI    | 3521 | A2M  | O3'-C3' | -3.04 | 1.35        | 1.43     |
| 45  | LF    | 1815 | A2M  | C5-C4   | -3.04 | 1.33        | 1.39     |
| 44  | LE    | 1106 | A2M  | O3'-C3' | -3.03 | 1.35        | 1.43     |
| 45  | LF    | 1891 | A2M  | O3'-C3' | -3.03 | 1.35        | 1.43     |
| 46  | LG    | 2005 | A2M  | C5-C4   | -3.03 | 1.33        | 1.39     |
| 1   | S1    | 2046 | A2M  | O3'-C3' | -3.02 | 1.35        | 1.43     |
| 45  | LF    | 1929 | A2M  | C5-C4   | -3.02 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 47  | LH    | 2746 | PSU  | O2-C2   | -3.02 | 1.17        | 1.23     |
| 44  | LE    | 1039 | A2M  | C5-C4   | -3.02 | 1.33        | 1.39     |
| 1   | S1    | 533  | A2M  | O3'-C3' | -3.01 | 1.35        | 1.43     |
| 47  | LH    | 2744 | A2M  | C5-N7   | -3.01 | 1.33        | 1.39     |
| 47  | LH    | 2814 | A2M  | C5-C4   | -3.01 | 1.33        | 1.39     |
| 47  | LH    | 2904 | B8H  | C4-N3   | -3.01 | 1.33        | 1.38     |
| 47  | LH    | 2768 | A2M  | O3'-C3' | -3.00 | 1.35        | 1.43     |
| 1   | S1    | 110  | A2M  | O3'-C3' | -3.00 | 1.35        | 1.43     |
| 41  | LB    | 183  | A2M  | C5-C4   | -3.00 | 1.33        | 1.39     |
| 48  | LI    | 3315 | A2M  | C5-C4   | -3.00 | 1.33        | 1.39     |
| 1   | S1    | 1096 | A2M  | O3'-C3' | -3.00 | 1.35        | 1.43     |
| 48  | LI    | 3145 | PSU  | O4'-C1' | -3.00 | 1.39        | 1.43     |
| 1   | S1    | 565  | A2M  | C5-C4   | -2.99 | 1.33        | 1.39     |
| 47  | LH    | 2809 | A2M  | O3'-C3' | -2.99 | 1.35        | 1.43     |
| 47  | LH    | 2708 | A2M  | C5-C4   | -2.99 | 1.33        | 1.39     |
| 1   | S1    | 1900 | A2M  | C5-C4   | -2.99 | 1.33        | 1.39     |
| 47  | LH    | 2812 | A2M  | O3'-C3' | -2.99 | 1.35        | 1.43     |
| 46  | LG    | 2005 | A2M  | O3'-C3' | -2.98 | 1.36        | 1.43     |
| 1   | S1    | 533  | A2M  | C5-C4   | -2.97 | 1.33        | 1.39     |
| 47  | LH    | 2766 | 5MC  | C2-N3   | 2.97  | 1.42        | 1.36     |
| 47  | LH    | 2768 | A2M  | C5-C4   | -2.97 | 1.33        | 1.39     |
| 47  | LH    | 2812 | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 1   | S1    | 645  | A2M  | O3'-C3' | -2.96 | 1.36        | 1.43     |
| 46  | LG    | 2022 | A2M  | C5-C4   | -2.96 | 1.33        | 1.39     |
| 1   | S1    | 533  | A2M  | C5-N7   | -2.95 | 1.33        | 1.39     |
| 47  | LH    | 2849 | A2M  | O3'-C3' | -2.95 | 1.36        | 1.43     |
| 47  | LH    | 2742 | PSU  | O4-C4   | -2.95 | 1.18        | 1.23     |
| 48  | LI    | 3367 | A2M  | O3'-C3' | -2.95 | 1.36        | 1.43     |
| 44  | LE    | 931  | 1MA  | C6-N6   | 2.94  | 1.35        | 1.28     |
| 42  | LC    | 421  | PSU  | O4-C4   | -2.94 | 1.18        | 1.23     |
| 47  | LH    | 2920 | A2M  | O3'-C3' | -2.94 | 1.36        | 1.43     |
| 1   | S1    | 1096 | A2M  | C5-C4   | -2.93 | 1.33        | 1.39     |
| 1   | S1    | 2144 | 5MC  | C6-N1   | -2.92 | 1.33        | 1.38     |
| 45  | LF    | 1856 | OMG  | C6-N1   | 2.92  | 1.44        | 1.38     |
| 1   | S1    | 649  | A2M  | O3'-C3' | -2.92 | 1.36        | 1.43     |
| 1   | S1    | 1900 | A2M  | O3'-C3' | -2.91 | 1.36        | 1.43     |
| 48  | LI    | 3355 | OMC  | C2-N1   | 2.91  | 1.46        | 1.40     |
| 1   | S1    | 38   | OMC  | C2-N1   | 2.90  | 1.46        | 1.40     |
| 46  | LG    | 2022 | A2M  | C5-N7   | -2.90 | 1.33        | 1.39     |
| 48  | LI    | 3348 | A2M  | O3'-C3' | -2.90 | 1.36        | 1.43     |
| 1   | S1    | 1396 | PSU  | O4-C4   | -2.89 | 1.18        | 1.23     |
| 44  | LE    | 1204 | A2M  | C5-N7   | -2.89 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | LG    | 2022 | A2M  | O3'-C3' | -2.89 | 1.36        | 1.43     |
| 47  | LH    | 2769 | A2M  | O3'-C3' | -2.89 | 1.36        | 1.43     |
| 42  | LC    | 594  | A2M  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 1   | S1    | 180  | OMG  | C6-N1   | 2.88  | 1.44        | 1.38     |
| 1   | S1    | 407  | A2M  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 48  | LI    | 3531 | PSU  | O4-C4   | -2.88 | 1.18        | 1.23     |
| 47  | LH    | 2812 | A2M  | C5-N7   | -2.87 | 1.33        | 1.39     |
| 1   | S1    | 403  | PSU  | O4-C4   | -2.87 | 1.18        | 1.23     |
| 44  | LE    | 1121 | A2M  | C5-C4   | -2.87 | 1.33        | 1.39     |
| 47  | LH    | 2920 | A2M  | C5-N7   | -2.86 | 1.33        | 1.39     |
| 48  | LI    | 3521 | A2M  | C5-N7   | -2.86 | 1.33        | 1.39     |
| 1   | S1    | 121  | PSU  | C6-C5   | 2.86  | 1.38        | 1.35     |
| 44  | LE    | 931  | 1MA  | C5-C4   | 2.86  | 1.46        | 1.38     |
| 44  | LE    | 1208 | OMG  | C5-C4   | 2.86  | 1.46        | 1.38     |
| 1   | S1    | 407  | A2M  | C5-C4   | -2.85 | 1.33        | 1.39     |
| 48  | LI    | 3500 | A2M  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 1   | S1    | 32   | PSU  | O4-C4   | -2.85 | 1.18        | 1.23     |
| 47  | LH    | 2814 | A2M  | O2'-C2' | 2.85  | 1.49        | 1.42     |
| 45  | LF    | 1926 | PSU  | O4-C4   | -2.84 | 1.18        | 1.23     |
| 47  | LH    | 2361 | PSU  | O4-C4   | -2.84 | 1.18        | 1.23     |
| 47  | LH    | 2744 | A2M  | O2'-C2' | 2.84  | 1.49        | 1.42     |
| 48  | LI    | 3456 | 5MC  | C6-N1   | -2.84 | 1.33        | 1.38     |
| 1   | S1    | 1063 | A2M  | C5-C4   | -2.83 | 1.33        | 1.39     |
| 1   | S1    | 121  | PSU  | C4-N3   | -2.82 | 1.33        | 1.38     |
| 45  | LF    | 1738 | A2M  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 1   | S1    | 565  | A2M  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 44  | LE    | 1260 | PSU  | O4-C4   | -2.82 | 1.18        | 1.23     |
| 2   | S2    | 37   | MIA  | C5-N7   | -2.81 | 1.33        | 1.39     |
| 44  | LE    | 1126 | PSU  | O4-C4   | -2.81 | 1.18        | 1.23     |
| 1   | S1    | 1371 | A2M  | C5-N7   | -2.81 | 1.33        | 1.39     |
| 1   | S1    | 723  | A2M  | O2'-C2' | 2.81  | 1.49        | 1.42     |
| 47  | LH    | 2920 | A2M  | O2'-C2' | 2.80  | 1.49        | 1.42     |
| 1   | S1    | 1096 | A2M  | O2'-C2' | 2.80  | 1.49        | 1.42     |
| 45  | LF    | 1888 | A2M  | C5-N7   | -2.80 | 1.33        | 1.39     |
| 47  | LH    | 2925 | OMG  | C6-N1   | 2.80  | 1.44        | 1.38     |
| 45  | LF    | 1815 | A2M  | O2'-C2' | 2.80  | 1.49        | 1.42     |
| 47  | LH    | 2766 | 5MC  | C6-N1   | -2.79 | 1.33        | 1.38     |
| 1   | S1    | 2101 | PSU  | O4-C4   | -2.79 | 1.18        | 1.23     |
| 48  | LI    | 3533 | A2M  | C5-N7   | -2.79 | 1.33        | 1.39     |
| 1   | S1    | 1591 | PSU  | O4-C4   | -2.79 | 1.18        | 1.23     |
| 44  | LE    | 1121 | A2M  | C5-N7   | -2.79 | 1.33        | 1.39     |
| 51  | LL    | 3906 | A2M  | C5-C4   | -2.79 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 645  | A2M  | C5-C4   | -2.79 | 1.33        | 1.39     |
| 42  | LC    | 498  | PSU  | O4-C4   | -2.79 | 1.18        | 1.23     |
| 45  | LF    | 1815 | A2M  | C5-N7   | -2.79 | 1.33        | 1.39     |
| 44  | LE    | 1204 | A2M  | O2'-C2' | 2.79  | 1.49        | 1.42     |
| 1   | S1    | 1554 | PSU  | O4-C4   | -2.78 | 1.18        | 1.23     |
| 47  | LH    | 2591 | PSU  | O4-C4   | -2.78 | 1.18        | 1.23     |
| 48  | LI    | 3367 | A2M  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 1   | S1    | 2131 | PSU  | O4-C4   | -2.78 | 1.18        | 1.23     |
| 1   | S1    | 649  | A2M  | O2'-C2' | 2.77  | 1.49        | 1.42     |
| 48  | LI    | 3206 | PSU  | O4-C4   | -2.77 | 1.18        | 1.23     |
| 44  | LE    | 1324 | OMG  | C6-N1   | 2.77  | 1.44        | 1.38     |
| 1   | S1    | 89   | PSU  | O4-C4   | -2.77 | 1.18        | 1.23     |
| 47  | LH    | 2769 | A2M  | C5-N7   | -2.77 | 1.33        | 1.39     |
| 45  | LF    | 1876 | PSU  | O4-C4   | -2.77 | 1.18        | 1.23     |
| 44  | LE    | 1106 | A2M  | C5-N7   | -2.77 | 1.33        | 1.39     |
| 44  | LE    | 1260 | PSU  | O4'-C1' | -2.76 | 1.40        | 1.43     |
| 1   | S1    | 641  | OMG  | C6-N1   | 2.76  | 1.44        | 1.38     |
| 1   | S1    | 110  | A2M  | O2'-C2' | 2.76  | 1.49        | 1.42     |
| 1   | S1    | 390  | OMG  | C6-N1   | 2.76  | 1.44        | 1.38     |
| 44  | LE    | 1222 | OMU  | C2-N1   | 2.76  | 1.42        | 1.38     |
| 40  | LA    | 97   | A2M  | O2'-C2' | 2.76  | 1.49        | 1.42     |
| 40  | LA    | 39   | A2M  | C5-N7   | -2.75 | 1.33        | 1.39     |
| 1   | S1    | 649  | A2M  | C5-N7   | -2.75 | 1.33        | 1.39     |
| 1   | S1    | 2075 | OMG  | C6-N1   | 2.75  | 1.43        | 1.38     |
| 42  | LC    | 594  | A2M  | O2'-C2' | 2.75  | 1.49        | 1.42     |
| 1   | S1    | 1549 | A2M  | C5-N7   | -2.75 | 1.33        | 1.39     |
| 1   | S1    | 2116 | PSU  | O4-C4   | -2.75 | 1.18        | 1.23     |
| 42  | LC    | 480  | PSU  | O4-C4   | -2.75 | 1.18        | 1.23     |
| 1   | S1    | 2129 | PSU  | O4-C4   | -2.75 | 1.18        | 1.23     |
| 45  | LF    | 1738 | A2M  | O2'-C2' | 2.75  | 1.49        | 1.42     |
| 47  | LH    | 2623 | PSU  | O4-C4   | -2.75 | 1.18        | 1.23     |
| 48  | LI    | 3185 | PSU  | O4-C4   | -2.75 | 1.18        | 1.23     |
| 45  | LF    | 1929 | A2M  | C5-N7   | -2.75 | 1.33        | 1.39     |
| 47  | LH    | 2887 | A2M  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 44  | LE    | 935  | A2M  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 48  | LI    | 3533 | A2M  | O2'-C2' | 2.74  | 1.49        | 1.42     |
| 2   | S2    | 37   | MIA  | C8-N9   | -2.74 | 1.32        | 1.37     |
| 48  | LI    | 3562 | PSU  | O4-C4   | -2.74 | 1.18        | 1.23     |
| 1   | S1    | 1900 | A2M  | O2'-C2' | 2.74  | 1.49        | 1.42     |
| 47  | LH    | 2849 | A2M  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 47  | LH    | 2914 | PSU  | O4-C4   | -2.74 | 1.18        | 1.23     |
| 44  | LE    | 1222 | OMU  | C4-N3   | -2.74 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 44  | LE    | 1235 | PSU  | O4-C4   | -2.74 | 1.18        | 1.23     |
| 1   | S1    | 28   | A2M  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 45  | LF    | 1891 | A2M  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 47  | LH    | 2642 | PSU  | O4-C4   | -2.73 | 1.18        | 1.23     |
| 51  | LL    | 3906 | A2M  | O2'-C2' | 2.73  | 1.49        | 1.42     |
| 47  | LH    | 2883 | OMG  | C6-N1   | 2.73  | 1.43        | 1.38     |
| 48  | LI    | 3412 | PSU  | O4-C4   | -2.73 | 1.18        | 1.23     |
| 1   | S1    | 42   | OMG  | C6-N1   | 2.73  | 1.43        | 1.38     |
| 44  | LE    | 1171 | PSU  | O4-C4   | -2.73 | 1.18        | 1.23     |
| 47  | LH    | 2621 | PSU  | O4-C4   | -2.73 | 1.18        | 1.23     |
| 46  | LG    | 2119 | PSU  | O4-C4   | -2.73 | 1.18        | 1.23     |
| 1   | S1    | 105  | PSU  | O4-C4   | -2.73 | 1.18        | 1.23     |
| 1   | S1    | 723  | A2M  | C5-N7   | -2.73 | 1.33        | 1.39     |
| 47  | LH    | 2837 | PSU  | O4-C4   | -2.73 | 1.18        | 1.23     |
| 47  | LH    | 2915 | PSU  | O4-C4   | -2.72 | 1.18        | 1.23     |
| 47  | LH    | 2708 | A2M  | O2'-C2' | 2.72  | 1.49        | 1.42     |
| 1   | S1    | 1624 | PSU  | O4-C4   | -2.72 | 1.18        | 1.23     |
| 41  | LB    | 183  | A2M  | C5-N7   | -2.72 | 1.33        | 1.39     |
| 44  | LE    | 1039 | A2M  | C5-N7   | -2.72 | 1.33        | 1.39     |
| 48  | LI    | 3521 | A2M  | O2'-C2' | 2.71  | 1.49        | 1.42     |
| 48  | LI    | 3315 | A2M  | C5-N7   | -2.71 | 1.33        | 1.39     |
| 1   | S1    | 40   | A2M  | O2'-C2' | 2.71  | 1.49        | 1.42     |
| 47  | LH    | 2330 | PSU  | O4-C4   | -2.71 | 1.18        | 1.23     |
| 47  | LH    | 2624 | PSU  | O4-C4   | -2.71 | 1.18        | 1.23     |
| 41  | LB    | 234  | PSU  | O4-C4   | -2.71 | 1.18        | 1.23     |
| 47  | LH    | 2809 | A2M  | C5-N7   | -2.70 | 1.33        | 1.39     |
| 47  | LH    | 2814 | A2M  | C5-N7   | -2.70 | 1.33        | 1.39     |
| 47  | LH    | 2349 | A2M  | C5-N7   | -2.70 | 1.33        | 1.39     |
| 47  | LH    | 2809 | A2M  | O2'-C2' | 2.70  | 1.49        | 1.42     |
| 47  | LH    | 2768 | A2M  | C5-N7   | -2.70 | 1.33        | 1.39     |
| 1   | S1    | 1068 | PSU  | O4-C4   | -2.70 | 1.18        | 1.23     |
| 40  | LA    | 74   | OMG  | C6-N1   | 2.70  | 1.43        | 1.38     |
| 40  | LA    | 16   | PSU  | O4-C4   | -2.70 | 1.18        | 1.23     |
| 48  | LI    | 3348 | A2M  | C5-N7   | -2.70 | 1.33        | 1.39     |
| 44  | LE    | 1039 | A2M  | O2'-C2' | 2.70  | 1.49        | 1.42     |
| 48  | LI    | 3503 | PSU  | O4-C4   | -2.70 | 1.18        | 1.23     |
| 48  | LI    | 3518 | 5MC  | C2-N3   | 2.70  | 1.41        | 1.36     |
| 48  | LI    | 3167 | PSU  | O4-C4   | -2.70 | 1.18        | 1.23     |
| 48  | LI    | 3509 | OMG  | C6-N1   | 2.70  | 1.43        | 1.38     |
| 47  | LH    | 2768 | A2M  | O2'-C2' | 2.69  | 1.49        | 1.42     |
| 1   | S1    | 645  | A2M  | C5-N7   | -2.69 | 1.33        | 1.39     |
| 44  | LE    | 1184 | PSU  | O4-C4   | -2.69 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 40   | A2M  | C5-N7   | -2.69 | 1.33        | 1.39     |
| 44  | LE    | 935  | A2M  | O2'-C2' | 2.69  | 1.49        | 1.42     |
| 47  | LH    | 2754 | PSU  | O4-C4   | -2.69 | 1.18        | 1.23     |
| 48  | LI    | 3204 | PSU  | O4-C4   | -2.69 | 1.18        | 1.23     |
| 1   | S1    | 2287 | MA6  | C5-N7   | -2.69 | 1.33        | 1.39     |
| 42  | LC    | 628  | OMG  | C6-N1   | 2.69  | 1.43        | 1.38     |
| 1   | S1    | 645  | A2M  | O2'-C2' | 2.69  | 1.49        | 1.42     |
| 48  | LI    | 3315 | A2M  | O2'-C2' | 2.69  | 1.49        | 1.42     |
| 48  | LI    | 3440 | PSU  | O4-C4   | -2.69 | 1.18        | 1.23     |
| 1   | S1    | 1711 | PSU  | O4-C4   | -2.69 | 1.18        | 1.23     |
| 47  | LH    | 2769 | A2M  | O2'-C2' | 2.69  | 1.49        | 1.42     |
| 42  | LC    | 537  | OMC  | C2-N1   | 2.68  | 1.45        | 1.40     |
| 45  | LF    | 1888 | A2M  | O2'-C2' | 2.68  | 1.49        | 1.42     |
| 48  | LI    | 3348 | A2M  | O2'-C2' | 2.68  | 1.49        | 1.42     |
| 1   | S1    | 110  | A2M  | C5-N7   | -2.68 | 1.34        | 1.39     |
| 48  | LI    | 3223 | OMG  | C6-N1   | 2.68  | 1.43        | 1.38     |
| 1   | S1    | 407  | A2M  | O2'-C2' | 2.68  | 1.49        | 1.42     |
| 44  | LE    | 1075 | PSU  | O4-C4   | -2.68 | 1.18        | 1.23     |
| 47  | LH    | 2874 | PSU  | O4-C4   | -2.68 | 1.18        | 1.23     |
| 1   | S1    | 1597 | UR3  | C3U-N3  | -2.68 | 1.42        | 1.47     |
| 48  | LI    | 3444 | PSU  | O4-C4   | -2.68 | 1.18        | 1.23     |
| 48  | LI    | 3518 | 5MC  | C6-N1   | -2.68 | 1.33        | 1.38     |
| 1   | S1    | 544  | PSU  | O4-C4   | -2.68 | 1.18        | 1.23     |
| 46  | LG    | 2171 | PSU  | O4-C4   | -2.68 | 1.18        | 1.23     |
| 46  | LG    | 2022 | A2M  | O2'-C2' | 2.68  | 1.49        | 1.42     |
| 52  | LM    | 3963 | PSU  | O4-C4   | -2.68 | 1.18        | 1.23     |
| 49  | LJ    | 3688 | OMG  | C6-N1   | 2.67  | 1.43        | 1.38     |
| 1   | S1    | 1681 | OMG  | C6-N1   | 2.67  | 1.43        | 1.38     |
| 45  | LF    | 1826 | OMG  | C6-N1   | 2.67  | 1.43        | 1.38     |
| 1   | S1    | 1660 | PSU  | O4-C4   | -2.67 | 1.18        | 1.23     |
| 49  | LJ    | 3697 | PSU  | O4-C4   | -2.67 | 1.18        | 1.23     |
| 48  | LI    | 3451 | PSU  | O4-C4   | -2.67 | 1.18        | 1.23     |
| 48  | LI    | 3367 | A2M  | O2'-C2' | 2.67  | 1.49        | 1.42     |
| 1   | S1    | 2065 | PSU  | O4-C4   | -2.67 | 1.18        | 1.23     |
| 48  | LI    | 3568 | PSU  | O4-C4   | -2.67 | 1.18        | 1.23     |
| 44  | LE    | 1121 | A2M  | O2'-C2' | 2.66  | 1.49        | 1.42     |
| 42  | LC    | 631  | OMG  | C6-N1   | 2.66  | 1.43        | 1.38     |
| 46  | LG    | 2009 | OMG  | C6-N1   | 2.66  | 1.43        | 1.38     |
| 1   | S1    | 1096 | A2M  | C5-N7   | -2.66 | 1.34        | 1.39     |
| 1   | S1    | 1063 | A2M  | C5-N7   | -2.66 | 1.34        | 1.39     |
| 41  | LB    | 215  | OMG  | C6-N1   | 2.66  | 1.43        | 1.38     |
| 45  | LF    | 1662 | OMG  | C6-N1   | 2.66  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 45  | LF    | 1502 | A2M  | O2'-C2' | 2.66  | 1.49        | 1.42     |
| 1   | S1    | 533  | A2M  | O2'-C2' | 2.65  | 1.49        | 1.42     |
| 1   | S1    | 2046 | A2M  | O2'-C2' | 2.65  | 1.49        | 1.42     |
| 47  | LH    | 2897 | OMG  | C6-N1   | 2.65  | 1.43        | 1.38     |
| 45  | LF    | 1692 | PSU  | O4-C4   | -2.65 | 1.18        | 1.23     |
| 45  | LF    | 1502 | A2M  | C5-N7   | -2.65 | 1.34        | 1.39     |
| 40  | LA    | 97   | A2M  | C5-N7   | -2.65 | 1.34        | 1.39     |
| 52  | LM    | 3953 | PSU  | O4-C4   | -2.65 | 1.18        | 1.23     |
| 48  | LI    | 3332 | PSU  | O4-C4   | -2.65 | 1.18        | 1.23     |
| 49  | LJ    | 3680 | PSU  | O4-C4   | -2.65 | 1.18        | 1.23     |
| 1   | S1    | 1378 | PSU  | O4-C4   | -2.64 | 1.18        | 1.23     |
| 47  | LH    | 2879 | OMG  | C6-N1   | 2.64  | 1.43        | 1.38     |
| 45  | LF    | 1859 | PSU  | O4-C4   | -2.64 | 1.18        | 1.23     |
| 44  | LE    | 1201 | OMG  | C6-N1   | 2.64  | 1.43        | 1.38     |
| 48  | LI    | 3214 | 6MZ  | C5-N7   | -2.64 | 1.34        | 1.39     |
| 45  | LF    | 1883 | OMG  | C6-N1   | 2.64  | 1.43        | 1.38     |
| 48  | LI    | 3446 | PSU  | O4-C4   | -2.64 | 1.18        | 1.23     |
| 48  | LI    | 3187 | OMG  | C6-N1   | 2.64  | 1.43        | 1.38     |
| 1   | S1    | 1371 | A2M  | O2'-C2' | 2.64  | 1.49        | 1.42     |
| 49  | LJ    | 3591 | PSU  | O4-C4   | -2.63 | 1.18        | 1.23     |
| 51  | LL    | 3906 | A2M  | C5-N7   | -2.63 | 1.34        | 1.39     |
| 47  | LH    | 2708 | A2M  | C5-N7   | -2.63 | 1.34        | 1.39     |
| 1   | S1    | 1900 | A2M  | C5-N7   | -2.63 | 1.34        | 1.39     |
| 1   | S1    | 1393 | PSU  | O4-C4   | -2.63 | 1.18        | 1.23     |
| 47  | LH    | 2752 | PSU  | O4-C4   | -2.63 | 1.18        | 1.23     |
| 44  | LE    | 1363 | PSU  | O4-C4   | -2.63 | 1.18        | 1.23     |
| 47  | LH    | 2349 | A2M  | O2'-C2' | 2.63  | 1.49        | 1.42     |
| 47  | LH    | 2358 | A2M  | C5-N7   | -2.63 | 1.34        | 1.39     |
| 45  | LF    | 1568 | PSU  | O4-C4   | -2.63 | 1.18        | 1.23     |
| 48  | LI    | 3510 | PSU  | O4-C4   | -2.62 | 1.18        | 1.23     |
| 45  | LF    | 1891 | A2M  | O2'-C2' | 2.62  | 1.49        | 1.42     |
| 47  | LH    | 2899 | PSU  | O4-C4   | -2.62 | 1.18        | 1.23     |
| 49  | LJ    | 3701 | PSU  | O4-C4   | -2.62 | 1.18        | 1.23     |
| 47  | LH    | 2617 | PSU  | O4-C4   | -2.61 | 1.18        | 1.23     |
| 1   | S1    | 2144 | 5MC  | C2-N3   | 2.61  | 1.41        | 1.36     |
| 44  | LE    | 1198 | PSU  | O4-C4   | -2.61 | 1.18        | 1.23     |
| 47  | LH    | 2842 | PSU  | O4-C4   | -2.61 | 1.18        | 1.23     |
| 1   | S1    | 2081 | PSU  | O4-C4   | -2.61 | 1.18        | 1.23     |
| 1   | S1    | 1705 | OMG  | C6-N1   | 2.61  | 1.43        | 1.38     |
| 40  | LA    | 68   | PSU  | O4-C4   | -2.61 | 1.18        | 1.23     |
| 40  | LA    | 41   | OMG  | C6-N1   | 2.61  | 1.43        | 1.38     |
| 47  | LH    | 2870 | OMG  | C6-N1   | 2.61  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 47  | LH    | 2887 | A2M  | O2'-C2' | 2.61  | 1.49        | 1.42     |
| 48  | LI    | 3434 | OMG  | C6-N1   | 2.61  | 1.43        | 1.38     |
| 45  | LF    | 1586 | PSU  | O4-C4   | -2.61 | 1.18        | 1.23     |
| 48  | LI    | 3500 | A2M  | O2'-C2' | 2.61  | 1.49        | 1.42     |
| 45  | LF    | 1929 | A2M  | O2'-C2' | 2.61  | 1.49        | 1.42     |
| 42  | LC    | 308  | PSU  | O4-C4   | -2.60 | 1.18        | 1.23     |
| 45  | LF    | 1582 | PSU  | O4-C4   | -2.60 | 1.18        | 1.23     |
| 42  | LC    | 567  | PSU  | O4-C4   | -2.60 | 1.18        | 1.23     |
| 48  | LI    | 3175 | PSU  | O4-C4   | -2.60 | 1.18        | 1.23     |
| 1   | S1    | 1960 | PSU  | O4-C4   | -2.60 | 1.18        | 1.23     |
| 1   | S1    | 2046 | A2M  | C5-N7   | -2.60 | 1.34        | 1.39     |
| 47  | LH    | 2679 | PSU  | O4-C4   | -2.60 | 1.18        | 1.23     |
| 48  | LI    | 3347 | OMC  | C2-N1   | 2.59  | 1.45        | 1.40     |
| 1   | S1    | 1536 | OMG  | C6-N1   | 2.59  | 1.43        | 1.38     |
| 1   | S1    | 1901 | OMG  | C6-N1   | 2.59  | 1.43        | 1.38     |
| 44  | LE    | 1217 | OMG  | C6-N1   | 2.59  | 1.43        | 1.38     |
| 45  | LF    | 1819 | OMG  | C6-N1   | 2.59  | 1.43        | 1.38     |
| 46  | LG    | 2154 | PSU  | O4-C4   | -2.59 | 1.18        | 1.23     |
| 46  | LG    | 2005 | A2M  | C5-N7   | -2.59 | 1.34        | 1.39     |
| 44  | LE    | 1266 | PSU  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 48  | LI    | 3191 | OMG  | C6-N1   | 2.58  | 1.43        | 1.38     |
| 1   | S1    | 2180 | A2M  | C5-C6   | 2.58  | 1.48        | 1.41     |
| 47  | LH    | 2802 | PSU  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 41  | LB    | 183  | A2M  | O2'-C2' | 2.58  | 1.49        | 1.42     |
| 46  | LG    | 2146 | OMG  | C6-N1   | 2.58  | 1.43        | 1.38     |
| 49  | LJ    | 3644 | PSU  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 1   | S1    | 27   | PSU  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 40  | LA    | 39   | A2M  | O2'-C2' | 2.58  | 1.49        | 1.42     |
| 1   | S1    | 485  | OMG  | C6-N1   | 2.58  | 1.43        | 1.38     |
| 44  | LE    | 1365 | PSU  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 47  | LH    | 2904 | B8H  | C2-N3   | -2.58 | 1.33        | 1.38     |
| 47  | LH    | 2744 | A2M  | C8-N9   | -2.58 | 1.32        | 1.37     |
| 44  | LE    | 1407 | PSU  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 46  | LG    | 2005 | A2M  | O2'-C2' | 2.58  | 1.49        | 1.42     |
| 44  | LE    | 1208 | OMG  | C6-N1   | -2.58 | 1.34        | 1.38     |
| 1   | S1    | 2305 | PSU  | O4-C4   | -2.57 | 1.18        | 1.23     |
| 47  | LH    | 2586 | PSU  | O4-C4   | -2.57 | 1.18        | 1.23     |
| 1   | S1    | 1715 | PSU  | O4-C4   | -2.57 | 1.18        | 1.23     |
| 48  | LI    | 3504 | OMG  | C6-N1   | 2.57  | 1.43        | 1.38     |
| 42  | LC    | 302  | PSU  | O4-C4   | -2.57 | 1.18        | 1.23     |
| 52  | LM    | 3957 | OMC  | C2-N1   | 2.57  | 1.45        | 1.40     |
| 48  | LI    | 3456 | 5MC  | O2-C2   | -2.57 | 1.19        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 48  | LI    | 3145 | PSU  | O4-C4   | -2.56 | 1.18        | 1.23     |
| 47  | LH    | 2776 | OMG  | C6-N1   | 2.56  | 1.43        | 1.38     |
| 46  | LG    | 2022 | A2M  | C8-N9   | -2.56 | 1.32        | 1.37     |
| 44  | LE    | 1204 | A2M  | C8-N9   | -2.56 | 1.32        | 1.37     |
| 1   | S1    | 640  | PSU  | O4-C4   | -2.56 | 1.18        | 1.23     |
| 1   | S1    | 2288 | MA6  | C5-N7   | -2.56 | 1.34        | 1.39     |
| 47  | LH    | 2610 | OMG  | C6-N1   | 2.56  | 1.43        | 1.38     |
| 1   | S1    | 565  | A2M  | O2'-C2' | 2.55  | 1.49        | 1.42     |
| 44  | LE    | 1118 | PSU  | O2-C2   | -2.55 | 1.18        | 1.23     |
| 1   | S1    | 280  | PSU  | O4-C4   | -2.55 | 1.18        | 1.23     |
| 1   | S1    | 28   | A2M  | O2'-C2' | 2.55  | 1.49        | 1.42     |
| 1   | S1    | 176  | PSU  | O4-C4   | -2.55 | 1.18        | 1.23     |
| 48  | LI    | 3379 | OMG  | C6-N1   | 2.55  | 1.43        | 1.38     |
| 45  | LF    | 1835 | OMG  | C6-N1   | 2.55  | 1.43        | 1.38     |
| 48  | LI    | 3377 | OMG  | C6-N1   | 2.55  | 1.43        | 1.38     |
| 1   | S1    | 2287 | MA6  | C8-N9   | -2.55 | 1.32        | 1.37     |
| 45  | LF    | 1667 | OMG  | C6-N1   | 2.54  | 1.43        | 1.38     |
| 1   | S1    | 2144 | 5MC  | O2-C2   | -2.54 | 1.19        | 1.23     |
| 53  | LN    | 3969 | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 42  | LC    | 541  | OMG  | C6-N1   | 2.53  | 1.43        | 1.38     |
| 44  | LE    | 1023 | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 41  | LB    | 281  | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 41  | LB    | 280  | PSU  | O4-C4   | -2.52 | 1.18        | 1.23     |
| 42  | LC    | 577  | OMC  | C2-N1   | 2.52  | 1.45        | 1.40     |
| 48  | LI    | 3542 | PSU  | O4-C4   | -2.52 | 1.18        | 1.23     |
| 45  | LF    | 1956 | OMG  | C6-N1   | 2.51  | 1.43        | 1.38     |
| 48  | LI    | 3521 | A2M  | C8-N9   | -2.51 | 1.33        | 1.37     |
| 1   | S1    | 1037 | OMC  | C2-N1   | 2.51  | 1.45        | 1.40     |
| 44  | LE    | 1106 | A2M  | O2'-C2' | 2.51  | 1.49        | 1.42     |
| 48  | LI    | 3412 | PSU  | O4'-C1' | -2.51 | 1.40        | 1.43     |
| 1   | S1    | 723  | A2M  | C8-N9   | -2.50 | 1.33        | 1.37     |
| 49  | LJ    | 3644 | PSU  | O2-C2   | -2.50 | 1.18        | 1.23     |
| 1   | S1    | 1371 | A2M  | C8-N9   | -2.49 | 1.33        | 1.37     |
| 48  | LI    | 3456 | 5MC  | C2-N3   | 2.49  | 1.41        | 1.36     |
| 44  | LE    | 931  | 1MA  | C5-N7   | -2.49 | 1.34        | 1.39     |
| 44  | LE    | 1104 | OMG  | C6-N1   | 2.49  | 1.43        | 1.38     |
| 1   | S1    | 2046 | A2M  | C8-N9   | -2.49 | 1.33        | 1.37     |
| 40  | LA    | 68   | PSU  | O2-C2   | -2.49 | 1.18        | 1.23     |
| 1   | S1    | 465  | PSU  | O4-C4   | -2.49 | 1.18        | 1.23     |
| 1   | S1    | 2288 | MA6  | C8-N9   | -2.48 | 1.33        | 1.37     |
| 48  | LI    | 3222 | OMC  | C2-N1   | 2.48  | 1.45        | 1.40     |
| 1   | S1    | 1592 | PSU  | O2-C2   | -2.48 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 1549 | A2M  | O2'-C2' | 2.48  | 1.49        | 1.42     |
| 1   | S1    | 1601 | B8N  | C6-C5   | 2.47  | 1.38        | 1.34     |
| 47  | LH    | 2623 | PSU  | O2-C2   | -2.47 | 1.18        | 1.23     |
| 45  | LF    | 1683 | OMG  | C6-N1   | 2.47  | 1.43        | 1.38     |
| 1   | S1    | 1549 | A2M  | O5'-C5' | -2.47 | 1.38        | 1.44     |
| 49  | LJ    | 3701 | PSU  | O2-C2   | -2.46 | 1.18        | 1.23     |
| 42  | LC    | 483  | OMC  | C2-N1   | 2.46  | 1.45        | 1.40     |
| 47  | LH    | 2812 | A2M  | C8-N9   | -2.46 | 1.33        | 1.37     |
| 48  | LI    | 2999 | PSU  | O4-C4   | -2.46 | 1.18        | 1.23     |
| 1   | S1    | 57   | OMG  | C6-N1   | 2.46  | 1.43        | 1.38     |
| 46  | LG    | 2119 | PSU  | O2-C2   | -2.45 | 1.18        | 1.23     |
| 51  | LL    | 3865 | PSU  | O4-C4   | -2.45 | 1.18        | 1.23     |
| 1   | S1    | 110  | A2M  | C8-N9   | -2.44 | 1.33        | 1.37     |
| 1   | S1    | 1711 | PSU  | O2-C2   | -2.44 | 1.18        | 1.23     |
| 47  | LH    | 2361 | PSU  | O2-C2   | -2.44 | 1.18        | 1.23     |
| 45  | LF    | 1815 | A2M  | C8-N9   | -2.43 | 1.33        | 1.37     |
| 44  | LE    | 1365 | PSU  | O2-C2   | -2.42 | 1.18        | 1.23     |
| 1   | S1    | 649  | A2M  | C8-N9   | -2.42 | 1.33        | 1.37     |
| 48  | LI    | 3042 | PSU  | O4-C4   | -2.42 | 1.19        | 1.23     |
| 48  | LI    | 3204 | PSU  | O2-C2   | -2.42 | 1.18        | 1.23     |
| 42  | LC    | 421  | PSU  | O2-C2   | -2.42 | 1.18        | 1.23     |
| 48  | LI    | 3444 | PSU  | O2-C2   | -2.42 | 1.18        | 1.23     |
| 46  | LG    | 2125 | PSU  | O4-C4   | -2.42 | 1.19        | 1.23     |
| 45  | LF    | 1582 | PSU  | O2-C2   | -2.42 | 1.18        | 1.23     |
| 44  | LE    | 1208 | OMG  | C5-N7   | -2.41 | 1.34        | 1.39     |
| 47  | LH    | 2679 | PSU  | O2-C2   | -2.41 | 1.18        | 1.23     |
| 49  | LJ    | 3680 | PSU  | O2-C2   | -2.41 | 1.18        | 1.23     |
| 47  | LH    | 2349 | A2M  | C8-N9   | -2.41 | 1.33        | 1.37     |
| 46  | LG    | 2125 | PSU  | O2-C2   | -2.40 | 1.18        | 1.23     |
| 44  | LE    | 1266 | PSU  | O2-C2   | -2.40 | 1.18        | 1.23     |
| 47  | LH    | 2899 | PSU  | O2-C2   | -2.40 | 1.18        | 1.23     |
| 1   | S1    | 1371 | A2M  | O5'-C5' | -2.40 | 1.38        | 1.44     |
| 49  | LJ    | 3591 | PSU  | O2-C2   | -2.40 | 1.18        | 1.23     |
| 47  | LH    | 2904 | B8H  | C6-C5   | 2.39  | 1.38        | 1.34     |
| 45  | LF    | 1888 | A2M  | C8-N9   | -2.39 | 1.33        | 1.37     |
| 44  | LE    | 1126 | PSU  | O2-C2   | -2.39 | 1.18        | 1.23     |
| 47  | LH    | 2624 | PSU  | O4'-C1' | -2.39 | 1.40        | 1.43     |
| 48  | LI    | 3332 | PSU  | O2-C2   | -2.39 | 1.18        | 1.23     |
| 47  | LH    | 2358 | A2M  | C8-N9   | -2.38 | 1.33        | 1.37     |
| 47  | LH    | 2769 | A2M  | C8-N9   | -2.38 | 1.33        | 1.37     |
| 47  | LH    | 2617 | PSU  | O2-C2   | -2.38 | 1.18        | 1.23     |
| 46  | LG    | 2171 | PSU  | O4'-C1' | -2.38 | 1.40        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 44  | LE    | 1075 | PSU  | O4'-C1' | -2.38 | 1.40        | 1.43     |
| 47  | LH    | 2920 | A2M  | C8-N9   | -2.38 | 1.33        | 1.37     |
| 1   | S1    | 1378 | PSU  | O2-C2   | -2.38 | 1.18        | 1.23     |
| 41  | LB    | 234  | PSU  | O2-C2   | -2.38 | 1.18        | 1.23     |
| 42  | LC    | 480  | PSU  | O2-C2   | -2.38 | 1.18        | 1.23     |
| 1   | S1    | 565  | A2M  | C8-N9   | -2.38 | 1.33        | 1.37     |
| 1   | S1    | 544  | PSU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 47  | LH    | 2914 | PSU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 1   | S1    | 1591 | PSU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 44  | LE    | 1075 | PSU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 47  | LH    | 2754 | PSU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 48  | LI    | 3562 | PSU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 48  | LI    | 3533 | A2M  | C8-N9   | -2.37 | 1.33        | 1.37     |
| 1   | S1    | 465  | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 45  | LF    | 1891 | A2M  | C8-N9   | -2.36 | 1.33        | 1.37     |
| 44  | LE    | 1260 | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 48  | LI    | 3503 | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 47  | LH    | 2887 | A2M  | C8-N9   | -2.36 | 1.33        | 1.37     |
| 1   | S1    | 2305 | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 48  | LI    | 3206 | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 1   | S1    | 1660 | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 45  | LF    | 1876 | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 42  | LC    | 594  | A2M  | C8-N9   | -2.36 | 1.33        | 1.37     |
| 47  | LH    | 2349 | A2M  | O5'-C5' | -2.35 | 1.39        | 1.44     |
| 1   | S1    | 27   | PSU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 44  | LE    | 1235 | PSU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 1   | S1    | 533  | A2M  | C8-N9   | -2.35 | 1.33        | 1.37     |
| 1   | S1    | 2180 | A2M  | C5-N7   | -2.35 | 1.34        | 1.39     |
| 45  | LF    | 1692 | PSU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 44  | LE    | 1184 | PSU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 47  | LH    | 2752 | PSU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 44  | LE    | 1198 | PSU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 47  | LH    | 2814 | A2M  | O5'-C5' | -2.35 | 1.39        | 1.44     |
| 47  | LH    | 2915 | PSU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 42  | LC    | 567  | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 45  | LF    | 1502 | A2M  | C8-N9   | -2.34 | 1.33        | 1.37     |
| 47  | LH    | 2874 | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 48  | LI    | 3451 | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 1   | S1    | 2131 | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 48  | LI    | 3412 | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 1   | S1    | 407  | A2M  | O5'-C5' | -2.34 | 1.39        | 1.44     |
| 44  | LE    | 1023 | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 89   | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 1   | S1    | 2101 | PSU  | O2-C2   | -2.33 | 1.18        | 1.23     |
| 44  | LE    | 1407 | PSU  | O2-C2   | -2.33 | 1.18        | 1.23     |
| 48  | LI    | 3531 | PSU  | O2-C2   | -2.33 | 1.18        | 1.23     |
| 41  | LB    | 183  | A2M  | C8-N9   | -2.33 | 1.33        | 1.37     |
| 45  | LF    | 1738 | A2M  | C8-N9   | -2.33 | 1.33        | 1.37     |
| 1   | S1    | 1393 | PSU  | O2-C2   | -2.33 | 1.18        | 1.23     |
| 47  | LH    | 2837 | PSU  | O2-C2   | -2.33 | 1.18        | 1.23     |
| 47  | LH    | 2708 | A2M  | C8-N9   | -2.32 | 1.33        | 1.37     |
| 44  | LE    | 1363 | PSU  | O2-C2   | -2.32 | 1.18        | 1.23     |
| 1   | S1    | 2129 | PSU  | O2-C2   | -2.32 | 1.18        | 1.23     |
| 45  | LF    | 1859 | PSU  | O2-C2   | -2.32 | 1.18        | 1.23     |
| 47  | LH    | 2642 | PSU  | O2-C2   | -2.32 | 1.18        | 1.23     |
| 1   | S1    | 28   | A2M  | C8-N9   | -2.32 | 1.33        | 1.37     |
| 42  | LC    | 498  | PSU  | O2-C2   | -2.32 | 1.18        | 1.23     |
| 44  | LE    | 1222 | OMU  | C2-N3   | -2.32 | 1.33        | 1.38     |
| 51  | LL    | 3865 | PSU  | O2-C2   | -2.32 | 1.18        | 1.23     |
| 48  | LI    | 3401 | OMG  | C6-N1   | 2.31  | 1.43        | 1.38     |
| 48  | LI    | 3348 | A2M  | C8-N9   | -2.31 | 1.33        | 1.37     |
| 1   | S1    | 2116 | PSU  | O2-C2   | -2.31 | 1.18        | 1.23     |
| 48  | LI    | 3175 | PSU  | O2-C2   | -2.31 | 1.18        | 1.23     |
| 49  | LJ    | 3697 | PSU  | O2-C2   | -2.31 | 1.18        | 1.23     |
| 44  | LE    | 935  | A2M  | C8-N9   | -2.31 | 1.33        | 1.37     |
| 1   | S1    | 1960 | PSU  | O2-C2   | -2.31 | 1.18        | 1.23     |
| 1   | S1    | 407  | A2M  | C8-N9   | -2.30 | 1.33        | 1.37     |
| 1   | S1    | 1554 | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 47  | LH    | 2849 | A2M  | C8-N9   | -2.30 | 1.33        | 1.37     |
| 41  | LB    | 280  | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 46  | LG    | 2154 | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 44  | LE    | 1222 | OMU  | C5-C4   | -2.30 | 1.38        | 1.43     |
| 48  | LI    | 3542 | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 48  | LI    | 3185 | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 45  | LF    | 1568 | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 1   | S1    | 2081 | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 47  | LH    | 2744 | A2M  | O3'-C3' | -2.29 | 1.37        | 1.43     |
| 47  | LH    | 2849 | A2M  | O5'-C5' | -2.29 | 1.39        | 1.44     |
| 40  | LA    | 16   | PSU  | O2-C2   | -2.29 | 1.18        | 1.23     |
| 45  | LF    | 1586 | PSU  | O2-C2   | -2.29 | 1.18        | 1.23     |
| 47  | LH    | 2586 | PSU  | O2-C2   | -2.29 | 1.18        | 1.23     |
| 48  | LI    | 3518 | 5MC  | O2-C2   | -2.29 | 1.19        | 1.23     |
| 48  | LI    | 3568 | PSU  | O2-C2   | -2.28 | 1.18        | 1.23     |
| 47  | LH    | 2742 | PSU  | O2-C2   | -2.28 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 44  | LE    | 1121 | A2M  | C8-N9   | -2.28 | 1.33        | 1.37     |
| 44  | LE    | 1324 | OMG  | C8-N9   | 2.28  | 1.42        | 1.37     |
| 45  | LF    | 1976 | OMC  | C2-N1   | 2.28  | 1.44        | 1.40     |
| 48  | LI    | 3535 | OMC  | C2-N1   | 2.28  | 1.44        | 1.40     |
| 1   | S1    | 176  | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 44  | LE    | 1106 | A2M  | C8-N9   | -2.27 | 1.33        | 1.37     |
| 1   | S1    | 1715 | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 48  | LI    | 3315 | A2M  | O5'-C5' | -2.27 | 1.39        | 1.44     |
| 47  | LH    | 2842 | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 1   | S1    | 1900 | A2M  | C8-N9   | -2.27 | 1.33        | 1.37     |
| 41  | LB    | 281  | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 1   | S1    | 105  | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 44  | LE    | 1171 | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 45  | LF    | 1926 | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 42  | LC    | 302  | PSU  | O2-C2   | -2.27 | 1.18        | 1.23     |
| 48  | LI    | 3500 | A2M  | C8-N9   | -2.26 | 1.33        | 1.37     |
| 1   | S1    | 32   | PSU  | O2-C2   | -2.26 | 1.18        | 1.23     |
| 47  | LH    | 2330 | PSU  | O2-C2   | -2.26 | 1.18        | 1.23     |
| 44  | LE    | 1217 | OMG  | C4-N3   | 2.26  | 1.39        | 1.34     |
| 45  | LF    | 1819 | OMG  | C4-N3   | 2.26  | 1.39        | 1.34     |
| 1   | S1    | 621  | OMC  | C2-N1   | 2.26  | 1.44        | 1.40     |
| 48  | LI    | 3440 | PSU  | O2-C2   | -2.26 | 1.18        | 1.23     |
| 47  | LH    | 2768 | A2M  | C8-N9   | -2.26 | 1.33        | 1.37     |
| 47  | LH    | 2636 | JMH  | C2-N1   | 2.25  | 1.41        | 1.38     |
| 45  | LF    | 1929 | A2M  | C8-N9   | -2.25 | 1.33        | 1.37     |
| 47  | LH    | 2809 | A2M  | C8-N9   | -2.25 | 1.33        | 1.37     |
| 45  | LF    | 1815 | A2M  | O5'-C5' | -2.25 | 1.39        | 1.44     |
| 1   | S1    | 390  | OMG  | C8-N9   | 2.25  | 1.42        | 1.37     |
| 1   | S1    | 403  | PSU  | O2-C2   | -2.25 | 1.18        | 1.23     |
| 1   | S1    | 2065 | PSU  | O2-C2   | -2.25 | 1.18        | 1.23     |
| 1   | S1    | 40   | A2M  | C8-N9   | -2.24 | 1.33        | 1.37     |
| 48  | LI    | 3315 | A2M  | C8-N9   | -2.24 | 1.33        | 1.37     |
| 1   | S1    | 280  | PSU  | O2-C2   | -2.24 | 1.18        | 1.23     |
| 1   | S1    | 1396 | PSU  | O2-C2   | -2.24 | 1.18        | 1.23     |
| 48  | LI    | 3446 | PSU  | O2-C2   | -2.23 | 1.18        | 1.23     |
| 47  | LH    | 2348 | OMC  | C2-N1   | 2.23  | 1.44        | 1.40     |
| 1   | S1    | 645  | A2M  | C8-N9   | -2.23 | 1.33        | 1.37     |
| 1   | S1    | 1068 | PSU  | O2-C2   | -2.23 | 1.18        | 1.23     |
| 46  | LG    | 2005 | A2M  | C8-N9   | -2.23 | 1.33        | 1.37     |
| 47  | LH    | 2802 | PSU  | O2-C2   | -2.23 | 1.18        | 1.23     |
| 48  | LI    | 3167 | PSU  | O2-C2   | -2.23 | 1.18        | 1.23     |
| 1   | S1    | 565  | A2M  | O5'-C5' | -2.23 | 1.39        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 640  | PSU  | O2-C2   | -2.22 | 1.18        | 1.23     |
| 47  | LH    | 2814 | A2M  | C8-N9   | -2.22 | 1.33        | 1.37     |
| 44  | LE    | 1039 | A2M  | C8-N9   | -2.22 | 1.33        | 1.37     |
| 1   | S1    | 1096 | A2M  | C8-N9   | -2.22 | 1.33        | 1.37     |
| 48  | LI    | 3510 | PSU  | O2-C2   | -2.22 | 1.18        | 1.23     |
| 48  | LI    | 3214 | 6MZ  | C5-C6   | 2.22  | 1.47        | 1.41     |
| 1   | S1    | 723  | A2M  | O5'-C5' | -2.22 | 1.39        | 1.44     |
| 49  | LJ    | 3680 | PSU  | O4'-C1' | -2.22 | 1.40        | 1.43     |
| 40  | LA    | 97   | A2M  | C8-N9   | -2.22 | 1.33        | 1.37     |
| 48  | LI    | 3145 | PSU  | O2-C2   | -2.22 | 1.18        | 1.23     |
| 47  | LH    | 2591 | PSU  | O2-C2   | -2.21 | 1.18        | 1.23     |
| 52  | LM    | 3953 | PSU  | O2-C2   | -2.21 | 1.18        | 1.23     |
| 1   | S1    | 649  | A2M  | O5'-C5' | -2.21 | 1.39        | 1.44     |
| 1   | S1    | 2046 | A2M  | O5'-C5' | -2.20 | 1.39        | 1.44     |
| 44  | LE    | 1201 | OMG  | C4-N3   | 2.20  | 1.39        | 1.34     |
| 45  | LF    | 1856 | OMG  | C8-N9   | 2.20  | 1.42        | 1.37     |
| 42  | LC    | 308  | PSU  | O2-C2   | -2.20 | 1.18        | 1.23     |
| 44  | LE    | 1324 | OMG  | C4-N3   | 2.20  | 1.39        | 1.34     |
| 45  | LF    | 1822 | OMC  | C2-N1   | 2.19  | 1.44        | 1.40     |
| 45  | LF    | 1929 | A2M  | O5'-C5' | -2.19 | 1.39        | 1.44     |
| 1   | S1    | 180  | OMG  | C4-N3   | 2.19  | 1.39        | 1.34     |
| 1   | S1    | 1063 | A2M  | C8-N9   | -2.19 | 1.33        | 1.37     |
| 1   | S1    | 2180 | A2M  | C8-N7   | 2.19  | 1.35        | 1.31     |
| 42  | LC    | 541  | OMG  | C4-N3   | 2.19  | 1.39        | 1.34     |
| 47  | LH    | 2925 | OMG  | C4-N3   | 2.18  | 1.39        | 1.34     |
| 44  | LE    | 1204 | A2M  | O5'-C5' | -2.18 | 1.39        | 1.44     |
| 48  | LI    | 3367 | A2M  | C8-N9   | -2.18 | 1.33        | 1.37     |
| 48  | LI    | 3042 | PSU  | O2-C2   | -2.18 | 1.18        | 1.23     |
| 40  | LA    | 39   | A2M  | C8-N9   | -2.18 | 1.33        | 1.37     |
| 47  | LH    | 2776 | OMG  | C4-N3   | 2.18  | 1.39        | 1.34     |
| 47  | LH    | 2853 | OMC  | C2-N1   | 2.18  | 1.44        | 1.40     |
| 1   | S1    | 1624 | PSU  | O2-C2   | -2.18 | 1.18        | 1.23     |
| 48  | LI    | 2999 | PSU  | O2-C2   | -2.18 | 1.18        | 1.23     |
| 47  | LH    | 2358 | A2M  | O5'-C5' | -2.18 | 1.39        | 1.44     |
| 1   | S1    | 40   | A2M  | O5'-C5' | -2.17 | 1.39        | 1.44     |
| 1   | S1    | 28   | A2M  | O5'-C5' | -2.17 | 1.39        | 1.44     |
| 52  | LM    | 3963 | PSU  | O2-C2   | -2.17 | 1.18        | 1.23     |
| 46  | LG    | 2171 | PSU  | O2-C2   | -2.17 | 1.18        | 1.23     |
| 47  | LH    | 2624 | PSU  | O2-C2   | -2.17 | 1.18        | 1.23     |
| 42  | LC    | 631  | OMG  | C4-N3   | 2.16  | 1.39        | 1.34     |
| 47  | LH    | 2835 | OMU  | C2-N1   | 2.16  | 1.41        | 1.38     |
| 42  | LC    | 541  | OMG  | C8-N9   | 2.16  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | LL    | 3906 | A2M  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 45  | LF    | 1662 | OMG  | C4-N3   | 2.16  | 1.39        | 1.34     |
| 53  | LN    | 3969 | PSU  | O2-C2   | -2.16 | 1.18        | 1.23     |
| 48  | LI    | 3509 | OMG  | C8-N9   | 2.15  | 1.42        | 1.37     |
| 47  | LH    | 2809 | A2M  | O5'-C5' | -2.15 | 1.39        | 1.44     |
| 42  | LC    | 594  | A2M  | O5'-C5' | -2.15 | 1.39        | 1.44     |
| 45  | LF    | 1662 | OMG  | C8-N9   | 2.15  | 1.42        | 1.37     |
| 1   | S1    | 641  | OMG  | C4-N3   | 2.15  | 1.39        | 1.34     |
| 1   | S1    | 485  | OMG  | C8-N9   | 2.15  | 1.42        | 1.37     |
| 1   | S1    | 485  | OMG  | C4-N3   | 2.14  | 1.39        | 1.34     |
| 45  | LF    | 1926 | PSU  | O4'-C1' | -2.14 | 1.40        | 1.43     |
| 1   | S1    | 1549 | A2M  | C8-N9   | -2.14 | 1.33        | 1.37     |
| 1   | S1    | 2123 | OMC  | C2-N1   | 2.14  | 1.44        | 1.40     |
| 44  | LE    | 935  | A2M  | O5'-C5' | -2.14 | 1.39        | 1.44     |
| 41  | LB    | 215  | OMG  | C4-N3   | 2.14  | 1.39        | 1.34     |
| 1   | S1    | 2075 | OMG  | C8-N9   | 2.14  | 1.42        | 1.37     |
| 1   | S1    | 641  | OMG  | C8-N9   | 2.14  | 1.42        | 1.37     |
| 47  | LH    | 2744 | A2M  | O5'-C5' | -2.14 | 1.39        | 1.44     |
| 46  | LG    | 2005 | A2M  | O5'-C5' | -2.13 | 1.39        | 1.44     |
| 47  | LH    | 2883 | OMG  | C8-N9   | 2.13  | 1.42        | 1.37     |
| 45  | LF    | 1835 | OMG  | C4-N3   | 2.13  | 1.39        | 1.34     |
| 40  | LA    | 74   | OMG  | C8-N9   | 2.13  | 1.42        | 1.37     |
| 1   | S1    | 1601 | B8N  | O4'-C1' | -2.13 | 1.40        | 1.43     |
| 47  | LH    | 2769 | A2M  | O5'-C5' | -2.12 | 1.39        | 1.44     |
| 47  | LH    | 2610 | OMG  | C4-N3   | 2.12  | 1.39        | 1.34     |
| 44  | LE    | 1121 | A2M  | O5'-C5' | -2.12 | 1.39        | 1.44     |
| 48  | LI    | 3500 | A2M  | O5'-C5' | -2.12 | 1.39        | 1.44     |
| 42  | LC    | 628  | OMG  | C4-N3   | 2.12  | 1.39        | 1.34     |
| 45  | LF    | 1883 | OMG  | C4-N3   | 2.12  | 1.39        | 1.34     |
| 47  | LH    | 2883 | OMG  | C4-N3   | 2.12  | 1.39        | 1.34     |
| 46  | LG    | 2022 | A2M  | O5'-C5' | -2.12 | 1.39        | 1.44     |
| 1   | S1    | 121  | PSU  | C2-N3   | -2.12 | 1.33        | 1.37     |
| 48  | LI    | 3214 | 6MZ  | C8-N7   | 2.12  | 1.35        | 1.31     |
| 47  | LH    | 2925 | OMG  | C8-N9   | 2.12  | 1.42        | 1.37     |
| 45  | LF    | 1662 | OMG  | C2-N2   | 2.12  | 1.39        | 1.34     |
| 42  | LC    | 631  | OMG  | C8-N9   | 2.12  | 1.42        | 1.37     |
| 1   | S1    | 2075 | OMG  | C4-N3   | 2.11  | 1.39        | 1.34     |
| 1   | S1    | 1681 | OMG  | C4-N3   | 2.11  | 1.39        | 1.34     |
| 45  | LF    | 1683 | OMG  | C8-N9   | 2.11  | 1.42        | 1.37     |
| 1   | S1    | 42   | OMG  | C4-N3   | 2.11  | 1.39        | 1.34     |
| 40  | LA    | 74   | OMG  | C4-N3   | 2.11  | 1.39        | 1.34     |
| 48  | LI    | 3223 | OMG  | C4-N3   | 2.11  | 1.39        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 1705 | OMG  | C4-N3   | 2.11  | 1.39        | 1.34     |
| 47  | LH    | 2887 | A2M  | O5'-C5' | -2.11 | 1.39        | 1.44     |
| 48  | LI    | 3444 | PSU  | O4'-C1' | -2.11 | 1.40        | 1.43     |
| 47  | LH    | 2776 | OMG  | C2-N2   | 2.10  | 1.39        | 1.34     |
| 48  | LI    | 3465 | OMC  | C2-N1   | 2.10  | 1.44        | 1.40     |
| 47  | LH    | 2920 | A2M  | O5'-C5' | -2.10 | 1.39        | 1.44     |
| 49  | LJ    | 3688 | OMG  | C4-N3   | 2.10  | 1.39        | 1.34     |
| 45  | LF    | 1667 | OMG  | C4-N3   | 2.10  | 1.39        | 1.34     |
| 48  | LI    | 3223 | OMG  | C2-N2   | 2.10  | 1.39        | 1.34     |
| 41  | LB    | 183  | A2M  | O5'-C5' | -2.10 | 1.39        | 1.44     |
| 47  | LH    | 2621 | PSU  | O2-C2   | -2.09 | 1.19        | 1.23     |
| 47  | LH    | 2768 | A2M  | O5'-C5' | -2.08 | 1.39        | 1.44     |
| 45  | LF    | 1819 | OMG  | C8-N9   | 2.08  | 1.42        | 1.37     |
| 1   | S1    | 533  | A2M  | O5'-C5' | -2.08 | 1.39        | 1.44     |
| 47  | LH    | 2313 | OMC  | C2-N1   | 2.08  | 1.44        | 1.40     |
| 1   | S1    | 390  | OMG  | C4-N3   | 2.08  | 1.39        | 1.34     |
| 48  | LI    | 3187 | OMG  | C4-N3   | 2.08  | 1.39        | 1.34     |
| 48  | LI    | 3377 | OMG  | C4-N3   | 2.08  | 1.39        | 1.34     |
| 45  | LF    | 1883 | OMG  | C8-N9   | 2.08  | 1.42        | 1.37     |
| 45  | LF    | 1738 | A2M  | O5'-C5' | -2.08 | 1.39        | 1.44     |
| 45  | LF    | 1683 | OMG  | C4-N3   | 2.08  | 1.39        | 1.34     |
| 45  | LF    | 1502 | A2M  | O5'-C5' | -2.07 | 1.39        | 1.44     |
| 42  | LC    | 628  | OMG  | C8-N9   | 2.07  | 1.42        | 1.37     |
| 45  | LF    | 1835 | OMG  | C8-N9   | 2.07  | 1.42        | 1.37     |
| 40  | LA    | 39   | A2M  | O5'-C5' | -2.07 | 1.39        | 1.44     |
| 45  | LF    | 1891 | A2M  | O5'-C5' | -2.07 | 1.39        | 1.44     |
| 47  | LH    | 2897 | OMG  | C4-N3   | 2.06  | 1.39        | 1.34     |
| 1   | S1    | 110  | A2M  | O5'-C5' | -2.06 | 1.39        | 1.44     |
| 1   | S1    | 641  | OMG  | C2-N2   | 2.06  | 1.39        | 1.34     |
| 47  | LH    | 2610 | OMG  | C8-N9   | 2.06  | 1.42        | 1.37     |
| 47  | LH    | 2776 | OMG  | C8-N9   | 2.06  | 1.42        | 1.37     |
| 40  | LA    | 68   | PSU  | O4'-C1' | -2.06 | 1.41        | 1.43     |
| 45  | LF    | 1956 | OMG  | C8-N9   | 2.06  | 1.42        | 1.37     |
| 48  | LI    | 3434 | OMG  | C8-N9   | 2.05  | 1.42        | 1.37     |
| 47  | LH    | 2842 | PSU  | O4'-C1' | -2.05 | 1.41        | 1.43     |
| 45  | LF    | 1836 | OMC  | C2-N1   | 2.05  | 1.44        | 1.40     |
| 1   | S1    | 1536 | OMG  | C4-N3   | 2.05  | 1.39        | 1.34     |
| 40  | LA    | 41   | OMG  | C4-N3   | 2.05  | 1.39        | 1.34     |
| 44  | LE    | 1106 | A2M  | O5'-C5' | -2.05 | 1.39        | 1.44     |
| 48  | LI    | 3379 | OMG  | C4-N3   | 2.05  | 1.39        | 1.34     |
| 46  | LG    | 2146 | OMG  | C4-N3   | 2.05  | 1.39        | 1.34     |
| 48  | LI    | 3504 | OMG  | C4-N3   | 2.05  | 1.39        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | S1    | 1681 | OMG  | C8-N9   | 2.05  | 1.42        | 1.37     |
| 45  | LF    | 1667 | OMG  | C8-N9   | 2.05  | 1.42        | 1.37     |
| 1   | S1    | 99   | OMC  | C2-N1   | 2.04  | 1.44        | 1.40     |
| 44  | LE    | 1324 | OMG  | C2-N2   | 2.04  | 1.39        | 1.34     |
| 44  | LE    | 1201 | OMG  | C8-N9   | 2.04  | 1.42        | 1.37     |
| 47  | LH    | 2744 | A2M  | C4-N9   | -2.04 | 1.33        | 1.37     |
| 46  | LG    | 2146 | OMG  | C2-N2   | 2.04  | 1.39        | 1.34     |
| 48  | LI    | 3401 | OMG  | C8-N9   | 2.04  | 1.42        | 1.37     |
| 42  | LC    | 631  | OMG  | C2-N2   | 2.04  | 1.39        | 1.34     |
| 52  | LM    | 3957 | OMC  | C2-N3   | 2.04  | 1.40        | 1.36     |
| 48  | LI    | 3367 | A2M  | O5'-C5' | -2.04 | 1.39        | 1.44     |
| 1   | S1    | 1901 | OMG  | C4-N3   | 2.04  | 1.39        | 1.34     |
| 1   | S1    | 42   | OMG  | C2-N2   | 2.03  | 1.39        | 1.34     |
| 48  | LI    | 3191 | OMG  | C4-N3   | 2.03  | 1.39        | 1.34     |
| 48  | LI    | 3533 | A2M  | O5'-C5' | -2.03 | 1.39        | 1.44     |
| 47  | LH    | 2879 | OMG  | C8-N9   | 2.03  | 1.42        | 1.37     |
| 1   | S1    | 57   | OMG  | C8-N9   | 2.03  | 1.42        | 1.37     |
| 1   | S1    | 57   | OMG  | C4-N3   | 2.03  | 1.39        | 1.34     |
| 1   | S1    | 2101 | PSU  | O4'-C1' | -2.02 | 1.41        | 1.43     |
| 47  | LH    | 2812 | A2M  | O5'-C5' | -2.02 | 1.39        | 1.44     |
| 48  | LI    | 3348 | A2M  | O5'-C5' | -2.02 | 1.39        | 1.44     |
| 1   | S1    | 180  | OMG  | C8-N9   | 2.02  | 1.42        | 1.37     |
| 1   | S1    | 180  | OMG  | C2-N2   | 2.02  | 1.39        | 1.34     |
| 44  | LE    | 1312 | OMC  | C2-N1   | 2.02  | 1.44        | 1.40     |
| 48  | LI    | 3451 | PSU  | O4'-C1' | -2.02 | 1.41        | 1.43     |
| 45  | LF    | 1826 | OMG  | C4-N3   | 2.02  | 1.39        | 1.34     |
| 49  | LJ    | 3688 | OMG  | C8-N9   | 2.02  | 1.42        | 1.37     |
| 48  | LI    | 3374 | OMC  | C2-N1   | 2.02  | 1.44        | 1.40     |
| 2   | S2    | 37   | MIA  | C4-N9   | -2.02 | 1.33        | 1.37     |
| 1   | S1    | 42   | OMG  | C8-N9   | 2.01  | 1.42        | 1.37     |
| 46  | LG    | 2009 | OMG  | C8-N9   | 2.01  | 1.42        | 1.37     |
| 45  | LF    | 1883 | OMG  | C2-N2   | 2.01  | 1.39        | 1.34     |
| 1   | S1    | 121  | PSU  | C2-N1   | -2.00 | 1.34        | 1.36     |
| 47  | LH    | 2870 | OMG  | C8-N9   | 2.00  | 1.42        | 1.37     |
| 45  | LF    | 1856 | OMG  | C2-N2   | 2.00  | 1.39        | 1.34     |

All (1534) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | S1    | 2288 | MA6  | N1-C6-N6    | -13.99 | 101.79      | 117.08   |
| 1   | S1    | 2287 | MA6  | N1-C6-N6    | -13.27 | 102.57      | 117.08   |
| 2   | S2    | 37   | MIA  | C12-C13-C14 | -9.01  | 109.61      | 127.14   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | S1    | 2288 | MA6  | C5-C6-N6   | 7.56  | 138.47      | 125.30   |
| 1   | S1    | 2287 | MA6  | C5-C6-N6   | 7.03  | 137.55      | 125.30   |
| 1   | S1    | 1601 | B8N  | C31-N3-C4  | 6.99  | 127.61      | 117.31   |
| 2   | S2    | 37   | MIA  | C11-S10-C2 | 6.68  | 107.26      | 102.27   |
| 1   | S1    | 2180 | A2M  | C5-C4-N3   | -6.66 | 118.06      | 126.75   |
| 48  | LI    | 3214 | 6MZ  | C5-C4-N3   | -6.52 | 118.24      | 126.75   |
| 1   | S1    | 407  | A2M  | C5-C4-N3   | -6.41 | 118.39      | 126.75   |
| 46  | LG    | 2005 | A2M  | N6-C6-N1   | -6.14 | 104.90      | 118.35   |
| 47  | LH    | 2358 | A2M  | N6-C6-N1   | -6.13 | 104.92      | 118.35   |
| 1   | S1    | 110  | A2M  | N6-C6-N1   | -6.12 | 104.95      | 118.35   |
| 1   | S1    | 2046 | A2M  | N6-C6-N1   | -6.11 | 104.97      | 118.35   |
| 47  | LH    | 2769 | A2M  | N6-C6-N1   | -6.09 | 105.02      | 118.35   |
| 47  | LH    | 2809 | A2M  | N6-C6-N1   | -6.07 | 105.06      | 118.35   |
| 44  | LE    | 935  | A2M  | N6-C6-N1   | -6.03 | 105.14      | 118.35   |
| 47  | LH    | 2814 | A2M  | N6-C6-N1   | -6.01 | 105.18      | 118.35   |
| 48  | LI    | 3348 | A2M  | N6-C6-N1   | -6.00 | 105.20      | 118.35   |
| 1   | S1    | 1549 | A2M  | N6-C6-N1   | -5.96 | 105.29      | 118.35   |
| 47  | LH    | 2887 | A2M  | N3-C2-N1   | -5.96 | 119.28      | 128.60   |
| 48  | LI    | 3521 | A2M  | N6-C6-N1   | -5.96 | 105.30      | 118.35   |
| 45  | LF    | 1502 | A2M  | N6-C6-N1   | -5.95 | 105.32      | 118.35   |
| 1   | S1    | 645  | A2M  | N6-C6-N1   | -5.95 | 105.32      | 118.35   |
| 1   | S1    | 121  | PSU  | N1-C2-N3   | 5.94  | 121.86      | 115.13   |
| 2   | S2    | 37   | MIA  | C5-C4-N3   | -5.94 | 120.50      | 127.19   |
| 45  | LF    | 1891 | A2M  | N3-C2-N1   | -5.94 | 119.32      | 128.60   |
| 1   | S1    | 1371 | A2M  | N6-C6-N1   | -5.93 | 105.36      | 118.35   |
| 1   | S1    | 1601 | B8N  | C4-N3-C2   | -5.92 | 117.97      | 125.46   |
| 47  | LH    | 2744 | A2M  | N6-C6-N1   | -5.92 | 105.38      | 118.35   |
| 1   | S1    | 565  | A2M  | N6-C6-N1   | -5.90 | 105.43      | 118.35   |
| 48  | LI    | 3315 | A2M  | N6-C6-N1   | -5.90 | 105.43      | 118.35   |
| 45  | LF    | 1738 | A2M  | N6-C6-N1   | -5.89 | 105.44      | 118.35   |
| 44  | LE    | 1039 | A2M  | N6-C6-N1   | -5.88 | 105.48      | 118.35   |
| 44  | LE    | 1121 | A2M  | N6-C6-N1   | -5.87 | 105.49      | 118.35   |
| 44  | LE    | 1204 | A2M  | N6-C6-N1   | -5.86 | 105.52      | 118.35   |
| 40  | LA    | 39   | A2M  | N6-C6-N1   | -5.84 | 105.56      | 118.35   |
| 1   | S1    | 2288 | MA6  | N1-C2-N3   | -5.83 | 119.48      | 128.60   |
| 1   | S1    | 28   | A2M  | N6-C6-N1   | -5.83 | 105.58      | 118.35   |
| 1   | S1    | 649  | A2M  | N6-C6-N1   | -5.83 | 105.59      | 118.35   |
| 1   | S1    | 40   | A2M  | N6-C6-N1   | -5.82 | 105.60      | 118.35   |
| 47  | LH    | 2812 | A2M  | C5-C4-N3   | -5.82 | 119.16      | 126.75   |
| 40  | LA    | 97   | A2M  | N6-C6-N1   | -5.82 | 105.61      | 118.35   |
| 47  | LH    | 2904 | B8H  | N3-C2-N1   | 5.81  | 121.42      | 115.14   |
| 44  | LE    | 935  | A2M  | N3-C2-N1   | -5.80 | 119.53      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 47  | LH    | 2349 | A2M  | N6-C6-N1 | -5.80 | 105.66      | 118.35   |
| 47  | LH    | 2768 | A2M  | N6-C6-N1 | -5.79 | 105.67      | 118.35   |
| 1   | S1    | 407  | A2M  | N6-C6-N1 | -5.78 | 105.70      | 118.35   |
| 1   | S1    | 645  | A2M  | C5-C4-N3 | -5.78 | 119.21      | 126.75   |
| 47  | LH    | 2887 | A2M  | N6-C6-N1 | -5.78 | 105.70      | 118.35   |
| 45  | LF    | 1502 | A2M  | N3-C2-N1 | -5.77 | 119.57      | 128.60   |
| 48  | LI    | 3367 | A2M  | N6-C6-N1 | -5.77 | 105.72      | 118.35   |
| 1   | S1    | 2046 | A2M  | N3-C2-N1 | -5.76 | 119.60      | 128.60   |
| 47  | LH    | 2809 | A2M  | N3-C2-N1 | -5.76 | 119.60      | 128.60   |
| 47  | LH    | 2920 | A2M  | N6-C6-N1 | -5.75 | 105.75      | 118.35   |
| 1   | S1    | 1900 | A2M  | N6-C6-N1 | -5.74 | 105.79      | 118.35   |
| 41  | LB    | 183  | A2M  | N6-C6-N1 | -5.74 | 105.79      | 118.35   |
| 47  | LH    | 2849 | A2M  | N6-C6-N1 | -5.71 | 105.83      | 118.35   |
| 47  | LH    | 2744 | A2M  | N3-C2-N1 | -5.71 | 119.66      | 128.60   |
| 40  | LA    | 97   | A2M  | N3-C2-N1 | -5.71 | 119.67      | 128.60   |
| 1   | S1    | 1371 | A2M  | N3-C2-N1 | -5.71 | 119.67      | 128.60   |
| 47  | LH    | 2708 | A2M  | N6-C6-N1 | -5.70 | 105.86      | 118.35   |
| 46  | LG    | 2022 | A2M  | N6-C6-N1 | -5.70 | 105.87      | 118.35   |
| 47  | LH    | 2812 | A2M  | N6-C6-N1 | -5.69 | 105.88      | 118.35   |
| 47  | LH    | 2349 | A2M  | N3-C2-N1 | -5.69 | 119.70      | 128.60   |
| 45  | LF    | 1891 | A2M  | N6-C6-N1 | -5.69 | 105.89      | 118.35   |
| 45  | LF    | 1815 | A2M  | N6-C6-N1 | -5.68 | 105.91      | 118.35   |
| 45  | LF    | 1888 | A2M  | N6-C6-N1 | -5.68 | 105.92      | 118.35   |
| 1   | S1    | 723  | A2M  | N6-C6-N1 | -5.67 | 105.92      | 118.35   |
| 40  | LA    | 39   | A2M  | C5-C4-N3 | -5.67 | 119.36      | 126.75   |
| 44  | LE    | 1204 | A2M  | C5-C4-N3 | -5.67 | 119.36      | 126.75   |
| 47  | LH    | 2920 | A2M  | C5-C4-N3 | -5.67 | 119.36      | 126.75   |
| 48  | LI    | 3367 | A2M  | N3-C2-N1 | -5.66 | 119.75      | 128.60   |
| 48  | LI    | 3533 | A2M  | N6-C6-N1 | -5.66 | 105.96      | 118.35   |
| 1   | S1    | 723  | A2M  | N3-C2-N1 | -5.65 | 119.76      | 128.60   |
| 46  | LG    | 2005 | A2M  | N3-C2-N1 | -5.65 | 119.76      | 128.60   |
| 1   | S1    | 407  | A2M  | N3-C2-N1 | -5.65 | 119.76      | 128.60   |
| 44  | LE    | 1208 | OMG  | C5-C4-N3 | -5.65 | 119.30      | 128.46   |
| 1   | S1    | 1549 | A2M  | C5-C4-N3 | -5.65 | 119.38      | 126.75   |
| 44  | LE    | 1106 | A2M  | N6-C6-N1 | -5.65 | 105.98      | 118.35   |
| 47  | LH    | 2358 | A2M  | N3-C2-N1 | -5.64 | 119.78      | 128.60   |
| 1   | S1    | 28   | A2M  | N3-C2-N1 | -5.63 | 119.79      | 128.60   |
| 48  | LI    | 3500 | A2M  | N3-C2-N1 | -5.63 | 119.79      | 128.60   |
| 1   | S1    | 1063 | A2M  | N6-C6-N1 | -5.63 | 106.02      | 118.35   |
| 1   | S1    | 645  | A2M  | N3-C2-N1 | -5.62 | 119.80      | 128.60   |
| 45  | LF    | 1929 | A2M  | N6-C6-N1 | -5.62 | 106.04      | 118.35   |
| 47  | LH    | 2769 | A2M  | C5-C4-N3 | -5.62 | 119.42      | 126.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 44  | LE    | 1204 | A2M  | N3-C2-N1 | -5.61 | 119.83      | 128.60   |
| 1   | S1    | 565  | A2M  | N3-C2-N1 | -5.61 | 119.83      | 128.60   |
| 48  | LI    | 3533 | A2M  | N3-C2-N1 | -5.60 | 119.83      | 128.60   |
| 1   | S1    | 1096 | A2M  | N6-C6-N1 | -5.59 | 106.11      | 118.35   |
| 46  | LG    | 2022 | A2M  | C5-C4-N3 | -5.59 | 119.46      | 126.75   |
| 44  | LE    | 1039 | A2M  | N3-C2-N1 | -5.58 | 119.87      | 128.60   |
| 45  | LF    | 1738 | A2M  | N3-C2-N1 | -5.58 | 119.88      | 128.60   |
| 45  | LF    | 1888 | A2M  | N3-C2-N1 | -5.58 | 119.88      | 128.60   |
| 1   | S1    | 649  | A2M  | N3-C2-N1 | -5.56 | 119.90      | 128.60   |
| 1   | S1    | 2287 | MA6  | N1-C2-N3 | -5.55 | 119.92      | 128.60   |
| 1   | S1    | 1371 | A2M  | C5-C4-N3 | -5.55 | 119.51      | 126.75   |
| 1   | S1    | 1096 | A2M  | N3-C2-N1 | -5.54 | 119.94      | 128.60   |
| 45  | LF    | 1929 | A2M  | N3-C2-N1 | -5.53 | 119.95      | 128.60   |
| 44  | LE    | 1121 | A2M  | N3-C2-N1 | -5.53 | 119.95      | 128.60   |
| 45  | LF    | 1891 | A2M  | C5-C4-N3 | -5.52 | 119.54      | 126.75   |
| 41  | LB    | 183  | A2M  | N3-C2-N1 | -5.51 | 119.98      | 128.60   |
| 48  | LI    | 3315 | A2M  | C5-C4-N3 | -5.51 | 119.57      | 126.75   |
| 47  | LH    | 2920 | A2M  | N3-C2-N1 | -5.51 | 119.99      | 128.60   |
| 47  | LH    | 2849 | A2M  | N3-C2-N1 | -5.50 | 120.00      | 128.60   |
| 1   | S1    | 40   | A2M  | N3-C2-N1 | -5.50 | 120.00      | 128.60   |
| 48  | LI    | 3315 | A2M  | N3-C2-N1 | -5.49 | 120.02      | 128.60   |
| 48  | LI    | 3500 | A2M  | N6-C6-N1 | -5.49 | 106.33      | 118.35   |
| 47  | LH    | 2768 | A2M  | C5-C4-N3 | -5.48 | 119.61      | 126.75   |
| 46  | LG    | 2005 | A2M  | C5-C4-N3 | -5.48 | 119.61      | 126.75   |
| 51  | LL    | 3906 | A2M  | N6-C6-N1 | -5.47 | 106.36      | 118.35   |
| 1   | S1    | 1900 | A2M  | N3-C2-N1 | -5.47 | 120.04      | 128.60   |
| 47  | LH    | 2746 | PSU  | N1-C2-N3 | 5.47  | 121.32      | 115.13   |
| 42  | LC    | 594  | A2M  | N3-C2-N1 | -5.47 | 120.05      | 128.60   |
| 44  | LE    | 1121 | A2M  | C5-C4-N3 | -5.46 | 119.63      | 126.75   |
| 1   | S1    | 533  | A2M  | N6-C6-N1 | -5.46 | 106.39      | 118.35   |
| 45  | LF    | 1815 | A2M  | N3-C2-N1 | -5.45 | 120.07      | 128.60   |
| 42  | LC    | 594  | A2M  | N6-C6-N1 | -5.45 | 106.42      | 118.35   |
| 47  | LH    | 2812 | A2M  | N3-C2-N1 | -5.45 | 120.08      | 128.60   |
| 1   | S1    | 1096 | A2M  | C5-C4-N3 | -5.44 | 119.65      | 126.75   |
| 47  | LH    | 2708 | A2M  | N3-C2-N1 | -5.43 | 120.10      | 128.60   |
| 47  | LH    | 2814 | A2M  | N3-C2-N1 | -5.42 | 120.12      | 128.60   |
| 51  | LL    | 3906 | A2M  | N3-C2-N1 | -5.42 | 120.12      | 128.60   |
| 48  | LI    | 3521 | A2M  | N3-C2-N1 | -5.42 | 120.13      | 128.60   |
| 47  | LH    | 2746 | PSU  | C4-N3-C2 | -5.41 | 118.55      | 126.34   |
| 1   | S1    | 1900 | A2M  | C5-C4-N3 | -5.41 | 119.69      | 126.75   |
| 45  | LF    | 1888 | A2M  | C5-C4-N3 | -5.39 | 119.72      | 126.75   |
| 1   | S1    | 110  | A2M  | N3-C2-N1 | -5.38 | 120.19      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 45  | LF    | 1738 | A2M  | C5-C4-N3 | -5.37 | 119.74      | 126.75   |
| 44  | LE    | 935  | A2M  | C5-C4-N3 | -5.37 | 119.75      | 126.75   |
| 48  | LI    | 3348 | A2M  | C5-C4-N3 | -5.36 | 119.76      | 126.75   |
| 47  | LH    | 2349 | A2M  | C5-C4-N3 | -5.35 | 119.77      | 126.75   |
| 44  | LE    | 931  | 1MA  | C5-C4-N3 | -5.35 | 119.27      | 127.26   |
| 1   | S1    | 533  | A2M  | C5-C4-N3 | -5.35 | 119.77      | 126.75   |
| 46  | LG    | 2022 | A2M  | N3-C2-N1 | -5.34 | 120.24      | 128.60   |
| 47  | LH    | 2768 | A2M  | N3-C2-N1 | -5.33 | 120.27      | 128.60   |
| 45  | LF    | 1815 | A2M  | C5-C4-N3 | -5.33 | 119.80      | 126.75   |
| 44  | LE    | 1106 | A2M  | N3-C2-N1 | -5.32 | 120.28      | 128.60   |
| 51  | LL    | 3906 | A2M  | C5-C4-N3 | -5.32 | 119.81      | 126.75   |
| 48  | LI    | 3348 | A2M  | N3-C2-N1 | -5.31 | 120.30      | 128.60   |
| 47  | LH    | 2708 | A2M  | C5-C4-N3 | -5.30 | 119.84      | 126.75   |
| 1   | S1    | 2180 | A2M  | N3-C4-N9 | 5.29  | 135.80      | 127.08   |
| 1   | S1    | 110  | A2M  | C5-C4-N3 | -5.29 | 119.85      | 126.75   |
| 47  | LH    | 2769 | A2M  | N3-C2-N1 | -5.28 | 120.34      | 128.60   |
| 1   | S1    | 40   | A2M  | C5-C4-N3 | -5.28 | 119.86      | 126.75   |
| 1   | S1    | 1549 | A2M  | N3-C2-N1 | -5.28 | 120.34      | 128.60   |
| 1   | S1    | 110  | A2M  | C5-C6-N6 | 5.27  | 134.90      | 123.43   |
| 1   | S1    | 2287 | MA6  | C5-C4-N3 | -5.27 | 119.88      | 126.75   |
| 1   | S1    | 1063 | A2M  | N3-C2-N1 | -5.26 | 120.37      | 128.60   |
| 1   | S1    | 2046 | A2M  | C5-C4-N3 | -5.26 | 119.89      | 126.75   |
| 1   | S1    | 1063 | A2M  | C5-C4-N3 | -5.25 | 119.90      | 126.75   |
| 1   | S1    | 28   | A2M  | C5-C4-N3 | -5.25 | 119.90      | 126.75   |
| 1   | S1    | 565  | A2M  | C5-C4-N3 | -5.25 | 119.90      | 126.75   |
| 45  | LF    | 1929 | A2M  | C5-C4-N3 | -5.23 | 119.93      | 126.75   |
| 40  | LA    | 39   | A2M  | N3-C2-N1 | -5.20 | 120.47      | 128.60   |
| 1   | S1    | 565  | A2M  | C5-C6-N6 | 5.19  | 134.72      | 123.43   |
| 42  | LC    | 594  | A2M  | C5-C4-N3 | -5.18 | 119.99      | 126.75   |
| 47  | LH    | 2358 | A2M  | C5-C4-N3 | -5.18 | 119.99      | 126.75   |
| 1   | S1    | 533  | A2M  | N3-C2-N1 | -5.17 | 120.51      | 128.60   |
| 41  | LB    | 183  | A2M  | C5-C4-N3 | -5.17 | 120.01      | 126.75   |
| 47  | LH    | 2809 | A2M  | C5-C6-N6 | 5.16  | 134.66      | 123.43   |
| 46  | LG    | 2005 | A2M  | C5-C6-N6 | 5.16  | 134.66      | 123.43   |
| 44  | LE    | 1039 | A2M  | C5-C4-N3 | -5.15 | 120.03      | 126.75   |
| 48  | LI    | 3521 | A2M  | C5-C6-N6 | 5.15  | 134.64      | 123.43   |
| 47  | LH    | 2904 | B8H  | C4-N3-C2 | -5.15 | 120.68      | 127.35   |
| 1   | S1    | 2046 | A2M  | C5-C6-N6 | 5.14  | 134.62      | 123.43   |
| 47  | LH    | 2814 | A2M  | C5-C6-N6 | 5.14  | 134.61      | 123.43   |
| 45  | LF    | 1502 | A2M  | C5-C6-N6 | 5.14  | 134.61      | 123.43   |
| 1   | S1    | 649  | A2M  | C5-C4-N3 | -5.13 | 120.05      | 126.75   |
| 1   | S1    | 1549 | A2M  | C5-C6-N6 | 5.13  | 134.60      | 123.43   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 48  | LI    | 3521 | A2M  | C5-C4-N3  | -5.10 | 120.09      | 126.75   |
| 48  | LI    | 3500 | A2M  | C5-C4-N3  | -5.10 | 120.10      | 126.75   |
| 47  | LH    | 2358 | A2M  | C5-C6-N6  | 5.08  | 134.50      | 123.43   |
| 47  | LH    | 2887 | A2M  | C5-C6-N6  | 5.08  | 134.49      | 123.43   |
| 44  | LE    | 1118 | PSU  | C4-N3-C2  | -5.08 | 119.03      | 126.34   |
| 40  | LA    | 97   | A2M  | C5-C6-N6  | 5.06  | 134.44      | 123.43   |
| 1   | S1    | 649  | A2M  | C5-C6-N6  | 5.05  | 134.42      | 123.43   |
| 48  | LI    | 3348 | A2M  | C5-C6-N6  | 5.05  | 134.41      | 123.43   |
| 44  | LE    | 1106 | A2M  | C5-C4-N3  | -5.05 | 120.17      | 126.75   |
| 47  | LH    | 2744 | A2M  | C5-C4-N3  | -5.03 | 120.18      | 126.75   |
| 48  | LI    | 3367 | A2M  | C5-C4-N3  | -5.03 | 120.19      | 126.75   |
| 1   | S1    | 645  | A2M  | C5-C6-N6  | 5.03  | 134.37      | 123.43   |
| 48  | LI    | 3214 | 6MZ  | N3-C4-N9  | 5.02  | 135.36      | 127.08   |
| 47  | LH    | 2744 | A2M  | C5-C6-N6  | 5.02  | 134.36      | 123.43   |
| 47  | LH    | 2809 | A2M  | C5-C4-N3  | -5.02 | 120.20      | 126.75   |
| 45  | LF    | 1502 | A2M  | C5-C4-N3  | -5.01 | 120.22      | 126.75   |
| 48  | LI    | 3315 | A2M  | C5-C6-N6  | 5.00  | 134.32      | 123.43   |
| 1   | S1    | 1592 | PSU  | C4-N3-C2  | -5.00 | 119.13      | 126.34   |
| 44  | LE    | 1222 | OMU  | C1'-N1-C2 | 5.00  | 126.62      | 117.57   |
| 47  | LH    | 2814 | A2M  | C5-C4-N3  | -4.98 | 120.25      | 126.75   |
| 44  | LE    | 1121 | A2M  | C5-C6-N6  | 4.97  | 134.24      | 123.43   |
| 1   | S1    | 1371 | A2M  | C5-C6-N6  | 4.96  | 134.22      | 123.43   |
| 47  | LH    | 2849 | A2M  | C5-C4-N3  | -4.95 | 120.29      | 126.75   |
| 44  | LE    | 935  | A2M  | C5-C6-N6  | 4.95  | 134.20      | 123.43   |
| 48  | LI    | 3214 | 6MZ  | C9-N6-C6  | -4.94 | 118.61      | 122.87   |
| 1   | S1    | 28   | A2M  | C5-C6-N6  | 4.94  | 134.18      | 123.43   |
| 44  | LE    | 1204 | A2M  | C5-C6-N6  | 4.94  | 134.18      | 123.43   |
| 46  | LG    | 2119 | PSU  | C4-N3-C2  | -4.93 | 119.23      | 126.34   |
| 47  | LH    | 2769 | A2M  | C5-C6-N6  | 4.93  | 134.15      | 123.43   |
| 1   | S1    | 723  | A2M  | C5-C4-N3  | -4.92 | 120.33      | 126.75   |
| 45  | LF    | 1738 | A2M  | C5-C6-N6  | 4.92  | 134.14      | 123.43   |
| 48  | LI    | 3533 | A2M  | C5-C4-N3  | -4.92 | 120.33      | 126.75   |
| 1   | S1    | 2131 | PSU  | C4-N3-C2  | -4.92 | 119.25      | 126.34   |
| 47  | LH    | 2849 | A2M  | C5-C6-N6  | 4.90  | 134.10      | 123.43   |
| 48  | LI    | 3367 | A2M  | C5-C6-N6  | 4.90  | 134.10      | 123.43   |
| 47  | LH    | 2768 | A2M  | C5-C6-N6  | 4.89  | 134.08      | 123.43   |
| 45  | LF    | 1815 | A2M  | C5-C6-N6  | 4.89  | 134.08      | 123.43   |
| 40  | LA    | 97   | A2M  | C5-C4-N3  | -4.89 | 120.37      | 126.75   |
| 1   | S1    | 1063 | A2M  | C5-C6-N6  | 4.89  | 134.07      | 123.43   |
| 44  | LE    | 1039 | A2M  | C5-C6-N6  | 4.89  | 134.07      | 123.43   |
| 1   | S1    | 40   | A2M  | C5-C6-N6  | 4.89  | 134.07      | 123.43   |
| 44  | LE    | 1106 | A2M  | C5-C6-N6  | 4.88  | 134.04      | 123.43   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 40  | LA    | 68   | PSU  | N1-C2-N3 | 4.87  | 120.64      | 115.13   |
| 47  | LH    | 2642 | PSU  | C4-N3-C2 | -4.87 | 119.33      | 126.34   |
| 47  | LH    | 2349 | A2M  | C5-C6-N6 | 4.87  | 134.02      | 123.43   |
| 48  | LI    | 3332 | PSU  | C4-N3-C2 | -4.85 | 119.35      | 126.34   |
| 49  | LJ    | 3644 | PSU  | C4-N3-C2 | -4.85 | 119.35      | 126.34   |
| 1   | S1    | 723  | A2M  | C5-C6-N6 | 4.85  | 133.97      | 123.43   |
| 46  | LG    | 2022 | A2M  | C5-C6-N6 | 4.84  | 133.96      | 123.43   |
| 48  | LI    | 3533 | A2M  | C5-C6-N6 | 4.84  | 133.95      | 123.43   |
| 41  | LB    | 183  | A2M  | C5-C6-N6 | 4.83  | 133.95      | 123.43   |
| 45  | LF    | 1876 | PSU  | C4-N3-C2 | -4.83 | 119.38      | 126.34   |
| 1   | S1    | 1900 | A2M  | C5-C6-N6 | 4.83  | 133.94      | 123.43   |
| 47  | LH    | 2708 | A2M  | C5-C6-N6 | 4.83  | 133.93      | 123.43   |
| 45  | LF    | 1929 | A2M  | C5-C6-N6 | 4.81  | 133.91      | 123.43   |
| 48  | LI    | 3206 | PSU  | C4-N3-C2 | -4.81 | 119.41      | 126.34   |
| 44  | LE    | 1260 | PSU  | C4-N3-C2 | -4.81 | 119.42      | 126.34   |
| 45  | LF    | 1891 | A2M  | C5-C6-N6 | 4.79  | 133.85      | 123.43   |
| 47  | LH    | 2874 | PSU  | C4-N3-C2 | -4.79 | 119.44      | 126.34   |
| 48  | LI    | 3451 | PSU  | C4-N3-C2 | -4.79 | 119.44      | 126.34   |
| 51  | LL    | 3865 | PSU  | C4-N3-C2 | -4.78 | 119.45      | 126.34   |
| 49  | LJ    | 3680 | PSU  | N1-C2-N3 | 4.78  | 120.55      | 115.13   |
| 47  | LH    | 2812 | A2M  | C5-C6-N6 | 4.78  | 133.83      | 123.43   |
| 48  | LI    | 3444 | PSU  | C4-N3-C2 | -4.78 | 119.46      | 126.34   |
| 48  | LI    | 3145 | PSU  | C4-N3-C2 | -4.77 | 119.46      | 126.34   |
| 1   | S1    | 2288 | MA6  | C5-C4-N3 | -4.77 | 120.53      | 126.75   |
| 47  | LH    | 2617 | PSU  | C4-N3-C2 | -4.77 | 119.47      | 126.34   |
| 48  | LI    | 3185 | PSU  | C4-N3-C2 | -4.76 | 119.47      | 126.34   |
| 45  | LF    | 1888 | A2M  | C5-C6-N6 | 4.76  | 133.79      | 123.43   |
| 47  | LH    | 2742 | PSU  | C4-N3-C2 | -4.76 | 119.48      | 126.34   |
| 47  | LH    | 2920 | A2M  | C5-C6-N6 | 4.76  | 133.78      | 123.43   |
| 48  | LI    | 3175 | PSU  | C4-N3-C2 | -4.75 | 119.49      | 126.34   |
| 42  | LC    | 594  | A2M  | C5-C6-N6 | 4.74  | 133.75      | 123.43   |
| 1   | S1    | 407  | A2M  | C5-C6-N6 | 4.74  | 133.74      | 123.43   |
| 42  | LC    | 480  | PSU  | C4-N3-C2 | -4.74 | 119.52      | 126.34   |
| 1   | S1    | 1096 | A2M  | C5-C6-N6 | 4.73  | 133.73      | 123.43   |
| 48  | LI    | 3542 | PSU  | C4-N3-C2 | -4.73 | 119.52      | 126.34   |
| 1   | S1    | 544  | PSU  | C4-N3-C2 | -4.73 | 119.53      | 126.34   |
| 47  | LH    | 2837 | PSU  | C4-N3-C2 | -4.73 | 119.53      | 126.34   |
| 1   | S1    | 1660 | PSU  | C4-N3-C2 | -4.73 | 119.53      | 126.34   |
| 47  | LH    | 2887 | A2M  | C5-C4-N3 | -4.72 | 120.59      | 126.75   |
| 47  | LH    | 2621 | PSU  | C4-N3-C2 | -4.72 | 119.53      | 126.34   |
| 48  | LI    | 3500 | A2M  | C5-C6-N6 | 4.72  | 133.71      | 123.43   |
| 44  | LE    | 1407 | PSU  | C4-N3-C2 | -4.72 | 119.54      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 49  | LJ    | 3591 | PSU  | C4-N3-C2 | -4.71 | 119.56      | 126.34   |
| 1   | S1    | 105  | PSU  | C4-N3-C2 | -4.70 | 119.56      | 126.34   |
| 1   | S1    | 1396 | PSU  | C4-N3-C2 | -4.70 | 119.57      | 126.34   |
| 40  | LA    | 16   | PSU  | C4-N3-C2 | -4.70 | 119.57      | 126.34   |
| 1   | S1    | 1393 | PSU  | C4-N3-C2 | -4.69 | 119.58      | 126.34   |
| 42  | LC    | 308  | PSU  | C4-N3-C2 | -4.68 | 119.59      | 126.34   |
| 44  | LE    | 931  | 1MA  | C2-N3-C4 | 4.68  | 121.62      | 112.41   |
| 48  | LI    | 2999 | PSU  | C4-N3-C2 | -4.68 | 119.60      | 126.34   |
| 44  | LE    | 1260 | PSU  | N1-C2-N3 | 4.68  | 120.43      | 115.13   |
| 42  | LC    | 498  | PSU  | C4-N3-C2 | -4.68 | 119.60      | 126.34   |
| 48  | LI    | 3510 | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |
| 48  | LI    | 3446 | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |
| 42  | LC    | 302  | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |
| 47  | LH    | 2899 | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |
| 48  | LI    | 3503 | PSU  | C4-N3-C2 | -4.67 | 119.62      | 126.34   |
| 52  | LM    | 3963 | PSU  | C4-N3-C2 | -4.67 | 119.62      | 126.34   |
| 47  | LH    | 2914 | PSU  | C4-N3-C2 | -4.66 | 119.62      | 126.34   |
| 47  | LH    | 2679 | PSU  | C4-N3-C2 | -4.64 | 119.65      | 126.34   |
| 1   | S1    | 1378 | PSU  | C4-N3-C2 | -4.64 | 119.65      | 126.34   |
| 48  | LI    | 3531 | PSU  | C4-N3-C2 | -4.64 | 119.65      | 126.34   |
| 1   | S1    | 533  | A2M  | C5-C6-N6 | 4.64  | 133.53      | 123.43   |
| 47  | LH    | 2330 | PSU  | C4-N3-C2 | -4.64 | 119.66      | 126.34   |
| 49  | LJ    | 3701 | PSU  | C4-N3-C2 | -4.64 | 119.66      | 126.34   |
| 48  | LI    | 3412 | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 49  | LJ    | 3697 | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 44  | LE    | 1365 | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 49  | LJ    | 3680 | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 45  | LF    | 1586 | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 1   | S1    | 544  | PSU  | N1-C2-N3 | 4.62  | 120.37      | 115.13   |
| 40  | LA    | 39   | A2M  | C5-C6-N6 | 4.62  | 133.49      | 123.43   |
| 48  | LI    | 3562 | PSU  | N1-C2-N3 | 4.62  | 120.36      | 115.13   |
| 47  | LH    | 2623 | PSU  | C4-N3-C2 | -4.62 | 119.68      | 126.34   |
| 44  | LE    | 1126 | PSU  | C4-N3-C2 | -4.62 | 119.68      | 126.34   |
| 45  | LF    | 1582 | PSU  | C4-N3-C2 | -4.62 | 119.68      | 126.34   |
| 45  | LF    | 1692 | PSU  | C4-N3-C2 | -4.62 | 119.69      | 126.34   |
| 51  | LL    | 3906 | A2M  | C5-C6-N6 | 4.61  | 133.47      | 123.43   |
| 48  | LI    | 3412 | PSU  | N1-C2-N3 | 4.61  | 120.36      | 115.13   |
| 47  | LH    | 2887 | A2M  | N9-C8-N7 | -4.61 | 107.61      | 113.91   |
| 40  | LA    | 68   | PSU  | C4-N3-C2 | -4.61 | 119.70      | 126.34   |
| 49  | LJ    | 3644 | PSU  | N1-C2-N3 | 4.60  | 120.35      | 115.13   |
| 1   | S1    | 2065 | PSU  | C4-N3-C2 | -4.60 | 119.71      | 126.34   |
| 47  | LH    | 2754 | PSU  | C4-N3-C2 | -4.60 | 119.71      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | S1    | 2129 | PSU  | C4-N3-C2  | -4.60 | 119.71      | 126.34   |
| 46  | LG    | 2119 | PSU  | N1-C2-N3  | 4.60  | 120.34      | 115.13   |
| 40  | LA    | 97   | A2M  | N9-C8-N7  | -4.59 | 107.63      | 113.91   |
| 1   | S1    | 280  | PSU  | C4-N3-C2  | -4.59 | 119.72      | 126.34   |
| 1   | S1    | 1591 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 1   | S1    | 2081 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 47  | LH    | 2874 | PSU  | N1-C2-N3  | 4.59  | 120.33      | 115.13   |
| 45  | LF    | 1859 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 47  | LH    | 2802 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 1   | S1    | 176  | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 2   | S2    | 37   | MIA  | N9-C8-N7  | -4.58 | 107.65      | 113.91   |
| 47  | LH    | 2636 | JMH  | C1'-N1-C2 | 4.58  | 124.72      | 116.99   |
| 44  | LE    | 1208 | OMG  | C2-N3-C4  | 4.58  | 120.45      | 112.30   |
| 46  | LG    | 2154 | PSU  | C4-N3-C2  | -4.58 | 119.75      | 126.34   |
| 47  | LH    | 2361 | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 47  | LH    | 2586 | PSU  | C4-N3-C2  | -4.56 | 119.76      | 126.34   |
| 1   | S1    | 465  | PSU  | N1-C2-N3  | 4.56  | 120.30      | 115.13   |
| 1   | S1    | 32   | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 1   | S1    | 1554 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 47  | LH    | 2624 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 48  | LI    | 3042 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 1   | S1    | 1960 | PSU  | C4-N3-C2  | -4.56 | 119.78      | 126.34   |
| 52  | LM    | 3953 | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 1   | S1    | 723  | A2M  | N9-C8-N7  | -4.55 | 107.69      | 113.91   |
| 47  | LH    | 2915 | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 42  | LC    | 480  | PSU  | N1-C2-N3  | 4.55  | 120.29      | 115.13   |
| 46  | LG    | 2125 | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 48  | LI    | 3562 | PSU  | C4-N3-C2  | -4.55 | 119.79      | 126.34   |
| 44  | LE    | 1208 | OMG  | N9-C4-N3  | 4.55  | 135.07      | 125.94   |
| 47  | LH    | 2623 | PSU  | N1-C2-N3  | 4.55  | 120.28      | 115.13   |
| 1   | S1    | 403  | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 48  | LI    | 3440 | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 1   | S1    | 1068 | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 47  | LH    | 2752 | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 45  | LF    | 1926 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 1   | S1    | 465  | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 44  | LE    | 1363 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 44  | LE    | 1198 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 47  | LH    | 2769 | A2M  | N9-C8-N7  | -4.53 | 107.72      | 113.91   |
| 1   | S1    | 2046 | A2M  | N9-C8-N7  | -4.53 | 107.72      | 113.91   |
| 47  | LH    | 2744 | A2M  | N9-C8-N7  | -4.52 | 107.73      | 113.91   |
| 44  | LE    | 1171 | PSU  | C4-N3-C2  | -4.52 | 119.83      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 47  | LH    | 2591 | PSU  | C4-N3-C2 | -4.52 | 119.83      | 126.34   |
| 47  | LH    | 2349 | A2M  | N9-C8-N7 | -4.51 | 107.75      | 113.91   |
| 1   | S1    | 89   | PSU  | C4-N3-C2 | -4.51 | 119.85      | 126.34   |
| 41  | LB    | 280  | PSU  | C4-N3-C2 | -4.51 | 119.85      | 126.34   |
| 45  | LF    | 1568 | PSU  | C4-N3-C2 | -4.50 | 119.85      | 126.34   |
| 48  | LI    | 2999 | PSU  | N1-C2-N3 | 4.50  | 120.23      | 115.13   |
| 48  | LI    | 3167 | PSU  | C4-N3-C2 | -4.50 | 119.86      | 126.34   |
| 44  | LE    | 1126 | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 1   | S1    | 649  | A2M  | N9-C8-N7 | -4.49 | 107.77      | 113.91   |
| 45  | LF    | 1502 | A2M  | N9-C8-N7 | -4.49 | 107.78      | 113.91   |
| 1   | S1    | 27   | PSU  | C4-N3-C2 | -4.49 | 119.88      | 126.34   |
| 49  | LJ    | 3680 | PSU  | C6-C5-C4 | 4.48  | 121.33      | 118.20   |
| 47  | LH    | 2361 | PSU  | N1-C2-N3 | 4.48  | 120.21      | 115.13   |
| 1   | S1    | 1393 | PSU  | N1-C2-N3 | 4.48  | 120.20      | 115.13   |
| 1   | S1    | 1715 | PSU  | C4-N3-C2 | -4.48 | 119.89      | 126.34   |
| 1   | S1    | 110  | A2M  | N9-C8-N7 | -4.48 | 107.79      | 113.91   |
| 1   | S1    | 1660 | PSU  | N1-C2-N3 | 4.48  | 120.20      | 115.13   |
| 1   | S1    | 2288 | MA6  | N9-C8-N7 | -4.47 | 107.80      | 113.91   |
| 48  | LI    | 3568 | PSU  | C4-N3-C2 | -4.47 | 119.90      | 126.34   |
| 45  | LF    | 1891 | A2M  | N9-C8-N7 | -4.47 | 107.81      | 113.91   |
| 51  | LL    | 3865 | PSU  | N1-C2-N3 | 4.47  | 120.19      | 115.13   |
| 47  | LH    | 2752 | PSU  | N1-C2-N3 | 4.46  | 120.19      | 115.13   |
| 44  | LE    | 1266 | PSU  | C4-N3-C2 | -4.45 | 119.92      | 126.34   |
| 42  | LC    | 302  | PSU  | N1-C2-N3 | 4.45  | 120.17      | 115.13   |
| 44  | LE    | 1023 | PSU  | N1-C2-N3 | 4.45  | 120.17      | 115.13   |
| 48  | LI    | 3451 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 44  | LE    | 935  | A2M  | N9-C8-N7 | -4.44 | 107.84      | 113.91   |
| 42  | LC    | 567  | PSU  | C4-N3-C2 | -4.44 | 119.95      | 126.34   |
| 48  | LI    | 3204 | PSU  | C4-N3-C2 | -4.43 | 119.95      | 126.34   |
| 47  | LH    | 2617 | PSU  | N1-C2-N3 | 4.43  | 120.15      | 115.13   |
| 49  | LJ    | 3697 | PSU  | N1-C2-N3 | 4.43  | 120.15      | 115.13   |
| 1   | S1    | 1371 | A2M  | N9-C8-N7 | -4.42 | 107.86      | 113.91   |
| 45  | LF    | 1738 | A2M  | N9-C8-N7 | -4.42 | 107.87      | 113.91   |
| 1   | S1    | 1378 | PSU  | N1-C2-N3 | 4.41  | 120.13      | 115.13   |
| 1   | S1    | 2081 | PSU  | N1-C2-N3 | 4.41  | 120.13      | 115.13   |
| 47  | LH    | 2809 | A2M  | N9-C8-N7 | -4.41 | 107.88      | 113.91   |
| 44  | LE    | 1023 | PSU  | C4-N3-C2 | -4.41 | 119.98      | 126.34   |
| 48  | LI    | 3510 | PSU  | N1-C2-N3 | 4.41  | 120.12      | 115.13   |
| 47  | LH    | 2754 | PSU  | N1-C2-N3 | 4.41  | 120.12      | 115.13   |
| 48  | LI    | 3145 | PSU  | N1-C2-N3 | 4.41  | 120.12      | 115.13   |
| 1   | S1    | 1711 | PSU  | N1-C2-N3 | 4.41  | 120.12      | 115.13   |
| 40  | LA    | 16   | PSU  | N1-C2-N3 | 4.41  | 120.12      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | LI    | 3531 | PSU  | N1-C2-N3    | 4.39  | 120.11      | 115.13   |
| 41  | LB    | 234  | PSU  | C4-N3-C2    | -4.39 | 120.01      | 126.34   |
| 44  | LE    | 1235 | PSU  | C4-N3-C2    | -4.39 | 120.01      | 126.34   |
| 48  | LI    | 3175 | PSU  | N1-C2-N3    | 4.39  | 120.11      | 115.13   |
| 49  | LJ    | 3701 | PSU  | N1-C2-N3    | 4.39  | 120.10      | 115.13   |
| 1   | S1    | 40   | A2M  | N9-C8-N7    | -4.39 | 107.91      | 113.91   |
| 48  | LI    | 3206 | PSU  | N1-C2-N3    | 4.38  | 120.09      | 115.13   |
| 46  | LG    | 2171 | PSU  | C4-N3-C2    | -4.38 | 120.03      | 126.34   |
| 45  | LF    | 1586 | PSU  | N1-C2-N3    | 4.38  | 120.09      | 115.13   |
| 42  | LC    | 421  | PSU  | C4-N3-C2    | -4.38 | 120.03      | 126.34   |
| 47  | LH    | 2914 | PSU  | N1-C2-N3    | 4.38  | 120.09      | 115.13   |
| 1   | S1    | 2305 | PSU  | C4-N3-C2    | -4.37 | 120.04      | 126.34   |
| 1   | S1    | 640  | PSU  | C4-N3-C2    | -4.37 | 120.05      | 126.34   |
| 2   | S2    | 37   | MIA  | C15-C14-C13 | -4.37 | 110.03      | 122.65   |
| 45  | LF    | 1929 | A2M  | N9-C8-N7    | -4.36 | 107.95      | 113.91   |
| 1   | S1    | 1096 | A2M  | N9-C8-N7    | -4.36 | 107.95      | 113.91   |
| 1   | S1    | 1592 | PSU  | N1-C2-N3    | 4.35  | 120.06      | 115.13   |
| 46  | LG    | 2125 | PSU  | N1-C2-N3    | 4.35  | 120.06      | 115.13   |
| 1   | S1    | 1711 | PSU  | C4-N3-C2    | -4.35 | 120.08      | 126.34   |
| 44  | LE    | 1118 | PSU  | N1-C2-N3    | 4.34  | 120.05      | 115.13   |
| 47  | LH    | 2899 | PSU  | N1-C2-N3    | 4.34  | 120.05      | 115.13   |
| 48  | LI    | 3332 | PSU  | N1-C2-N3    | 4.34  | 120.05      | 115.13   |
| 1   | S1    | 2065 | PSU  | N1-C2-N3    | 4.34  | 120.04      | 115.13   |
| 44  | LE    | 1363 | PSU  | N1-C2-N3    | 4.32  | 120.03      | 115.13   |
| 49  | LJ    | 3591 | PSU  | N1-C2-N3    | 4.32  | 120.03      | 115.13   |
| 1   | S1    | 89   | PSU  | N1-C2-N3    | 4.32  | 120.03      | 115.13   |
| 1   | S1    | 1396 | PSU  | N1-C2-N3    | 4.32  | 120.03      | 115.13   |
| 44  | LE    | 1266 | PSU  | N1-C2-N3    | 4.32  | 120.03      | 115.13   |
| 44  | LE    | 1075 | PSU  | C4-N3-C2    | -4.32 | 120.11      | 126.34   |
| 48  | LI    | 3503 | PSU  | N1-C2-N3    | 4.32  | 120.02      | 115.13   |
| 1   | S1    | 1624 | PSU  | C4-N3-C2    | -4.32 | 120.12      | 126.34   |
| 1   | S1    | 1960 | PSU  | N1-C2-N3    | 4.32  | 120.02      | 115.13   |
| 47  | LH    | 2768 | A2M  | N9-C8-N7    | -4.31 | 108.01      | 113.91   |
| 44  | LE    | 1198 | PSU  | N1-C2-N3    | 4.31  | 120.02      | 115.13   |
| 42  | LC    | 308  | PSU  | N1-C2-N3    | 4.30  | 120.00      | 115.13   |
| 2   | S2    | 37   | MIA  | C16-C14-C13 | -4.30 | 110.22      | 122.65   |
| 47  | LH    | 2842 | PSU  | C4-N3-C2    | -4.30 | 120.15      | 126.34   |
| 1   | S1    | 2116 | PSU  | C4-N3-C2    | -4.30 | 120.15      | 126.34   |
| 48  | LI    | 3533 | A2M  | N9-C8-N7    | -4.29 | 108.05      | 113.91   |
| 47  | LH    | 2358 | A2M  | N9-C8-N7    | -4.29 | 108.05      | 113.91   |
| 48  | LI    | 3542 | PSU  | N1-C2-N3    | 4.29  | 119.99      | 115.13   |
| 48  | LI    | 3444 | PSU  | N1-C2-N3    | 4.28  | 119.98      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 47  | LH    | 2708 | A2M  | N9-C8-N7 | -4.28 | 108.06      | 113.91   |
| 45  | LF    | 1582 | PSU  | N1-C2-N3 | 4.28  | 119.98      | 115.13   |
| 1   | S1    | 1063 | A2M  | N9-C8-N7 | -4.28 | 108.06      | 113.91   |
| 1   | S1    | 407  | A2M  | N3-C4-N9 | 4.27  | 134.13      | 127.08   |
| 1   | S1    | 280  | PSU  | N1-C2-N3 | 4.27  | 119.97      | 115.13   |
| 47  | LH    | 2849 | A2M  | N9-C8-N7 | -4.27 | 108.07      | 113.91   |
| 48  | LI    | 3367 | A2M  | N9-C8-N7 | -4.27 | 108.07      | 113.91   |
| 1   | S1    | 2131 | PSU  | N1-C2-N3 | 4.27  | 119.97      | 115.13   |
| 44  | LE    | 1039 | A2M  | N9-C8-N7 | -4.27 | 108.08      | 113.91   |
| 1   | S1    | 1900 | A2M  | N9-C8-N7 | -4.27 | 108.08      | 113.91   |
| 1   | S1    | 176  | PSU  | N1-C2-N3 | 4.26  | 119.96      | 115.13   |
| 48  | LI    | 3185 | PSU  | N1-C2-N3 | 4.26  | 119.96      | 115.13   |
| 44  | LE    | 1106 | A2M  | N9-C8-N7 | -4.26 | 108.08      | 113.91   |
| 44  | LE    | 1075 | PSU  | N1-C2-N3 | 4.26  | 119.95      | 115.13   |
| 42  | LC    | 567  | PSU  | N1-C2-N3 | 4.26  | 119.95      | 115.13   |
| 1   | S1    | 2287 | MA6  | N9-C8-N7 | -4.25 | 108.10      | 113.91   |
| 44  | LE    | 1407 | PSU  | N1-C2-N3 | 4.24  | 119.94      | 115.13   |
| 1   | S1    | 105  | PSU  | N1-C2-N3 | 4.24  | 119.94      | 115.13   |
| 42  | LC    | 498  | PSU  | N1-C2-N3 | 4.24  | 119.94      | 115.13   |
| 47  | LH    | 2679 | PSU  | N1-C2-N3 | 4.24  | 119.93      | 115.13   |
| 47  | LH    | 2642 | PSU  | N1-C2-N3 | 4.23  | 119.93      | 115.13   |
| 51  | LL    | 3906 | A2M  | N9-C8-N7 | -4.22 | 108.14      | 113.91   |
| 48  | LI    | 3440 | PSU  | N1-C2-N3 | 4.22  | 119.91      | 115.13   |
| 45  | LF    | 1692 | PSU  | N1-C2-N3 | 4.22  | 119.91      | 115.13   |
| 1   | S1    | 2101 | PSU  | C4-N3-C2 | -4.22 | 120.27      | 126.34   |
| 44  | LE    | 1184 | PSU  | C4-N3-C2 | -4.21 | 120.27      | 126.34   |
| 46  | LG    | 2154 | PSU  | N1-C2-N3 | 4.21  | 119.90      | 115.13   |
| 1   | S1    | 32   | PSU  | N1-C2-N3 | 4.21  | 119.90      | 115.13   |
| 1   | S1    | 27   | PSU  | N1-C2-N3 | 4.21  | 119.90      | 115.13   |
| 44  | LE    | 1365 | PSU  | N1-C2-N3 | 4.21  | 119.90      | 115.13   |
| 53  | LN    | 3969 | PSU  | C4-N3-C2 | -4.21 | 120.28      | 126.34   |
| 48  | LI    | 3042 | PSU  | N1-C2-N3 | 4.20  | 119.89      | 115.13   |
| 1   | S1    | 1715 | PSU  | N1-C2-N3 | 4.20  | 119.89      | 115.13   |
| 45  | LF    | 1859 | PSU  | N1-C2-N3 | 4.20  | 119.89      | 115.13   |
| 47  | LH    | 2920 | A2M  | N9-C8-N7 | -4.19 | 108.18      | 113.91   |
| 1   | S1    | 28   | A2M  | N9-C8-N7 | -4.19 | 108.19      | 113.91   |
| 45  | LF    | 1876 | PSU  | N1-C2-N3 | 4.18  | 119.87      | 115.13   |
| 45  | LF    | 1888 | A2M  | N9-C8-N7 | -4.18 | 108.19      | 113.91   |
| 47  | LH    | 2915 | PSU  | N1-C2-N3 | 4.18  | 119.87      | 115.13   |
| 41  | LB    | 183  | A2M  | N9-C8-N7 | -4.18 | 108.20      | 113.91   |
| 47  | LH    | 2837 | PSU  | N1-C2-N3 | 4.18  | 119.86      | 115.13   |
| 48  | LI    | 3167 | PSU  | N1-C2-N3 | 4.18  | 119.86      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 41  | LB    | 280  | PSU  | N1-C2-N3   | 4.17  | 119.86      | 115.13   |
| 52  | LM    | 3953 | PSU  | N1-C2-N3   | 4.17  | 119.85      | 115.13   |
| 46  | LG    | 2005 | A2M  | N9-C8-N7   | -4.16 | 108.22      | 113.91   |
| 47  | LH    | 2769 | A2M  | C2'-C1'-N9 | -4.16 | 106.53      | 113.53   |
| 48  | LI    | 3315 | A2M  | N9-C8-N7   | -4.14 | 108.25      | 113.91   |
| 44  | LE    | 1204 | A2M  | N9-C8-N7   | -4.14 | 108.25      | 113.91   |
| 47  | LH    | 2591 | PSU  | N1-C2-N3   | 4.14  | 119.82      | 115.13   |
| 48  | LI    | 3204 | PSU  | N1-C2-N3   | 4.14  | 119.82      | 115.13   |
| 44  | LE    | 1184 | PSU  | N1-C2-N3   | 4.14  | 119.81      | 115.13   |
| 41  | LB    | 281  | PSU  | C4-N3-C2   | -4.13 | 120.39      | 126.34   |
| 1   | S1    | 2129 | PSU  | N1-C2-N3   | 4.12  | 119.80      | 115.13   |
| 45  | LF    | 1926 | PSU  | N1-C2-N3   | 4.12  | 119.80      | 115.13   |
| 48  | LI    | 3348 | A2M  | N9-C8-N7   | -4.12 | 108.28      | 113.91   |
| 1   | S1    | 1068 | PSU  | N1-C2-N3   | 4.12  | 119.80      | 115.13   |
| 1   | S1    | 2180 | A2M  | C2-N3-C4   | 4.11  | 121.47      | 111.75   |
| 44  | LE    | 1235 | PSU  | N1-C2-N3   | 4.11  | 119.79      | 115.13   |
| 52  | LM    | 3963 | PSU  | N1-C2-N3   | 4.11  | 119.79      | 115.13   |
| 45  | LF    | 1815 | A2M  | N9-C8-N7   | -4.10 | 108.31      | 113.91   |
| 41  | LB    | 281  | PSU  | N1-C2-N3   | 4.09  | 119.77      | 115.13   |
| 1   | S1    | 2305 | PSU  | N1-C2-N3   | 4.09  | 119.76      | 115.13   |
| 48  | LI    | 3568 | PSU  | N1-C2-N3   | 4.09  | 119.76      | 115.13   |
| 45  | LF    | 1568 | PSU  | N1-C2-N3   | 4.08  | 119.75      | 115.13   |
| 41  | LB    | 234  | PSU  | N1-C2-N3   | 4.07  | 119.74      | 115.13   |
| 47  | LH    | 2842 | PSU  | N1-C2-N3   | 4.07  | 119.74      | 115.13   |
| 44  | LE    | 1260 | PSU  | C6-C5-C4   | 4.07  | 121.04      | 118.20   |
| 44  | LE    | 1171 | PSU  | N1-C2-N3   | 4.07  | 119.74      | 115.13   |
| 47  | LH    | 2742 | PSU  | N1-C2-N3   | 4.07  | 119.74      | 115.13   |
| 42  | LC    | 594  | A2M  | N9-C8-N7   | -4.07 | 108.35      | 113.91   |
| 47  | LH    | 2814 | A2M  | N9-C8-N7   | -4.05 | 108.37      | 113.91   |
| 48  | LI    | 3446 | PSU  | N1-C2-N3   | 4.05  | 119.72      | 115.13   |
| 1   | S1    | 407  | A2M  | C2-N3-C4   | 4.04  | 121.29      | 111.75   |
| 1   | S1    | 1624 | PSU  | N1-C2-N3   | 4.03  | 119.70      | 115.13   |
| 46  | LG    | 2171 | PSU  | N1-C2-N3   | 4.02  | 119.69      | 115.13   |
| 47  | LH    | 2586 | PSU  | N1-C2-N3   | 4.02  | 119.68      | 115.13   |
| 1   | S1    | 645  | A2M  | N9-C8-N7   | -4.00 | 108.44      | 113.91   |
| 48  | LI    | 3521 | A2M  | N9-C8-N7   | -3.99 | 108.46      | 113.91   |
| 48  | LI    | 3500 | A2M  | N9-C8-N7   | -3.97 | 108.48      | 113.91   |
| 46  | LG    | 2022 | A2M  | N9-C8-N7   | -3.97 | 108.48      | 113.91   |
| 47  | LH    | 2330 | PSU  | N1-C2-N3   | 3.96  | 119.61      | 115.13   |
| 44  | LE    | 1121 | A2M  | N9-C8-N7   | -3.95 | 108.51      | 113.91   |
| 47  | LH    | 2802 | PSU  | N1-C2-N3   | 3.93  | 119.59      | 115.13   |
| 1   | S1    | 2116 | PSU  | N1-C2-N3   | 3.92  | 119.57      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 42  | LC    | 421  | PSU  | N1-C2-N3 | 3.92  | 119.57      | 115.13   |
| 1   | S1    | 2101 | PSU  | N1-C2-N3 | 3.91  | 119.56      | 115.13   |
| 53  | LN    | 3969 | PSU  | N1-C2-N3 | 3.90  | 119.55      | 115.13   |
| 1   | S1    | 407  | A2M  | N9-C8-N7 | -3.90 | 108.58      | 113.91   |
| 47  | LH    | 2621 | PSU  | N1-C2-N3 | 3.89  | 119.53      | 115.13   |
| 1   | S1    | 1591 | PSU  | N1-C2-N3 | 3.87  | 119.51      | 115.13   |
| 46  | LG    | 2005 | A2M  | C2-N3-C4 | 3.85  | 120.86      | 111.75   |
| 1   | S1    | 2287 | MA6  | C4-C5-C6 | 3.84  | 120.18      | 115.88   |
| 1   | S1    | 565  | A2M  | N9-C8-N7 | -3.84 | 108.67      | 113.91   |
| 40  | LA    | 68   | PSU  | C6-C5-C4 | 3.84  | 120.88      | 118.20   |
| 1   | S1    | 1554 | PSU  | N1-C2-N3 | 3.83  | 119.47      | 115.13   |
| 40  | LA    | 39   | A2M  | N9-C8-N7 | -3.83 | 108.68      | 113.91   |
| 45  | LF    | 1891 | A2M  | C2-N3-C4 | 3.81  | 120.76      | 111.75   |
| 1   | S1    | 640  | PSU  | N1-C2-N3 | 3.81  | 119.44      | 115.13   |
| 48  | LI    | 3214 | 6MZ  | C2-N3-C4 | 3.80  | 120.73      | 111.75   |
| 1   | S1    | 645  | A2M  | C2-N3-C4 | 3.80  | 120.72      | 111.75   |
| 1   | S1    | 403  | PSU  | N1-C2-N3 | 3.79  | 119.43      | 115.13   |
| 1   | S1    | 121  | PSU  | C4-N3-C2 | -3.79 | 120.88      | 126.34   |
| 1   | S1    | 1601 | B8N  | N3-C2-N1 | 3.79  | 122.11      | 116.76   |
| 47  | LH    | 2812 | A2M  | C2-N3-C4 | 3.76  | 120.64      | 111.75   |
| 44  | LE    | 935  | A2M  | C2-N3-C4 | 3.75  | 120.62      | 111.75   |
| 1   | S1    | 2288 | MA6  | C2-N1-C6 | 3.74  | 120.59      | 111.75   |
| 1   | S1    | 1371 | A2M  | C2-N3-C4 | 3.74  | 120.59      | 111.75   |
| 44  | LE    | 1023 | PSU  | C6-N1-C2 | -3.73 | 118.87      | 122.68   |
| 47  | LH    | 2624 | PSU  | N1-C2-N3 | 3.73  | 119.35      | 115.13   |
| 47  | LH    | 2358 | A2M  | C2-N3-C4 | 3.72  | 120.55      | 111.75   |
| 44  | LE    | 1204 | A2M  | C2-N3-C4 | 3.71  | 120.52      | 111.75   |
| 1   | S1    | 533  | A2M  | N9-C8-N7 | -3.71 | 108.84      | 113.91   |
| 1   | S1    | 1549 | A2M  | N9-C8-N7 | -3.70 | 108.85      | 113.91   |
| 1   | S1    | 1711 | PSU  | C6-N1-C2 | -3.70 | 118.90      | 122.68   |
| 48  | LI    | 3315 | A2M  | C2-N3-C4 | 3.69  | 120.46      | 111.75   |
| 47  | LH    | 2812 | A2M  | N9-C8-N7 | -3.68 | 108.88      | 113.91   |
| 1   | S1    | 645  | A2M  | N3-C4-N9 | 3.68  | 133.15      | 127.08   |
| 1   | S1    | 2046 | A2M  | C2-N3-C4 | 3.68  | 120.44      | 111.75   |
| 47  | LH    | 2920 | A2M  | C2-N3-C4 | 3.66  | 120.40      | 111.75   |
| 44  | LE    | 1222 | OMU  | N3-C2-N1 | 3.66  | 119.75      | 114.89   |
| 45  | LF    | 1738 | A2M  | C2-N3-C4 | 3.65  | 120.37      | 111.75   |
| 40  | LA    | 39   | A2M  | C2-N3-C4 | 3.63  | 120.33      | 111.75   |
| 47  | LH    | 2349 | A2M  | C2-N3-C4 | 3.63  | 120.32      | 111.75   |
| 2   | S2    | 37   | MIA  | C4-C5-C6 | 3.62  | 119.61      | 116.81   |
| 47  | LH    | 2809 | A2M  | C2-N3-C4 | 3.60  | 120.26      | 111.75   |
| 1   | S1    | 1096 | A2M  | C2-N3-C4 | 3.60  | 120.26      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 47  | LH    | 2769 | A2M  | C2-N3-C4 | 3.60  | 120.26      | 111.75   |
| 45  | LF    | 1502 | A2M  | C2-N3-C4 | 3.60  | 120.26      | 111.75   |
| 44  | LE    | 1121 | A2M  | C2-N3-C4 | 3.59  | 120.24      | 111.75   |
| 44  | LE    | 1198 | PSU  | C6-C5-C4 | 3.59  | 120.71      | 118.20   |
| 44  | LE    | 1266 | PSU  | C6-C5-C4 | 3.59  | 120.71      | 118.20   |
| 1   | S1    | 28   | A2M  | C2-N3-C4 | 3.59  | 120.23      | 111.75   |
| 2   | S2    | 37   | MIA  | N3-C2-N1 | -3.59 | 120.37      | 126.95   |
| 45  | LF    | 1888 | A2M  | C2-N3-C4 | 3.59  | 120.22      | 111.75   |
| 1   | S1    | 40   | A2M  | C2-N3-C4 | 3.58  | 120.22      | 111.75   |
| 47  | LH    | 2920 | A2M  | N3-C4-N9 | 3.58  | 132.99      | 127.08   |
| 44  | LE    | 1235 | PSU  | C6-N1-C2 | -3.58 | 119.02      | 122.68   |
| 1   | S1    | 1549 | A2M  | C2-N3-C4 | 3.58  | 120.20      | 111.75   |
| 44  | LE    | 1222 | OMU  | C4-N3-C2 | -3.57 | 121.87      | 126.58   |
| 47  | LH    | 2754 | PSU  | C6-C5-C4 | 3.57  | 120.69      | 118.20   |
| 44  | LE    | 1039 | A2M  | C2-N3-C4 | 3.57  | 120.18      | 111.75   |
| 2   | S2    | 37   | MIA  | N3-C4-N9 | 3.57  | 131.94      | 126.99   |
| 44  | LE    | 1184 | PSU  | C6-N1-C2 | -3.57 | 119.03      | 122.68   |
| 48  | LI    | 2999 | PSU  | C6-C5-C4 | 3.56  | 120.69      | 118.20   |
| 49  | LJ    | 3680 | PSU  | C6-N1-C2 | -3.56 | 119.04      | 122.68   |
| 48  | LI    | 3562 | PSU  | C6-N1-C2 | -3.56 | 119.05      | 122.68   |
| 1   | S1    | 2288 | MA6  | C2-N3-C4 | 3.55  | 120.15      | 111.75   |
| 47  | LH    | 2744 | A2M  | C2-N3-C4 | 3.55  | 120.14      | 111.75   |
| 1   | S1    | 1096 | A2M  | N3-C4-N9 | 3.55  | 132.93      | 127.08   |
| 1   | S1    | 110  | A2M  | C2-N3-C4 | 3.55  | 120.14      | 111.75   |
| 46  | LG    | 2022 | A2M  | C2-N3-C4 | 3.55  | 120.13      | 111.75   |
| 48  | LI    | 3367 | A2M  | C2-N3-C4 | 3.54  | 120.12      | 111.75   |
| 48  | LI    | 3503 | PSU  | C6-C5-C4 | 3.54  | 120.67      | 118.20   |
| 1   | S1    | 1900 | A2M  | C2-N3-C4 | 3.54  | 120.12      | 111.75   |
| 45  | LF    | 1929 | A2M  | C2-N3-C4 | 3.54  | 120.10      | 111.75   |
| 47  | LH    | 2768 | A2M  | C2-N3-C4 | 3.54  | 120.10      | 111.75   |
| 41  | LB    | 183  | A2M  | C2-N3-C4 | 3.53  | 120.10      | 111.75   |
| 1   | S1    | 2287 | MA6  | C2-N3-C4 | 3.53  | 120.08      | 111.75   |
| 48  | LI    | 3444 | PSU  | C6-C5-C4 | 3.52  | 120.66      | 118.20   |
| 48  | LI    | 3348 | A2M  | C2-N3-C4 | 3.52  | 120.07      | 111.75   |
| 1   | S1    | 2287 | MA6  | C2-N1-C6 | 3.52  | 120.06      | 111.75   |
| 1   | S1    | 565  | A2M  | C2-N3-C4 | 3.51  | 120.04      | 111.75   |
| 48  | LI    | 3500 | A2M  | C2-N3-C4 | 3.51  | 120.03      | 111.75   |
| 1   | S1    | 723  | A2M  | C2-N3-C4 | 3.50  | 120.03      | 111.75   |
| 47  | LH    | 2887 | A2M  | C2-N3-C4 | 3.50  | 120.02      | 111.75   |
| 40  | LA    | 68   | PSU  | C6-N1-C2 | -3.50 | 119.11      | 122.68   |
| 47  | LH    | 2623 | PSU  | C6-N1-C2 | -3.50 | 119.11      | 122.68   |
| 45  | LF    | 1815 | A2M  | C2-N3-C4 | 3.50  | 120.01      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | S1    | 2180 | A2M  | C2'-C1'-N9  | -3.50 | 107.64      | 113.53   |
| 1   | S1    | 649  | A2M  | C2-N3-C4    | 3.49  | 120.00      | 111.75   |
| 1   | S1    | 2081 | PSU  | C6-C5-C4    | 3.49  | 120.64      | 118.20   |
| 44  | LE    | 1204 | A2M  | N3-C4-N9    | 3.49  | 132.83      | 127.08   |
| 44  | LE    | 1106 | A2M  | C4'-O4'-C1' | -3.49 | 101.78      | 109.47   |
| 47  | LH    | 2708 | A2M  | C2-N3-C4    | 3.49  | 119.99      | 111.75   |
| 48  | LI    | 3518 | 5MC  | C5-C4-N3    | 3.48  | 125.43      | 121.67   |
| 47  | LH    | 2361 | PSU  | C6-N1-C2    | -3.48 | 119.12      | 122.68   |
| 1   | S1    | 1396 | PSU  | C6-C5-C4    | 3.48  | 120.63      | 118.20   |
| 45  | LF    | 1891 | A2M  | N3-C4-N9    | 3.48  | 132.81      | 127.08   |
| 44  | LE    | 1171 | PSU  | C6-C5-C4    | 3.48  | 120.63      | 118.20   |
| 40  | LA    | 39   | A2M  | N3-C4-N9    | 3.47  | 132.81      | 127.08   |
| 51  | LL    | 3906 | A2M  | C2-N3-C4    | 3.47  | 119.95      | 111.75   |
| 47  | LH    | 2904 | B8H  | O2-C2-N1    | -3.46 | 118.97      | 122.87   |
| 40  | LA    | 97   | A2M  | C2-N3-C4    | 3.46  | 119.93      | 111.75   |
| 48  | LI    | 3533 | A2M  | C2-N3-C4    | 3.46  | 119.93      | 111.75   |
| 1   | S1    | 465  | PSU  | C6-C5-C4    | 3.46  | 120.62      | 118.20   |
| 51  | LL    | 3906 | A2M  | N3-C4-N9    | 3.45  | 132.78      | 127.08   |
| 47  | LH    | 2617 | PSU  | C6-C5-C4    | 3.45  | 120.61      | 118.20   |
| 47  | LH    | 2842 | PSU  | C6-N1-C2    | -3.43 | 119.17      | 122.68   |
| 46  | LG    | 2022 | A2M  | N3-C4-N9    | 3.43  | 132.74      | 127.08   |
| 48  | LI    | 3412 | PSU  | C6-N1-C2    | -3.43 | 119.18      | 122.68   |
| 49  | LJ    | 3644 | PSU  | C6-C5-C4    | 3.43  | 120.59      | 118.20   |
| 48  | LI    | 3521 | A2M  | C2-N3-C4    | 3.42  | 119.84      | 111.75   |
| 46  | LG    | 2171 | PSU  | C6-N1-C2    | -3.42 | 119.19      | 122.68   |
| 47  | LH    | 2752 | PSU  | C6-N1-C2    | -3.41 | 119.19      | 122.68   |
| 42  | LC    | 594  | A2M  | C2-N3-C4    | 3.41  | 119.81      | 111.75   |
| 1   | S1    | 121  | PSU  | O2-C2-N1    | -3.41 | 119.03      | 122.79   |
| 47  | LH    | 2766 | 5MC  | C5-C4-N3    | 3.41  | 125.35      | 121.67   |
| 48  | LI    | 3451 | PSU  | C6-C5-C4    | 3.40  | 120.58      | 118.20   |
| 51  | LL    | 3865 | PSU  | C6-C5-C4    | 3.40  | 120.58      | 118.20   |
| 1   | S1    | 465  | PSU  | C6-N1-C2    | -3.39 | 119.21      | 122.68   |
| 1   | S1    | 2287 | MA6  | N3-C4-N9    | 3.39  | 132.66      | 127.08   |
| 47  | LH    | 2769 | A2M  | N3-C4-N9    | 3.38  | 132.65      | 127.08   |
| 48  | LI    | 3145 | PSU  | C6-C5-C4    | 3.38  | 120.56      | 118.20   |
| 1   | S1    | 533  | A2M  | C2-N3-C4    | 3.37  | 119.72      | 111.75   |
| 1   | S1    | 1711 | PSU  | C6-C5-C4    | 3.37  | 120.55      | 118.20   |
| 1   | S1    | 1063 | A2M  | C2-N3-C4    | 3.37  | 119.70      | 111.75   |
| 47  | LH    | 2849 | A2M  | C2-N3-C4    | 3.36  | 119.69      | 111.75   |
| 47  | LH    | 2814 | A2M  | C2-N3-C4    | 3.35  | 119.67      | 111.75   |
| 41  | LB    | 281  | PSU  | C6-N1-C2    | -3.35 | 119.26      | 122.68   |
| 45  | LF    | 1888 | A2M  | N3-C4-N9    | 3.35  | 132.60      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 49  | LJ    | 3701 | PSU  | C6-N1-C2 | -3.34 | 119.26      | 122.68   |
| 44  | LE    | 1106 | A2M  | C2-N3-C4 | 3.34  | 119.64      | 111.75   |
| 42  | LC    | 480  | PSU  | C6-C5-C4 | 3.34  | 120.53      | 118.20   |
| 44  | LE    | 931  | 1MA  | N9-C4-N3 | 3.34  | 134.72      | 126.94   |
| 1   | S1    | 1960 | PSU  | C6-N1-C2 | -3.34 | 119.27      | 122.68   |
| 1   | S1    | 1900 | A2M  | N3-C4-N9 | 3.34  | 132.58      | 127.08   |
| 1   | S1    | 2101 | PSU  | C6-N1-C2 | -3.34 | 119.27      | 122.68   |
| 45  | LF    | 1815 | A2M  | N3-C4-N9 | 3.33  | 132.58      | 127.08   |
| 1   | S1    | 1393 | PSU  | C6-N1-C2 | -3.33 | 119.28      | 122.68   |
| 44  | LE    | 1121 | A2M  | N3-C4-N9 | 3.33  | 132.56      | 127.08   |
| 1   | S1    | 32   | PSU  | C6-N1-C2 | -3.32 | 119.29      | 122.68   |
| 47  | LH    | 2812 | A2M  | N3-C4-N9 | 3.32  | 132.55      | 127.08   |
| 47  | LH    | 2746 | PSU  | C6-N1-C2 | -3.32 | 119.29      | 122.68   |
| 47  | LH    | 2349 | A2M  | N3-C4-N9 | 3.32  | 132.55      | 127.08   |
| 44  | LE    | 1266 | PSU  | C6-N1-C2 | -3.32 | 119.29      | 122.68   |
| 1   | S1    | 1371 | A2M  | N3-C4-N9 | 3.31  | 132.53      | 127.08   |
| 42  | LC    | 594  | A2M  | N3-C4-N9 | 3.31  | 132.53      | 127.08   |
| 42  | LC    | 421  | PSU  | C6-N1-C2 | -3.31 | 119.30      | 122.68   |
| 44  | LE    | 935  | A2M  | N3-C4-N9 | 3.31  | 132.53      | 127.08   |
| 44  | LE    | 1222 | OMU  | C5-C4-N3 | 3.30  | 119.77      | 114.84   |
| 48  | LI    | 3562 | PSU  | C6-C5-C4 | 3.29  | 120.50      | 118.20   |
| 1   | S1    | 1371 | A2M  | C5-N7-C8 | 3.29  | 108.19      | 103.51   |
| 1   | S1    | 2046 | A2M  | C5-N7-C8 | 3.29  | 108.18      | 103.51   |
| 1   | S1    | 2065 | PSU  | C6-N1-C2 | -3.29 | 119.32      | 122.68   |
| 1   | S1    | 110  | A2M  | C5-N7-C8 | 3.29  | 108.18      | 103.51   |
| 48  | LI    | 3315 | A2M  | N3-C4-N9 | 3.28  | 132.50      | 127.08   |
| 47  | LH    | 2754 | PSU  | C6-N1-C2 | -3.28 | 119.33      | 122.68   |
| 48  | LI    | 3531 | PSU  | C6-C5-C4 | 3.28  | 120.49      | 118.20   |
| 45  | LF    | 1738 | A2M  | N3-C4-N9 | 3.27  | 132.48      | 127.08   |
| 1   | S1    | 1660 | PSU  | C6-N1-C2 | -3.27 | 119.34      | 122.68   |
| 45  | LF    | 1586 | PSU  | C6-C5-C4 | 3.27  | 120.49      | 118.20   |
| 1   | S1    | 1063 | A2M  | N3-C4-N9 | 3.27  | 132.47      | 127.08   |
| 47  | LH    | 2768 | A2M  | C5-N7-C8 | 3.27  | 108.16      | 103.51   |
| 1   | S1    | 533  | A2M  | N3-C4-N9 | 3.27  | 132.47      | 127.08   |
| 45  | LF    | 1929 | A2M  | N3-C4-N9 | 3.27  | 132.47      | 127.08   |
| 1   | S1    | 544  | PSU  | C6-N1-C2 | -3.26 | 119.35      | 122.68   |
| 44  | LE    | 1363 | PSU  | C6-N1-C2 | -3.26 | 119.35      | 122.68   |
| 47  | LH    | 2768 | A2M  | N3-C4-N9 | 3.26  | 132.45      | 127.08   |
| 48  | LI    | 3167 | PSU  | C6-N1-C2 | -3.26 | 119.35      | 122.68   |
| 48  | LI    | 3042 | PSU  | C6-C5-C4 | 3.25  | 120.47      | 118.20   |
| 48  | LI    | 3531 | PSU  | C6-N1-C2 | -3.25 | 119.36      | 122.68   |
| 48  | LI    | 3175 | PSU  | C6-C5-C4 | 3.25  | 120.47      | 118.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | LH    | 2769 | A2M  | C5-N7-C8    | 3.25  | 108.12      | 103.51   |
| 1   | S1    | 2288 | MA6  | C4-C5-C6    | 3.24  | 119.51      | 115.88   |
| 42  | LC    | 302  | PSU  | C6-C5-C4    | 3.24  | 120.46      | 118.20   |
| 1   | S1    | 682  | OMU  | CM2-O2'-C2' | -3.23 | 106.04      | 114.52   |
| 45  | LF    | 1586 | PSU  | C6-N1-C2    | -3.23 | 119.38      | 122.68   |
| 47  | LH    | 2349 | A2M  | C5-N7-C8    | 3.23  | 108.10      | 103.51   |
| 44  | LE    | 1260 | PSU  | C6-N1-C2    | -3.23 | 119.38      | 122.68   |
| 1   | S1    | 2180 | A2M  | N3-C2-N1    | -3.23 | 123.55      | 128.60   |
| 1   | S1    | 89   | PSU  | C6-N1-C2    | -3.23 | 119.38      | 122.68   |
| 42  | LC    | 480  | PSU  | C6-N1-C2    | -3.22 | 119.39      | 122.68   |
| 1   | S1    | 1396 | PSU  | C6-N1-C2    | -3.22 | 119.39      | 122.68   |
| 44  | LE    | 1204 | A2M  | C5-N7-C8    | 3.22  | 108.08      | 103.51   |
| 42  | LC    | 308  | PSU  | C6-C5-C4    | 3.22  | 120.45      | 118.20   |
| 47  | LH    | 2899 | PSU  | C6-N1-C2    | -3.22 | 119.39      | 122.68   |
| 44  | LE    | 1106 | A2M  | C2'-C1'-N9  | -3.21 | 108.12      | 113.53   |
| 47  | LH    | 2708 | A2M  | N3-C4-N9    | 3.21  | 132.38      | 127.08   |
| 46  | LG    | 2125 | PSU  | C6-C5-C4    | 3.20  | 120.44      | 118.20   |
| 1   | S1    | 645  | A2M  | C4'-O4'-C1' | -3.20 | 102.41      | 109.47   |
| 1   | S1    | 40   | A2M  | C5-N7-C8    | 3.19  | 108.05      | 103.51   |
| 1   | S1    | 1624 | PSU  | C6-N1-C2    | -3.19 | 119.42      | 122.68   |
| 45  | LF    | 1859 | PSU  | C6-N1-C2    | -3.19 | 119.42      | 122.68   |
| 47  | LH    | 2809 | A2M  | C5-N7-C8    | 3.19  | 108.04      | 103.51   |
| 48  | LI    | 3175 | PSU  | C6-N1-C2    | -3.19 | 119.42      | 122.68   |
| 48  | LI    | 3542 | PSU  | C6-C5-C4    | 3.19  | 120.43      | 118.20   |
| 1   | S1    | 27   | PSU  | C6-N1-C2    | -3.19 | 119.42      | 122.68   |
| 47  | LH    | 2874 | PSU  | C6-N1-C2    | -3.19 | 119.42      | 122.68   |
| 47  | LH    | 2874 | PSU  | C6-C5-C4    | 3.19  | 120.43      | 118.20   |
| 47  | LH    | 2887 | A2M  | C5-N7-C8    | 3.19  | 108.03      | 103.51   |
| 45  | LF    | 1738 | A2M  | C5-N7-C8    | 3.18  | 108.03      | 103.51   |
| 47  | LH    | 2623 | PSU  | C6-C5-C4    | 3.18  | 120.42      | 118.20   |
| 44  | LE    | 1106 | A2M  | O4'-C1'-N9  | 3.18  | 114.33      | 108.06   |
| 1   | S1    | 2081 | PSU  | C6-N1-C2    | -3.18 | 119.43      | 122.68   |
| 1   | S1    | 28   | A2M  | N3-C4-N9    | 3.18  | 132.32      | 127.08   |
| 48  | LI    | 3440 | PSU  | C6-C5-C4    | 3.18  | 120.42      | 118.20   |
| 1   | S1    | 1378 | PSU  | C6-N1-C2    | -3.17 | 119.44      | 122.68   |
| 44  | LE    | 1365 | PSU  | C6-C5-C4    | 3.17  | 120.42      | 118.20   |
| 1   | S1    | 649  | A2M  | C5-N7-C8    | 3.17  | 108.02      | 103.51   |
| 1   | S1    | 1715 | PSU  | C6-N1-C2    | -3.16 | 119.45      | 122.68   |
| 48  | LI    | 3222 | OMC  | C5-C4-N3    | 3.16  | 126.71      | 121.33   |
| 1   | S1    | 280  | PSU  | C6-N1-C2    | -3.16 | 119.45      | 122.68   |
| 40  | LA    | 97   | A2M  | C5-N7-C8    | 3.16  | 108.00      | 103.51   |
| 2   | S2    | 37   | MIA  | N6-C6-N1    | 3.16  | 122.52      | 118.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | S1    | 40   | A2M  | N3-C4-N9    | 3.15  | 132.28      | 127.08   |
| 44  | LE    | 1075 | PSU  | C6-N1-C2    | -3.15 | 119.46      | 122.68   |
| 1   | S1    | 2288 | MA6  | C5-N7-C8    | 3.15  | 107.98      | 103.51   |
| 1   | S1    | 1378 | PSU  | C6-C5-C4    | 3.15  | 120.40      | 118.20   |
| 44  | LE    | 935  | A2M  | C5-N7-C8    | 3.14  | 107.98      | 103.51   |
| 1   | S1    | 544  | PSU  | C6-C5-C4    | 3.14  | 120.40      | 118.20   |
| 41  | LB    | 234  | PSU  | C6-N1-C2    | -3.14 | 119.47      | 122.68   |
| 41  | LB    | 183  | A2M  | N3-C4-N9    | 3.14  | 132.26      | 127.08   |
| 48  | LI    | 3510 | PSU  | C6-N1-C2    | -3.14 | 119.47      | 122.68   |
| 48  | LI    | 3500 | A2M  | N3-C4-N9    | 3.13  | 132.24      | 127.08   |
| 48  | LI    | 3456 | 5MC  | C5-C4-N3    | 3.13  | 125.05      | 121.67   |
| 48  | LI    | 3510 | PSU  | C6-C5-C4    | 3.13  | 120.39      | 118.20   |
| 45  | LF    | 1692 | PSU  | C6-N1-C2    | -3.13 | 119.48      | 122.68   |
| 49  | LJ    | 3697 | PSU  | C6-N1-C2    | -3.13 | 119.48      | 122.68   |
| 1   | S1    | 2046 | A2M  | N3-C4-N9    | 3.13  | 132.24      | 127.08   |
| 46  | LG    | 2119 | PSU  | C6-N1-C2    | -3.13 | 119.49      | 122.68   |
| 45  | LF    | 1891 | A2M  | C5-N7-C8    | 3.13  | 107.95      | 103.51   |
| 1   | S1    | 565  | A2M  | N3-C4-N9    | 3.12  | 132.23      | 127.08   |
| 45  | LF    | 1836 | OMC  | C5-C4-N3    | 3.12  | 126.64      | 121.33   |
| 47  | LH    | 2914 | PSU  | C6-N1-C2    | -3.12 | 119.49      | 122.68   |
| 48  | LI    | 3206 | PSU  | C6-C5-C4    | 3.12  | 120.38      | 118.20   |
| 47  | LH    | 2837 | PSU  | C6-N1-C2    | -3.12 | 119.49      | 122.68   |
| 44  | LE    | 1126 | PSU  | C6-N1-C2    | -3.12 | 119.49      | 122.68   |
| 47  | LH    | 2769 | A2M  | O4'-C1'-N9  | 3.12  | 114.21      | 108.06   |
| 1   | S1    | 407  | A2M  | C5-N7-C8    | 3.12  | 107.94      | 103.51   |
| 1   | S1    | 723  | A2M  | C5-N7-C8    | 3.12  | 107.94      | 103.51   |
| 44  | LE    | 1106 | A2M  | N3-C4-N9    | 3.12  | 132.22      | 127.08   |
| 48  | LI    | 3206 | PSU  | C6-N1-C2    | -3.12 | 119.50      | 122.68   |
| 48  | LI    | 3214 | 6MZ  | C4-C5-N7    | -3.12 | 106.82      | 110.62   |
| 53  | LN    | 3969 | PSU  | C6-N1-C2    | -3.11 | 119.50      | 122.68   |
| 1   | S1    | 1371 | A2M  | C2'-C1'-N9  | -3.11 | 108.29      | 113.53   |
| 2   | S2    | 37   | MIA  | C5-N7-C8    | 3.11  | 107.93      | 103.51   |
| 45  | LF    | 1929 | A2M  | C5-N7-C8    | 3.11  | 107.93      | 103.51   |
| 48  | LI    | 3546 | OMC  | C5-C4-N3    | 3.11  | 126.62      | 121.33   |
| 1   | S1    | 2144 | 5MC  | C5-C4-N3    | 3.11  | 125.03      | 121.67   |
| 47  | LH    | 2591 | PSU  | C6-N1-C2    | -3.10 | 119.51      | 122.68   |
| 1   | S1    | 649  | A2M  | N3-C4-N9    | 3.10  | 132.19      | 127.08   |
| 45  | LF    | 1502 | A2M  | C5-N7-C8    | 3.10  | 107.91      | 103.51   |
| 47  | LH    | 2358 | A2M  | O2'-C2'-C1' | 3.09  | 115.10      | 109.08   |
| 44  | LE    | 1039 | A2M  | N3-C4-N9    | 3.09  | 132.17      | 127.08   |
| 40  | LA    | 16   | PSU  | C6-N1-C2    | -3.09 | 119.53      | 122.68   |
| 48  | LI    | 3315 | A2M  | C5-N7-C8    | 3.08  | 107.89      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 48  | LI    | 3440 | PSU  | C6-N1-C2 | -3.08 | 119.53      | 122.68   |
| 48  | LI    | 3348 | A2M  | N3-C4-N9 | 3.08  | 132.16      | 127.08   |
| 48  | LI    | 3204 | PSU  | C6-N1-C2 | -3.08 | 119.53      | 122.68   |
| 42  | LC    | 567  | PSU  | C6-C5-C4 | 3.08  | 120.35      | 118.20   |
| 1   | S1    | 2180 | A2M  | C4-C5-N7 | -3.07 | 106.88      | 110.62   |
| 1   | S1    | 2142 | OMC  | C5-C4-N3 | 3.07  | 126.55      | 121.33   |
| 44  | LE    | 1039 | A2M  | C5-N7-C8 | 3.07  | 107.87      | 103.51   |
| 48  | LI    | 2999 | PSU  | C6-N1-C2 | -3.07 | 119.55      | 122.68   |
| 48  | LI    | 3374 | OMC  | C5-C4-N3 | 3.07  | 126.55      | 121.33   |
| 1   | S1    | 2129 | PSU  | C6-N1-C2 | -3.07 | 119.55      | 122.68   |
| 47  | LH    | 2849 | A2M  | N3-C4-N9 | 3.07  | 132.14      | 127.08   |
| 47  | LH    | 2920 | A2M  | C5-N7-C8 | 3.07  | 107.87      | 103.51   |
| 1   | S1    | 1096 | A2M  | C5-N7-C8 | 3.07  | 107.86      | 103.51   |
| 44  | LE    | 1363 | PSU  | C6-C5-C4 | 3.06  | 120.34      | 118.20   |
| 1   | S1    | 99   | OMC  | C5-C4-N3 | 3.06  | 126.53      | 121.33   |
| 47  | LH    | 2708 | A2M  | C5-N7-C8 | 3.06  | 107.85      | 103.51   |
| 1   | S1    | 2305 | PSU  | C6-N1-C2 | -3.06 | 119.56      | 122.68   |
| 47  | LH    | 2744 | A2M  | C5-N7-C8 | 3.06  | 107.85      | 103.51   |
| 1   | S1    | 2116 | PSU  | C6-N1-C2 | -3.06 | 119.56      | 122.68   |
| 45  | LF    | 1692 | PSU  | C6-C5-C4 | 3.05  | 120.33      | 118.20   |
| 1   | S1    | 1900 | A2M  | C5-N7-C8 | 3.05  | 107.85      | 103.51   |
| 42  | LC    | 498  | PSU  | C6-N1-C2 | -3.05 | 119.56      | 122.68   |
| 44  | LE    | 1208 | OMG  | C6-C5-N7 | 3.05  | 135.93      | 130.25   |
| 48  | LI    | 3412 | PSU  | C6-C5-C4 | 3.05  | 120.33      | 118.20   |
| 42  | LC    | 537  | OMC  | C5-C4-N3 | 3.05  | 126.52      | 121.33   |
| 1   | S1    | 176  | PSU  | C6-N1-C2 | -3.05 | 119.57      | 122.68   |
| 45  | LF    | 1926 | PSU  | C6-N1-C2 | -3.05 | 119.57      | 122.68   |
| 45  | LF    | 1573 | OMC  | C5-C4-N3 | 3.05  | 126.51      | 121.33   |
| 48  | LI    | 3367 | A2M  | C5-N7-C8 | 3.04  | 107.83      | 103.51   |
| 1   | S1    | 1549 | A2M  | N3-C4-N9 | 3.04  | 132.09      | 127.08   |
| 46  | LG    | 2005 | A2M  | C5-N7-C8 | 3.04  | 107.83      | 103.51   |
| 44  | LE    | 1171 | PSU  | C6-N1-C2 | -3.04 | 119.57      | 122.68   |
| 42  | LC    | 302  | PSU  | C6-N1-C2 | -3.04 | 119.58      | 122.68   |
| 44  | LE    | 1312 | OMC  | C5-C4-N3 | 3.03  | 126.49      | 121.33   |
| 1   | S1    | 176  | PSU  | C6-C5-C4 | 3.03  | 120.32      | 118.20   |
| 51  | LL    | 3906 | A2M  | C5-N7-C8 | 3.03  | 107.82      | 103.51   |
| 1   | S1    | 1063 | A2M  | C5-N7-C8 | 3.03  | 107.82      | 103.51   |
| 48  | LI    | 3568 | PSU  | C6-N1-C2 | -3.03 | 119.58      | 122.68   |
| 48  | LI    | 3355 | OMC  | C5-C4-N3 | 3.03  | 126.48      | 121.33   |
| 46  | LG    | 2119 | PSU  | C6-C5-C4 | 3.03  | 120.31      | 118.20   |
| 48  | LI    | 3332 | PSU  | C6-C5-C4 | 3.03  | 120.31      | 118.20   |
| 46  | LG    | 2154 | PSU  | C6-N1-C2 | -3.03 | 119.59      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 44  | LE    | 1165 | OMC  | C5-C4-N3  | 3.02  | 126.47      | 121.33   |
| 42  | LC    | 577  | OMC  | C5-C4-N3  | 3.02  | 126.47      | 121.33   |
| 46  | LG    | 2125 | PSU  | C6-N1-C2  | -3.02 | 119.59      | 122.68   |
| 42  | LC    | 567  | PSU  | C6-N1-C2  | -3.02 | 119.59      | 122.68   |
| 47  | LH    | 2914 | PSU  | C6-C5-C4  | 3.02  | 120.31      | 118.20   |
| 1   | S1    | 621  | OMC  | C5-C4-N3  | 3.02  | 126.47      | 121.33   |
| 48  | LI    | 3568 | PSU  | C6-C5-C4  | 3.01  | 120.31      | 118.20   |
| 41  | LB    | 280  | PSU  | C6-N1-C2  | -3.01 | 119.60      | 122.68   |
| 49  | LJ    | 3644 | PSU  | C6-N1-C2  | -3.01 | 119.61      | 122.68   |
| 47  | LH    | 2313 | OMC  | C5-C4-N3  | 3.01  | 126.44      | 121.33   |
| 47  | LH    | 2358 | A2M  | N3-C4-N9  | 3.00  | 132.03      | 127.08   |
| 48  | LI    | 3451 | PSU  | C6-N1-C2  | -3.00 | 119.61      | 122.68   |
| 48  | LI    | 3208 | OMC  | C5-C4-N3  | 3.00  | 126.43      | 121.33   |
| 45  | LF    | 1888 | A2M  | C5-N7-C8  | 3.00  | 107.77      | 103.51   |
| 48  | LI    | 3533 | A2M  | N3-C4-N9  | 2.99  | 132.01      | 127.08   |
| 1   | S1    | 1711 | PSU  | O2-C2-N1  | -2.99 | 119.50      | 122.79   |
| 1   | S1    | 105  | PSU  | C6-N1-C2  | -2.99 | 119.63      | 122.68   |
| 47  | LH    | 2348 | OMC  | C5-C4-N3  | 2.99  | 126.41      | 121.33   |
| 49  | LJ    | 3591 | PSU  | C6-C5-C4  | 2.98  | 120.28      | 118.20   |
| 44  | LE    | 1198 | PSU  | C6-N1-C2  | -2.98 | 119.64      | 122.68   |
| 48  | LI    | 3533 | A2M  | C5-N7-C8  | 2.98  | 107.74      | 103.51   |
| 45  | LF    | 1582 | PSU  | C6-N1-C2  | -2.98 | 119.64      | 122.68   |
| 47  | LH    | 2617 | PSU  | C6-N1-C2  | -2.97 | 119.64      | 122.68   |
| 52  | LM    | 3953 | PSU  | C6-N1-C2  | -2.97 | 119.64      | 122.68   |
| 46  | LG    | 2022 | A2M  | C5-N7-C8  | 2.97  | 107.73      | 103.51   |
| 47  | LH    | 2744 | A2M  | N3-C4-N9  | 2.97  | 131.97      | 127.08   |
| 1   | S1    | 1068 | PSU  | C6-N1-C2  | -2.97 | 119.65      | 122.68   |
| 1   | S1    | 103  | OMC  | C5-C4-N3  | 2.97  | 126.38      | 121.33   |
| 47  | LH    | 2915 | PSU  | C6-N1-C2  | -2.96 | 119.65      | 122.68   |
| 1   | S1    | 723  | A2M  | N3-C4-N9  | 2.96  | 131.97      | 127.08   |
| 48  | LI    | 3348 | A2M  | C5-N7-C8  | 2.96  | 107.72      | 103.51   |
| 44  | LE    | 1365 | PSU  | O2-C2-N1  | -2.96 | 119.53      | 122.79   |
| 44  | LE    | 1106 | A2M  | C5-N7-C8  | 2.96  | 107.72      | 103.51   |
| 47  | LH    | 2685 | OMC  | C5-C4-N3  | 2.96  | 126.36      | 121.33   |
| 47  | LH    | 2685 | OMC  | C1'-N1-C2 | 2.96  | 125.03      | 118.42   |
| 1   | S1    | 2131 | PSU  | C6-C5-C4  | 2.96  | 120.27      | 118.20   |
| 47  | LH    | 2358 | A2M  | C5-N7-C8  | 2.95  | 107.70      | 103.51   |
| 1   | S1    | 645  | A2M  | C5-N7-C8  | 2.95  | 107.70      | 103.51   |
| 48  | LI    | 3521 | A2M  | N3-C4-N9  | 2.95  | 131.95      | 127.08   |
| 45  | LF    | 1976 | OMC  | C5-C4-N3  | 2.95  | 126.35      | 121.33   |
| 46  | LG    | 2005 | A2M  | N3-C4-N9  | 2.95  | 131.94      | 127.08   |
| 47  | LH    | 2849 | A2M  | C5-N7-C8  | 2.95  | 107.70      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | LI    | 3446 | PSU  | C6-C5-C4    | 2.95  | 120.26      | 118.20   |
| 1   | S1    | 38   | OMC  | C5-C4-N3    | 2.94  | 126.34      | 121.33   |
| 1   | S1    | 1037 | OMC  | C5-C4-N3    | 2.94  | 126.33      | 121.33   |
| 1   | S1    | 393  | OMC  | C5-C4-N3    | 2.94  | 126.33      | 121.33   |
| 41  | LB    | 183  | A2M  | C5-N7-C8    | 2.94  | 107.69      | 103.51   |
| 44  | LE    | 1121 | A2M  | C5-N7-C8    | 2.94  | 107.69      | 103.51   |
| 52  | LM    | 3963 | PSU  | C6-N1-C2    | -2.94 | 119.68      | 122.68   |
| 1   | S1    | 186  | OMU  | CM2-O2'-C2' | -2.94 | 106.81      | 114.52   |
| 47  | LH    | 2814 | A2M  | C5-N7-C8    | 2.94  | 107.68      | 103.51   |
| 1   | S1    | 2078 | 7MG  | C5-C4-N9    | 2.93  | 110.16      | 106.35   |
| 44  | LE    | 1407 | PSU  | C6-N1-C2    | -2.93 | 119.68      | 122.68   |
| 51  | LL    | 3865 | PSU  | C6-N1-C2    | -2.93 | 119.69      | 122.68   |
| 44  | LE    | 1270 | OMU  | CM2-O2'-C2' | -2.93 | 106.84      | 114.52   |
| 48  | LI    | 3503 | PSU  | C6-N1-C2    | -2.93 | 119.69      | 122.68   |
| 48  | LI    | 3167 | PSU  | O2-C2-N1    | -2.93 | 119.57      | 122.79   |
| 48  | LI    | 3367 | A2M  | N3-C4-N9    | 2.92  | 131.90      | 127.08   |
| 44  | LE    | 949  | OMC  | C5-C4-N3    | 2.92  | 126.30      | 121.33   |
| 45  | LF    | 1822 | OMC  | C5-C4-N3    | 2.92  | 126.30      | 121.33   |
| 1   | S1    | 28   | A2M  | C5-N7-C8    | 2.92  | 107.66      | 103.51   |
| 47  | LH    | 2832 | OMC  | C5-C4-N3    | 2.92  | 126.30      | 121.33   |
| 40  | LA    | 68   | PSU  | O2-C2-N1    | -2.92 | 119.58      | 122.79   |
| 47  | LH    | 2642 | PSU  | C6-N1-C2    | -2.92 | 119.70      | 122.68   |
| 52  | LM    | 3957 | OMC  | C5-C4-N3    | 2.91  | 126.28      | 121.33   |
| 1   | S1    | 1549 | A2M  | C5-N7-C8    | 2.91  | 107.65      | 103.51   |
| 1   | S1    | 1624 | PSU  | O2-C2-N1    | -2.91 | 119.58      | 122.79   |
| 47  | LH    | 2897 | OMG  | CM2-O2'-C2' | -2.91 | 106.88      | 114.52   |
| 47  | LH    | 2853 | OMC  | C5-C4-N3    | 2.91  | 126.28      | 121.33   |
| 44  | LE    | 1106 | A2M  | O4'-C4'-C3' | -2.91 | 99.36       | 105.11   |
| 44  | LE    | 1222 | OMU  | O4-C4-C5    | -2.91 | 120.05      | 125.16   |
| 48  | LI    | 3145 | PSU  | C6-N1-C2    | -2.90 | 119.71      | 122.68   |
| 48  | LI    | 3347 | OMC  | C5-C4-N3    | 2.90  | 126.27      | 121.33   |
| 49  | LJ    | 3697 | PSU  | C6-C5-C4    | 2.90  | 120.23      | 118.20   |
| 44  | LE    | 936  | OMC  | CM2-O2'-C2' | -2.90 | 106.92      | 114.52   |
| 47  | LH    | 2802 | PSU  | C6-C5-C4    | 2.90  | 120.22      | 118.20   |
| 48  | LI    | 3185 | PSU  | C6-C5-C4    | 2.90  | 120.22      | 118.20   |
| 1   | S1    | 1592 | PSU  | C6-N1-C2    | -2.90 | 119.72      | 122.68   |
| 48  | LI    | 3185 | PSU  | C6-N1-C2    | -2.90 | 119.72      | 122.68   |
| 1   | S1    | 110  | A2M  | N3-C4-N9    | 2.89  | 131.85      | 127.08   |
| 42  | LC    | 483  | OMC  | C5-C4-N3    | 2.89  | 126.25      | 121.33   |
| 48  | LI    | 3521 | A2M  | C5-N7-C8    | 2.89  | 107.62      | 103.51   |
| 44  | LE    | 1218 | OMC  | C5-C4-N3    | 2.89  | 126.24      | 121.33   |
| 49  | LJ    | 3591 | PSU  | C6-N1-C2    | -2.89 | 119.73      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | LI    | 3214 | 6MZ  | C6-C5-N7    | 2.89  | 135.52      | 132.39   |
| 47  | LH    | 2242 | OMC  | C5-C4-N3    | 2.89  | 126.24      | 121.33   |
| 45  | LF    | 1582 | PSU  | C6-C5-C4    | 2.89  | 120.22      | 118.20   |
| 45  | LF    | 1815 | A2M  | C5-N7-C8    | 2.89  | 107.61      | 103.51   |
| 45  | LF    | 1859 | PSU  | C6-C5-C4    | 2.89  | 120.22      | 118.20   |
| 45  | LF    | 1582 | PSU  | O2-C2-N1    | -2.88 | 119.62      | 122.79   |
| 47  | LH    | 2679 | PSU  | C6-N1-C2    | -2.88 | 119.74      | 122.68   |
| 40  | LA    | 97   | A2M  | N3-C4-N9    | 2.88  | 131.83      | 127.08   |
| 47  | LH    | 2825 | OMC  | C5-C4-N3    | 2.88  | 126.22      | 121.33   |
| 48  | LI    | 3465 | OMC  | C5-C4-N3    | 2.88  | 126.22      | 121.33   |
| 45  | LF    | 1502 | A2M  | N3-C4-N9    | 2.87  | 131.82      | 127.08   |
| 1   | S1    | 1554 | PSU  | C6-N1-C2    | -2.87 | 119.75      | 122.68   |
| 47  | LH    | 2812 | A2M  | C5-N7-C8    | 2.87  | 107.59      | 103.51   |
| 44  | LE    | 1407 | PSU  | C6-C5-C4    | 2.86  | 120.20      | 118.20   |
| 45  | LF    | 1876 | PSU  | C6-N1-C2    | -2.86 | 119.75      | 122.68   |
| 1   | S1    | 1591 | PSU  | C6-N1-C2    | -2.86 | 119.76      | 122.68   |
| 1   | S1    | 2123 | OMC  | C5-C4-N3    | 2.86  | 126.19      | 121.33   |
| 1   | S1    | 280  | PSU  | C6-C5-C4    | 2.86  | 120.20      | 118.20   |
| 48  | LI    | 3332 | PSU  | C6-N1-C2    | -2.86 | 119.76      | 122.68   |
| 1   | S1    | 1625 | OMC  | C5-C4-N3    | 2.85  | 126.18      | 121.33   |
| 1   | S1    | 2287 | MA6  | C5-N7-C8    | 2.85  | 107.56      | 103.51   |
| 47  | LH    | 2754 | PSU  | O2-C2-N1    | -2.85 | 119.66      | 122.79   |
| 44  | LE    | 936  | OMC  | C5-C4-N3    | 2.84  | 126.17      | 121.33   |
| 1   | S1    | 1679 | OMU  | CM2-O2'-C2' | -2.84 | 107.07      | 114.52   |
| 1   | S1    | 565  | A2M  | C5-N7-C8    | 2.83  | 107.53      | 103.51   |
| 48  | LI    | 3500 | A2M  | C5-N7-C8    | 2.83  | 107.52      | 103.51   |
| 1   | S1    | 89   | PSU  | C6-C5-C4    | 2.82  | 120.17      | 118.20   |
| 44  | LE    | 1365 | PSU  | C6-N1-C2    | -2.82 | 119.80      | 122.68   |
| 47  | LH    | 2602 | OMC  | C5-C4-N3    | 2.82  | 126.12      | 121.33   |
| 44  | LE    | 1266 | PSU  | O2-C2-N1    | -2.81 | 119.69      | 122.79   |
| 1   | S1    | 1393 | PSU  | C6-C5-C4    | 2.81  | 120.17      | 118.20   |
| 1   | S1    | 1393 | PSU  | O2-C2-N1    | -2.81 | 119.69      | 122.79   |
| 48  | LI    | 3042 | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 44  | LE    | 1023 | PSU  | O2-C2-N1    | -2.80 | 119.70      | 122.79   |
| 1   | S1    | 32   | PSU  | C6-C5-C4    | 2.80  | 120.16      | 118.20   |
| 44  | LE    | 1222 | OMU  | O2-C2-N3    | -2.80 | 116.28      | 121.50   |
| 42  | LC    | 594  | A2M  | C5-N7-C8    | 2.80  | 107.49      | 103.51   |
| 42  | LC    | 308  | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 1   | S1    | 42   | OMG  | CM2-O2'-C2' | -2.79 | 107.19      | 114.52   |
| 45  | LF    | 1568 | PSU  | C6-N1-C2    | -2.79 | 119.83      | 122.68   |
| 47  | LH    | 2586 | PSU  | C6-N1-C2    | -2.79 | 119.83      | 122.68   |
| 2   | S2    | 37   | MIA  | C4-N9-C8    | 2.79  | 108.75      | 105.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | S1    | 1601 | B8N  | O4-C4-N3    | 2.78  | 124.70      | 119.98   |
| 52  | LM    | 3953 | PSU  | C6-C5-C4    | 2.78  | 120.14      | 118.20   |
| 41  | LB    | 234  | PSU  | C6-C5-C4    | 2.78  | 120.14      | 118.20   |
| 42  | LC    | 498  | PSU  | C6-C5-C4    | 2.78  | 120.14      | 118.20   |
| 47  | LH    | 2586 | PSU  | C6-C5-C4    | 2.78  | 120.14      | 118.20   |
| 47  | LH    | 2874 | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 48  | LI    | 3214 | 6MZ  | N1-C2-N3    | -2.77 | 124.27      | 128.60   |
| 48  | LI    | 3206 | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 46  | LG    | 2154 | PSU  | C6-C5-C4    | 2.77  | 120.13      | 118.20   |
| 45  | LF    | 1859 | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 44  | LE    | 1023 | PSU  | C6-C5-C4    | 2.76  | 120.13      | 118.20   |
| 44  | LE    | 938  | 7MG  | C5-C4-N9    | 2.76  | 109.94      | 106.35   |
| 47  | LH    | 2642 | PSU  | C6-C5-C4    | 2.76  | 120.13      | 118.20   |
| 47  | LH    | 2802 | PSU  | C6-N1-C2    | -2.76 | 119.86      | 122.68   |
| 47  | LH    | 2814 | A2M  | N3-C4-N9    | 2.76  | 131.63      | 127.08   |
| 1   | S1    | 1601 | B8N  | O2-C2-N3    | -2.76 | 118.16      | 121.99   |
| 47  | LH    | 2679 | PSU  | C6-C5-C4    | 2.76  | 120.13      | 118.20   |
| 48  | LI    | 3542 | PSU  | C6-N1-C2    | -2.75 | 119.87      | 122.68   |
| 1   | S1    | 1549 | A2M  | C5'-C4'-C3' | -2.75 | 104.87      | 115.18   |
| 49  | LJ    | 3701 | PSU  | O2-C2-N1    | -2.75 | 119.76      | 122.79   |
| 40  | LA    | 39   | A2M  | C5-N7-C8    | 2.75  | 107.41      | 103.51   |
| 48  | LI    | 3444 | PSU  | C6-N1-C2    | -2.74 | 119.88      | 122.68   |
| 45  | LF    | 1891 | A2M  | C2'-C1'-N9  | -2.74 | 108.92      | 113.53   |
| 40  | LA    | 97   | A2M  | C2'-C1'-N9  | -2.74 | 108.92      | 113.53   |
| 48  | LI    | 3535 | OMC  | C5-C4-N3    | 2.73  | 125.97      | 121.33   |
| 48  | LI    | 3042 | PSU  | O2-C2-N1    | -2.73 | 119.79      | 122.79   |
| 1   | S1    | 180  | OMG  | C6-C5-C4    | 2.72  | 122.96      | 118.77   |
| 44  | LE    | 1222 | OMU  | C1'-N1-C6   | -2.72 | 114.91      | 120.84   |
| 47  | LH    | 2809 | A2M  | N3-C4-N9    | 2.72  | 131.56      | 127.08   |
| 49  | LJ    | 3697 | PSU  | O2-C2-N1    | -2.72 | 119.80      | 122.79   |
| 47  | LH    | 2636 | JMH  | C6-N1-C2    | -2.72 | 119.36      | 121.79   |
| 47  | LH    | 2625 | OMU  | C4-N3-C2    | -2.71 | 123.01      | 126.58   |
| 1   | S1    | 280  | PSU  | O2-C2-N1    | -2.70 | 119.81      | 122.79   |
| 45  | LF    | 1586 | PSU  | O2-C2-N1    | -2.70 | 119.81      | 122.79   |
| 1   | S1    | 1549 | A2M  | O4'-C1'-N9  | 2.70  | 113.38      | 108.06   |
| 45  | LF    | 1876 | PSU  | C6-C5-C4    | 2.70  | 120.09      | 118.20   |
| 47  | LH    | 2887 | A2M  | N3-C4-N9    | 2.70  | 131.53      | 127.08   |
| 52  | LM    | 3963 | PSU  | C6-C5-C4    | 2.70  | 120.08      | 118.20   |
| 45  | LF    | 1836 | OMC  | CM2-O2'-C2' | -2.70 | 107.45      | 114.52   |
| 48  | LI    | 3208 | OMC  | C4-N3-C2    | -2.69 | 115.91      | 120.25   |
| 48  | LI    | 3518 | 5MC  | C1'-N1-C2   | -2.69 | 112.41      | 118.42   |
| 48  | LI    | 3208 | OMC  | CM2-O2'-C2' | -2.69 | 107.46      | 114.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | LH    | 2742 | PSU  | C6-N1-C2    | -2.69 | 119.93      | 122.68   |
| 48  | LI    | 3510 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 1   | S1    | 2081 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 2   | S2    | 37   | MIA  | C2-N3-C4    | 2.69  | 119.43      | 112.35   |
| 44  | LE    | 1126 | PSU  | C6-C5-C4    | 2.69  | 120.08      | 118.20   |
| 47  | LH    | 2330 | PSU  | C6-N1-C2    | -2.68 | 119.94      | 122.68   |
| 1   | S1    | 1660 | PSU  | C6-C5-C4    | 2.68  | 120.07      | 118.20   |
| 47  | LH    | 2685 | OMC  | CM2-O2'-C2' | -2.68 | 107.50      | 114.52   |
| 42  | LC    | 498  | PSU  | O2-C2-N1    | -2.67 | 119.85      | 122.79   |
| 1   | S1    | 105  | PSU  | C6-C5-C4    | 2.67  | 120.07      | 118.20   |
| 48  | LI    | 3446 | PSU  | C6-N1-C2    | -2.67 | 119.95      | 122.68   |
| 42  | LC    | 480  | PSU  | O2-C2-N1    | -2.67 | 119.85      | 122.79   |
| 42  | LC    | 421  | PSU  | O2-C2-N1    | -2.67 | 119.86      | 122.79   |
| 46  | LG    | 2125 | PSU  | O2-C2-N1    | -2.67 | 119.86      | 122.79   |
| 48  | LI    | 2999 | PSU  | O2-C2-N1    | -2.66 | 119.86      | 122.79   |
| 47  | LH    | 2591 | PSU  | C6-C5-C4    | 2.66  | 120.06      | 118.20   |
| 48  | LI    | 3348 | A2M  | C2'-C1'-N9  | -2.66 | 109.05      | 113.53   |
| 1   | S1    | 1591 | PSU  | C6-C5-C4    | 2.66  | 120.06      | 118.20   |
| 1   | S1    | 1068 | PSU  | C6-C5-C4    | 2.65  | 120.05      | 118.20   |
| 1   | S1    | 2129 | PSU  | C6-C5-C4    | 2.65  | 120.05      | 118.20   |
| 41  | LB    | 280  | PSU  | C6-C5-C4    | 2.65  | 120.05      | 118.20   |
| 48  | LI    | 3444 | PSU  | O2-C2-N1    | -2.65 | 119.88      | 122.79   |
| 1   | S1    | 465  | PSU  | O2-C2-N1    | -2.65 | 119.88      | 122.79   |
| 1   | S1    | 723  | A2M  | C4-N9-C8    | 2.65  | 108.60      | 105.73   |
| 1   | S1    | 621  | OMC  | CM2-O2'-C2' | -2.65 | 107.58      | 114.52   |
| 48  | LI    | 3300 | OMU  | CM2-O2'-C2' | -2.64 | 107.59      | 114.52   |
| 47  | LH    | 2899 | PSU  | C6-C5-C4    | 2.64  | 120.05      | 118.20   |
| 48  | LI    | 3367 | A2M  | C2'-C1'-N9  | -2.64 | 109.08      | 113.53   |
| 51  | LL    | 3906 | A2M  | C2'-C1'-N9  | -2.64 | 109.09      | 113.53   |
| 46  | LG    | 2154 | PSU  | O2-C2-N1    | -2.64 | 119.89      | 122.79   |
| 1   | S1    | 533  | A2M  | C5-N7-C8    | 2.64  | 107.25      | 103.51   |
| 1   | S1    | 2131 | PSU  | C6-N1-C2    | -2.63 | 119.99      | 122.68   |
| 48  | LI    | 3412 | PSU  | O2-C2-N1    | -2.63 | 119.90      | 122.79   |
| 47  | LH    | 2752 | PSU  | O2-C2-N1    | -2.63 | 119.90      | 122.79   |
| 45  | LF    | 1976 | OMC  | CM2-O2'-C2' | -2.62 | 107.65      | 114.52   |
| 1   | S1    | 2288 | MA6  | N3-C4-N9    | 2.62  | 131.39      | 127.08   |
| 1   | S1    | 2131 | PSU  | O2-C2-N1    | -2.62 | 119.91      | 122.79   |
| 47  | LH    | 2623 | PSU  | O2-C2-N1    | -2.61 | 119.92      | 122.79   |
| 42  | LC    | 308  | PSU  | O2-C2-N1    | -2.60 | 119.93      | 122.79   |
| 1   | S1    | 403  | PSU  | C6-N1-C2    | -2.60 | 120.03      | 122.68   |
| 1   | S1    | 1592 | PSU  | C6-C5-C4    | 2.60  | 120.02      | 118.20   |
| 1   | S1    | 38   | OMC  | CM2-O2'-C2' | -2.60 | 107.70      | 114.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | LH    | 2752 | PSU  | C6-C5-C4    | 2.60  | 120.01      | 118.20   |
| 48  | LI    | 3440 | PSU  | O2-C2-N1    | -2.59 | 119.93      | 122.79   |
| 1   | S1    | 1960 | PSU  | C6-C5-C4    | 2.59  | 120.01      | 118.20   |
| 1   | S1    | 2180 | A2M  | C5-N7-C8    | 2.59  | 107.19      | 103.51   |
| 42  | LC    | 567  | PSU  | O2-C2-N1    | -2.59 | 119.94      | 122.79   |
| 49  | LJ    | 3591 | PSU  | O2-C2-N1    | -2.59 | 119.94      | 122.79   |
| 1   | S1    | 1960 | PSU  | O2-C2-N1    | -2.59 | 119.94      | 122.79   |
| 47  | LH    | 2625 | OMU  | CM2-O2'-C2' | -2.58 | 107.75      | 114.52   |
| 47  | LH    | 2624 | PSU  | C6-N1-C2    | -2.58 | 120.04      | 122.68   |
| 44  | LE    | 1235 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 48  | LI    | 3562 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 46  | LG    | 1999 | OMU  | CM2-O2'-C2' | -2.58 | 107.76      | 114.52   |
| 48  | LI    | 3204 | PSU  | C6-C5-C4    | 2.58  | 120.00      | 118.20   |
| 44  | LE    | 1235 | PSU  | C6-C5-C4    | 2.57  | 120.00      | 118.20   |
| 45  | LF    | 1573 | OMC  | CM2-O2'-C2' | -2.57 | 107.77      | 114.52   |
| 45  | LF    | 1504 | OMU  | CM2-O2'-C2' | -2.57 | 107.78      | 114.52   |
| 44  | LE    | 1118 | PSU  | C6-N1-C2    | -2.57 | 120.06      | 122.68   |
| 1   | S1    | 27   | PSU  | C6-C5-C4    | 2.57  | 119.99      | 118.20   |
| 46  | LG    | 2171 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 1   | S1    | 1624 | PSU  | C6-C5-C4    | 2.56  | 119.99      | 118.20   |
| 1   | S1    | 1715 | PSU  | C6-C5-C4    | 2.56  | 119.99      | 118.20   |
| 1   | S1    | 2101 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 48  | LI    | 3159 | OMU  | CM2-O2'-C2' | -2.56 | 107.82      | 114.52   |
| 45  | LF    | 1692 | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 52  | LM    | 3963 | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 2   | S2    | 37   | MIA  | C5-C6-N6    | -2.55 | 117.47      | 121.76   |
| 1   | S1    | 103  | OMC  | CM2-O2'-C2' | -2.55 | 107.84      | 114.52   |
| 1   | S1    | 1378 | PSU  | O2-C2-N1    | -2.55 | 119.99      | 122.79   |
| 1   | S1    | 544  | PSU  | O2-C2-N1    | -2.54 | 119.99      | 122.79   |
| 45  | LF    | 1824 | OMU  | CM2-O2'-C2' | -2.54 | 107.85      | 114.52   |
| 48  | LI    | 3175 | PSU  | O2-C2-N1    | -2.54 | 119.99      | 122.79   |
| 45  | LF    | 1822 | OMC  | CM2-O2'-C2' | -2.54 | 107.85      | 114.52   |
| 47  | LH    | 2746 | PSU  | C6-C5-C4    | 2.54  | 119.97      | 118.20   |
| 47  | LH    | 2766 | 5MC  | C5-C4-N4    | -2.54 | 117.68      | 121.48   |
| 47  | LH    | 2624 | PSU  | C6-C5-C4    | 2.54  | 119.97      | 118.20   |
| 49  | LJ    | 3694 | OMU  | CM2-O2'-C2' | -2.54 | 107.87      | 114.52   |
| 1   | S1    | 1371 | A2M  | C4'-O4'-C1' | -2.53 | 103.88      | 109.47   |
| 47  | LH    | 2914 | PSU  | O2-C2-N1    | -2.53 | 120.00      | 122.79   |
| 42  | LC    | 491  | OMU  | CM2-O2'-C2' | -2.53 | 107.88      | 114.52   |
| 47  | LH    | 2842 | PSU  | O2-C2-N1    | -2.53 | 120.00      | 122.79   |
| 1   | S1    | 8    | OMU  | CM2-O2'-C2' | -2.53 | 107.89      | 114.52   |
| 44  | LE    | 938  | 7MG  | C4-C5-N7    | 2.53  | 109.04      | 105.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | LI    | 3451 | PSU  | O2-C2-N1    | -2.53 | 120.01      | 122.79   |
| 47  | LH    | 2832 | OMC  | C4-N3-C2    | -2.52 | 116.18      | 120.25   |
| 1   | S1    | 176  | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 47  | LH    | 2915 | PSU  | C6-C5-C4    | 2.52  | 119.96      | 118.20   |
| 40  | LA    | 97   | A2M  | C4-N9-C8    | 2.52  | 108.46      | 105.73   |
| 47  | LH    | 2825 | OMC  | CM2-O2'-C2' | -2.52 | 107.92      | 114.52   |
| 46  | LG    | 2119 | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 40  | LA    | 16   | PSU  | C6-C5-C4    | 2.51  | 119.95      | 118.20   |
| 47  | LH    | 2887 | A2M  | C4-N9-C8    | 2.51  | 108.45      | 105.73   |
| 1   | S1    | 1641 | OMU  | CM2-O2'-C2' | -2.51 | 107.95      | 114.52   |
| 49  | LJ    | 3701 | PSU  | C6-C5-C4    | 2.51  | 119.95      | 118.20   |
| 1   | S1    | 186  | OMU  | C4-N3-C2    | -2.50 | 123.28      | 126.58   |
| 47  | LH    | 2621 | PSU  | C6-N1-C2    | -2.50 | 120.13      | 122.68   |
| 47  | LH    | 2346 | OMU  | CM2-O2'-C2' | -2.49 | 107.98      | 114.52   |
| 48  | LI    | 3300 | OMU  | C4-N3-C2    | -2.49 | 123.29      | 126.58   |
| 48  | LI    | 3222 | OMC  | CM2-O2'-C2' | -2.49 | 107.98      | 114.52   |
| 1   | S1    | 2078 | 7MG  | C4-C5-N7    | 2.49  | 108.99      | 105.53   |
| 45  | LF    | 1976 | OMC  | C4-N3-C2    | -2.49 | 116.23      | 120.25   |
| 44  | LE    | 931  | 1MA  | C4-C5-N7    | -2.49 | 106.78      | 110.72   |
| 1   | S1    | 2305 | PSU  | C6-C5-C4    | 2.49  | 119.94      | 118.20   |
| 47  | LH    | 2842 | PSU  | C6-C5-C4    | 2.49  | 119.94      | 118.20   |
| 44  | LE    | 1363 | PSU  | O2-C2-N1    | -2.49 | 120.05      | 122.79   |
| 48  | LI    | 3355 | OMC  | CM2-O2'-C2' | -2.49 | 107.99      | 114.52   |
| 45  | LF    | 1898 | OMU  | C4-N3-C2    | -2.49 | 123.30      | 126.58   |
| 49  | LJ    | 3688 | OMG  | CM2-O2'-C2' | -2.48 | 108.02      | 114.52   |
| 44  | LE    | 1165 | OMC  | CM2-O2'-C2' | -2.48 | 108.02      | 114.52   |
| 48  | LI    | 3465 | OMC  | CM2-O2'-C2' | -2.48 | 108.03      | 114.52   |
| 48  | LI    | 3332 | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 48  | LI    | 3508 | OMU  | CM2-O2'-C2' | -2.47 | 108.03      | 114.52   |
| 44  | LE    | 1189 | OMU  | CM2-O2'-C2' | -2.47 | 108.04      | 114.52   |
| 1   | S1    | 2305 | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 47  | LH    | 2766 | 5MC  | N1-C2-N3    | -2.47 | 114.31      | 118.81   |
| 45  | LF    | 1836 | OMC  | C4-N3-C2    | -2.47 | 116.27      | 120.25   |
| 44  | LE    | 1198 | PSU  | O2-C2-N1    | -2.46 | 120.08      | 122.79   |
| 1   | S1    | 1037 | OMC  | CM2-O2'-C2' | -2.46 | 108.06      | 114.52   |
| 1   | S1    | 2046 | A2M  | C4-N9-C8    | 2.46  | 108.39      | 105.73   |
| 45  | LF    | 1876 | PSU  | O2-C2-N1    | -2.46 | 120.08      | 122.79   |
| 1   | S1    | 1601 | B8N  | C32-C31-N3  | 2.46  | 116.60      | 112.00   |
| 47  | LH    | 2909 | OMU  | C4-N3-C2    | -2.46 | 123.34      | 126.58   |
| 1   | S1    | 649  | A2M  | C4-N9-C8    | 2.45  | 108.38      | 105.73   |
| 1   | S1    | 621  | OMC  | C4-N3-C2    | -2.45 | 116.30      | 120.25   |
| 47  | LH    | 2586 | PSU  | O2-C2-N1    | -2.45 | 120.10      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | LH    | 2591 | PSU  | O2-C2-N1    | -2.45 | 120.10      | 122.79   |
| 1   | S1    | 1660 | PSU  | O2-C2-N1    | -2.44 | 120.10      | 122.79   |
| 1   | S1    | 2065 | PSU  | C6-C5-C4    | 2.44  | 119.91      | 118.20   |
| 51  | LL    | 3865 | PSU  | O2-C2-N1    | -2.44 | 120.10      | 122.79   |
| 1   | S1    | 8    | OMU  | C4-N3-C2    | -2.44 | 123.36      | 126.58   |
| 1   | S1    | 180  | OMG  | N1-C2-N3    | 2.44  | 127.88      | 123.32   |
| 45  | LF    | 1826 | OMG  | CM2-O2'-C2' | -2.44 | 108.13      | 114.52   |
| 42  | LC    | 577  | OMC  | C4-N3-C2    | -2.44 | 116.32      | 120.25   |
| 47  | LH    | 2346 | OMU  | C4-N3-C2    | -2.44 | 123.37      | 126.58   |
| 1   | S1    | 1096 | A2M  | C4-N9-C8    | 2.43  | 108.36      | 105.73   |
| 44  | LE    | 1218 | OMC  | CM2-O2'-C2' | -2.43 | 108.15      | 114.52   |
| 48  | LI    | 3204 | PSU  | O2-C2-N1    | -2.43 | 120.11      | 122.79   |
| 48  | LI    | 3503 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 1   | S1    | 640  | PSU  | C6-N1-C2    | -2.43 | 120.20      | 122.68   |
| 1   | S1    | 1396 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 1   | S1    | 110  | A2M  | C4-C5-N7    | -2.43 | 107.66      | 110.62   |
| 1   | S1    | 682  | OMU  | C4-N3-C2    | -2.43 | 123.38      | 126.58   |
| 44  | LE    | 1407 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 1   | S1    | 407  | A2M  | C6-C5-C4    | 2.43  | 120.44      | 117.18   |
| 52  | LM    | 3957 | OMC  | C4-N3-C2    | -2.42 | 116.34      | 120.25   |
| 44  | LE    | 1260 | PSU  | O2-C2-N1    | -2.42 | 120.12      | 122.79   |
| 48  | LI    | 3214 | 6MZ  | C5-N7-C8    | 2.42  | 106.94      | 103.51   |
| 48  | LI    | 3546 | OMC  | CM2-O2'-C2' | -2.42 | 108.18      | 114.52   |
| 44  | LE    | 1184 | PSU  | O2-C2-N1    | -2.42 | 120.13      | 122.79   |
| 48  | LI    | 3568 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 45  | LF    | 1835 | OMG  | C2-N1-C6    | -2.41 | 120.70      | 125.10   |
| 47  | LH    | 2713 | OMU  | CM2-O2'-C2' | -2.41 | 108.20      | 114.52   |
| 47  | LH    | 2617 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 53  | LN    | 3969 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 48  | LI    | 3222 | OMC  | C4-N3-C2    | -2.41 | 116.37      | 120.25   |
| 1   | S1    | 2287 | MA6  | C4-N9-C8    | 2.41  | 108.34      | 105.73   |
| 45  | LF    | 1819 | OMG  | O2'-C2'-C1' | 2.41  | 113.77      | 109.08   |
| 48  | LI    | 3145 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 2   | S2    | 37   | MIA  | C16-C14-C15 | -2.40 | 109.29      | 114.60   |
| 47  | LH    | 2744 | A2M  | C4-N9-C8    | 2.40  | 108.33      | 105.73   |
| 44  | LE    | 1315 | OMU  | CM2-O2'-C2' | -2.40 | 108.22      | 114.52   |
| 44  | LE    | 1208 | OMG  | C4-C5-N7    | -2.40 | 106.92      | 110.72   |
| 1   | S1    | 1641 | OMU  | C4-N3-C2    | -2.40 | 123.42      | 126.58   |
| 1   | S1    | 2142 | OMC  | N4-C4-N3    | -2.40 | 113.76      | 117.97   |
| 1   | S1    | 1616 | OMU  | CM2-O2'-C2' | -2.40 | 108.23      | 114.52   |
| 1   | S1    | 1068 | PSU  | O2-C2-N1    | -2.40 | 120.15      | 122.79   |
| 1   | S1    | 2123 | OMC  | C4-N3-C2    | -2.40 | 116.39      | 120.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 44  | LE    | 1452 | OMU  | C4-N3-C2    | -2.39 | 123.42      | 126.58   |
| 47  | LH    | 2349 | A2M  | C4-N9-C8    | 2.39  | 108.32      | 105.73   |
| 45  | LF    | 1926 | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 1   | S1    | 1715 | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 47  | LH    | 2636 | JMH  | O2-C2-N3    | -2.39 | 117.97      | 121.34   |
| 42  | LC    | 302  | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 44  | LE    | 1189 | OMU  | C4-N3-C2    | -2.38 | 123.44      | 126.58   |
| 1   | S1    | 393  | OMC  | C4-N3-C2    | -2.38 | 116.41      | 120.25   |
| 47  | LH    | 2832 | OMC  | CM2-O2'-C2' | -2.38 | 108.27      | 114.52   |
| 44  | LE    | 1270 | OMU  | C4-N3-C2    | -2.38 | 123.44      | 126.58   |
| 45  | LF    | 1502 | A2M  | C4-N9-C8    | 2.38  | 108.30      | 105.73   |
| 1   | S1    | 1901 | OMG  | N1-C2-N3    | 2.37  | 127.75      | 123.32   |
| 47  | LH    | 2361 | PSU  | C6-C5-C4    | 2.37  | 119.86      | 118.20   |
| 49  | LJ    | 3644 | PSU  | O2-C2-N1    | -2.37 | 120.19      | 122.79   |
| 44  | LE    | 1075 | PSU  | O2-C2-N1    | -2.37 | 120.19      | 122.79   |
| 47  | LH    | 2909 | OMU  | CM2-O2'-C2' | -2.37 | 108.32      | 114.52   |
| 1   | S1    | 704  | OMU  | C4-N3-C2    | -2.36 | 123.46      | 126.58   |
| 1   | S1    | 99   | OMC  | C4-N3-C2    | -2.36 | 116.44      | 120.25   |
| 48  | LI    | 3374 | OMC  | CM2-O2'-C2' | -2.36 | 108.32      | 114.52   |
| 45  | LF    | 1956 | OMG  | N1-C2-N3    | 2.36  | 127.73      | 123.32   |
| 47  | LH    | 2879 | OMG  | N2-C2-N3    | -2.36 | 115.14      | 119.73   |
| 1   | S1    | 1549 | A2M  | C5-C4-N9    | 2.36  | 108.53      | 105.78   |
| 1   | S1    | 2144 | 5MC  | N1-C2-N3    | -2.36 | 114.52      | 118.81   |
| 47  | LH    | 2849 | A2M  | C4-N9-C8    | 2.35  | 108.28      | 105.73   |
| 48  | LI    | 3222 | OMC  | N4-C4-N3    | -2.35 | 113.84      | 117.97   |
| 48  | LI    | 3355 | OMC  | C4-N3-C2    | -2.35 | 116.46      | 120.25   |
| 1   | S1    | 641  | OMG  | CM2-O2'-C2' | -2.35 | 108.35      | 114.52   |
| 47  | LH    | 2853 | OMC  | CM2-O2'-C2' | -2.35 | 108.36      | 114.52   |
| 45  | LF    | 1667 | OMG  | N1-C2-N3    | 2.35  | 127.71      | 123.32   |
| 53  | LN    | 3969 | PSU  | C6-C5-C4    | 2.35  | 119.84      | 118.20   |
| 1   | S1    | 1679 | OMU  | C4-N3-C2    | -2.35 | 123.48      | 126.58   |
| 48  | LI    | 3159 | OMU  | C4-N3-C2    | -2.35 | 123.48      | 126.58   |
| 45  | LF    | 1898 | OMU  | CM2-O2'-C2' | -2.34 | 108.38      | 114.52   |
| 46  | LG    | 2022 | A2M  | C2'-C1'-N9  | -2.34 | 109.59      | 113.53   |
| 48  | LI    | 3546 | OMC  | C4-N3-C2    | -2.34 | 116.48      | 120.25   |
| 44  | LE    | 1126 | PSU  | O2-C2-N1    | -2.34 | 120.22      | 122.79   |
| 1   | S1    | 57   | OMG  | N1-C2-N3    | 2.34  | 127.68      | 123.32   |
| 44  | LE    | 935  | A2M  | C4-N9-C8    | 2.33  | 108.26      | 105.73   |
| 48  | LI    | 3185 | PSU  | O2-C2-N1    | -2.33 | 120.22      | 122.79   |
| 41  | LB    | 247  | OMU  | CM2-O2'-C2' | -2.33 | 108.41      | 114.52   |
| 47  | LH    | 2348 | OMC  | C4-N3-C2    | -2.33 | 116.49      | 120.25   |
| 1   | S1    | 179  | OMU  | C4-N3-C2    | -2.33 | 123.51      | 126.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | LH    | 2361 | PSU  | O2-C2-N1    | -2.33 | 120.23      | 122.79   |
| 45  | LF    | 1957 | OMU  | C4-N3-C2    | -2.33 | 123.51      | 126.58   |
| 47  | LH    | 2837 | PSU  | C6-C5-C4    | 2.33  | 119.82      | 118.20   |
| 47  | LH    | 2349 | A2M  | C2'-C1'-N9  | -2.33 | 109.61      | 113.53   |
| 1   | S1    | 2144 | 5MC  | C5-C4-N4    | -2.33 | 118.00      | 121.48   |
| 47  | LH    | 2746 | PSU  | O2-C2-N1    | -2.33 | 120.23      | 122.79   |
| 40  | LA    | 16   | PSU  | O2-C2-N1    | -2.32 | 120.23      | 122.79   |
| 1   | S1    | 533  | A2M  | C6-C5-C4    | 2.32  | 120.31      | 117.18   |
| 47  | LH    | 2768 | A2M  | C3'-C2'-C1' | 2.32  | 107.25      | 102.89   |
| 46  | LG    | 2005 | A2M  | C4-C5-N7    | -2.32 | 107.79      | 110.62   |
| 1   | S1    | 2180 | A2M  | O4'-C1'-N9  | 2.32  | 112.63      | 108.06   |
| 1   | S1    | 1591 | PSU  | O2-C2-N1    | -2.32 | 120.24      | 122.79   |
| 48  | LI    | 3171 | OMU  | CM2-O2'-C2' | -2.32 | 108.44      | 114.52   |
| 44  | LE    | 1081 | OMU  | CM2-O2'-C2' | -2.32 | 108.44      | 114.52   |
| 1   | S1    | 1554 | PSU  | C6-C5-C4    | 2.32  | 119.82      | 118.20   |
| 1   | S1    | 105  | PSU  | O2-C2-N1    | -2.32 | 120.24      | 122.79   |
| 46  | LG    | 2129 | OMU  | C4-N3-C2    | -2.32 | 123.53      | 126.58   |
| 1   | S1    | 2180 | A2M  | C4-N9-C8    | 2.31  | 108.23      | 105.73   |
| 45  | LF    | 1891 | A2M  | C4-N9-C8    | 2.31  | 108.23      | 105.73   |
| 51  | LL    | 3906 | A2M  | C4-N9-C8    | 2.31  | 108.23      | 105.73   |
| 47  | LH    | 2802 | PSU  | O2-C2-N1    | -2.31 | 120.25      | 122.79   |
| 1   | S1    | 1549 | A2M  | C6-C5-C4    | 2.31  | 120.28      | 117.18   |
| 48  | LI    | 3401 | OMG  | N1-C2-N3    | 2.30  | 127.62      | 123.32   |
| 48  | LI    | 3377 | OMG  | CM2-O2'-C2' | -2.30 | 108.49      | 114.52   |
| 52  | LM    | 3953 | PSU  | O2-C2-N1    | -2.30 | 120.26      | 122.79   |
| 45  | LF    | 1929 | A2M  | C4-N9-C8    | 2.30  | 108.22      | 105.73   |
| 1   | S1    | 2288 | MA6  | C4-N9-C8    | 2.30  | 108.22      | 105.73   |
| 1   | S1    | 38   | OMC  | C4-N3-C2    | -2.30 | 116.55      | 120.25   |
| 47  | LH    | 2621 | PSU  | O2-C2-N1    | -2.30 | 120.26      | 122.79   |
| 47  | LH    | 2713 | OMU  | C4-N3-C2    | -2.30 | 123.55      | 126.58   |
| 46  | LG    | 2022 | A2M  | C6-C5-C4    | 2.30  | 120.27      | 117.18   |
| 1   | S1    | 704  | OMU  | CM2-O2'-C2' | -2.29 | 108.50      | 114.52   |
| 41  | LB    | 280  | PSU  | O2-C2-N1    | -2.29 | 120.27      | 122.79   |
| 46  | LG    | 2005 | A2M  | C5-C4-N9    | 2.29  | 108.45      | 105.78   |
| 48  | LI    | 3347 | OMC  | C4-N3-C2    | -2.29 | 116.55      | 120.25   |
| 1   | S1    | 2046 | A2M  | C4-C5-N7    | -2.29 | 107.83      | 110.62   |
| 47  | LH    | 2915 | PSU  | O2-C2-N1    | -2.29 | 120.27      | 122.79   |
| 1   | S1    | 2041 | OMU  | C4-N3-C2    | -2.29 | 123.56      | 126.58   |
| 1   | S1    | 1063 | A2M  | C6-C5-C4    | 2.29  | 120.25      | 117.18   |
| 47  | LH    | 2812 | A2M  | C6-C5-C4    | 2.29  | 120.25      | 117.18   |
| 46  | LG    | 2009 | OMG  | N1-C2-N3    | 2.28  | 127.59      | 123.32   |
| 1   | S1    | 1966 | OMU  | C4-N3-C2    | -2.28 | 123.57      | 126.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | S1    | 1063 | A2M  | C4-N9-C8    | 2.28  | 108.20      | 105.73   |
| 48  | LI    | 3434 | OMG  | N1-C2-N3    | 2.28  | 127.58      | 123.32   |
| 48  | LI    | 3456 | 5MC  | C1'-N1-C2   | -2.28 | 113.34      | 118.42   |
| 45  | LF    | 1956 | OMG  | C2-N1-C6    | -2.28 | 120.94      | 125.10   |
| 42  | LC    | 537  | OMC  | C4-N3-C2    | -2.28 | 116.58      | 120.25   |
| 42  | LC    | 483  | OMC  | CM2-O2'-C2' | -2.28 | 108.55      | 114.52   |
| 44  | LE    | 1106 | A2M  | C4-N9-C8    | 2.27  | 108.19      | 105.73   |
| 47  | LH    | 2769 | A2M  | C4-N9-C8    | 2.27  | 108.19      | 105.73   |
| 49  | LJ    | 3680 | PSU  | O4'-C1'-C2' | 2.27  | 108.35      | 105.14   |
| 48  | LI    | 3508 | OMU  | C4-N3-C2    | -2.27 | 123.58      | 126.58   |
| 44  | LE    | 1312 | OMC  | C4-N3-C2    | -2.27 | 116.59      | 120.25   |
| 47  | LH    | 2610 | OMG  | C2-N1-C6    | -2.27 | 120.96      | 125.10   |
| 1   | S1    | 2065 | PSU  | O2-C2-N1    | -2.27 | 120.29      | 122.79   |
| 1   | S1    | 1037 | OMC  | C4-N3-C2    | -2.27 | 116.59      | 120.25   |
| 47  | LH    | 2636 | JMH  | C1'-N1-C6   | -2.27 | 115.89      | 120.84   |
| 48  | LI    | 3374 | OMC  | C4-N3-C2    | -2.27 | 116.59      | 120.25   |
| 1   | S1    | 723  | A2M  | C3'-C2'-C1' | 2.27  | 107.16      | 102.89   |
| 48  | LI    | 3533 | A2M  | C4-N9-C8    | 2.27  | 108.19      | 105.73   |
| 44  | LE    | 936  | OMC  | C4-N3-C2    | -2.27 | 116.59      | 120.25   |
| 1   | S1    | 1591 | PSU  | O4-C4-C5    | -2.27 | 118.12      | 124.05   |
| 47  | LH    | 2744 | A2M  | C3'-C2'-C1' | 2.26  | 107.14      | 102.89   |
| 44  | LE    | 1218 | OMC  | C4-N3-C2    | -2.26 | 116.60      | 120.25   |
| 45  | LF    | 1553 | OMU  | C4-N3-C2    | -2.26 | 123.60      | 126.58   |
| 40  | LA    | 68   | PSU  | O4'-C1'-C2' | 2.26  | 108.33      | 105.14   |
| 47  | LH    | 2708 | A2M  | C4-N9-C8    | 2.26  | 108.18      | 105.73   |
| 1   | S1    | 702  | OMU  | C4-N3-C2    | -2.26 | 123.60      | 126.58   |
| 44  | LE    | 1184 | PSU  | C6-C5-C4    | 2.26  | 119.78      | 118.20   |
| 47  | LH    | 2825 | OMC  | N4-C4-N3    | -2.25 | 114.01      | 117.97   |
| 48  | LI    | 3171 | OMU  | C4-N3-C2    | -2.25 | 123.61      | 126.58   |
| 47  | LH    | 2809 | A2M  | C4-C5-N7    | -2.25 | 107.88      | 110.62   |
| 47  | LH    | 2853 | OMC  | C4-N3-C2    | -2.25 | 116.62      | 120.25   |
| 1   | S1    | 2078 | 7MG  | O6-C6-N1    | -2.25 | 115.80      | 120.12   |
| 48  | LI    | 3444 | PSU  | O4'-C1'-C2' | 2.25  | 108.32      | 105.14   |
| 47  | LH    | 2837 | PSU  | O2-C2-N1    | -2.25 | 120.31      | 122.79   |
| 48  | LI    | 3456 | 5MC  | C5-C4-N4    | -2.25 | 118.12      | 121.48   |
| 45  | LF    | 1835 | OMG  | N1-C2-N3    | 2.25  | 127.52      | 123.32   |
| 49  | LJ    | 3718 | OMU  | C4-N3-C2    | -2.25 | 123.62      | 126.58   |
| 44  | LE    | 1075 | PSU  | C6-C5-C4    | 2.25  | 119.77      | 118.20   |
| 1   | S1    | 1616 | OMU  | C4-N3-C2    | -2.24 | 123.63      | 126.58   |
| 44  | LE    | 1315 | OMU  | C4-N3-C2    | -2.24 | 123.63      | 126.58   |
| 1   | S1    | 99   | OMC  | CM2-O2'-C2' | -2.24 | 108.65      | 114.52   |
| 47  | LH    | 2330 | PSU  | C6-C5-C4    | 2.24  | 119.76      | 118.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | LI    | 3206 | PSU  | O4'-C1'-C2' | 2.24  | 108.30      | 105.14   |
| 47  | LH    | 2621 | PSU  | C6-C5-C4    | 2.24  | 119.76      | 118.20   |
| 1   | S1    | 485  | OMG  | N1-C2-N3    | 2.23  | 127.49      | 123.32   |
| 1   | S1    | 89   | PSU  | O2-C2-N1    | -2.23 | 120.33      | 122.79   |
| 1   | S1    | 1371 | A2M  | C4-C5-N7    | -2.23 | 107.90      | 110.62   |
| 1   | S1    | 1601 | B8N  | O4'-C1'-C2' | 2.23  | 108.29      | 105.14   |
| 1   | S1    | 2075 | OMG  | N1-C2-N3    | 2.23  | 127.49      | 123.32   |
| 47  | LH    | 2348 | OMC  | CM2-O2'-C2' | -2.23 | 108.67      | 114.52   |
| 42  | LC    | 537  | OMC  | CM2-O2'-C2' | -2.23 | 108.67      | 114.52   |
| 47  | LH    | 2806 | OMU  | C4-N3-C2    | -2.23 | 123.64      | 126.58   |
| 45  | LF    | 1667 | OMG  | C2-N1-C6    | -2.23 | 121.03      | 125.10   |
| 48  | LI    | 3401 | OMG  | C2-N1-C6    | -2.23 | 121.04      | 125.10   |
| 48  | LI    | 3533 | A2M  | C2'-C1'-N9  | -2.23 | 109.78      | 113.53   |
| 45  | LF    | 1883 | OMG  | N1-C2-N3    | 2.23  | 127.48      | 123.32   |
| 49  | LJ    | 3636 | OMU  | C4-N3-C2    | -2.23 | 123.64      | 126.58   |
| 47  | LH    | 2358 | A2M  | C4-N9-C8    | 2.23  | 108.14      | 105.73   |
| 47  | LH    | 2313 | OMC  | CM2-O2'-C2' | -2.22 | 108.69      | 114.52   |
| 1   | S1    | 121  | PSU  | C3'-C2'-C1' | 2.22  | 104.23      | 101.64   |
| 47  | LH    | 2313 | OMC  | C4-N3-C2    | -2.22 | 116.67      | 120.25   |
| 1   | S1    | 1900 | A2M  | C4-N9-C8    | 2.22  | 108.14      | 105.73   |
| 47  | LH    | 2742 | PSU  | C6-C5-C4    | 2.22  | 119.75      | 118.20   |
| 47  | LH    | 2835 | OMU  | C4-N3-C2    | -2.22 | 123.65      | 126.58   |
| 45  | LF    | 1681 | OMU  | C4-N3-C2    | -2.22 | 123.66      | 126.58   |
| 1   | S1    | 1901 | OMG  | C2-N1-C6    | -2.22 | 121.05      | 125.10   |
| 1   | S1    | 2288 | MA6  | C4-C5-N7    | -2.22 | 107.92      | 110.62   |
| 42  | LC    | 628  | OMG  | N1-C2-N3    | 2.22  | 127.46      | 123.32   |
| 45  | LF    | 1738 | A2M  | C4-N9-C8    | 2.21  | 108.13      | 105.73   |
| 1   | S1    | 27   | PSU  | O2-C2-N1    | -2.21 | 120.35      | 122.79   |
| 47  | LH    | 2330 | PSU  | O2-C2-N1    | -2.21 | 120.35      | 122.79   |
| 48  | LI    | 3377 | OMG  | N1-C2-N3    | 2.21  | 127.45      | 123.32   |
| 1   | S1    | 1536 | OMG  | N1-C2-N3    | 2.21  | 127.45      | 123.32   |
| 40  | LA    | 97   | A2M  | O4'-C1'-C2' | -2.21 | 102.69      | 106.57   |
| 48  | LI    | 3347 | OMC  | CM2-O2'-C2' | -2.21 | 108.72      | 114.52   |
| 1   | S1    | 2129 | PSU  | O2-C2-N1    | -2.21 | 120.36      | 122.79   |
| 47  | LH    | 2610 | OMG  | CM2-O2'-C2' | -2.21 | 108.73      | 114.52   |
| 48  | LI    | 3412 | PSU  | O4'-C1'-C2' | 2.21  | 108.26      | 105.14   |
| 1   | S1    | 57   | OMG  | N2-C2-N3    | -2.21 | 115.44      | 119.73   |
| 45  | LF    | 1504 | OMU  | C4-N3-C2    | -2.21 | 123.67      | 126.58   |
| 47  | LH    | 2768 | A2M  | C4-C5-N7    | -2.21 | 107.93      | 110.62   |
| 44  | LE    | 1208 | OMG  | O6-C6-C5    | -2.20 | 120.76      | 126.60   |
| 47  | LH    | 2744 | A2M  | C2'-C3'-C4' | 2.20  | 106.78      | 101.99   |
| 42  | LC    | 594  | A2M  | C6-C5-C4    | 2.20  | 120.14      | 117.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | S1    | 40   | A2M  | C4-N9-C8    | 2.20  | 108.11      | 105.73   |
| 41  | LB    | 183  | A2M  | C4-N9-C8    | 2.20  | 108.11      | 105.73   |
| 1   | S1    | 702  | OMU  | CM2-O2'-C2' | -2.20 | 108.75      | 114.52   |
| 1   | S1    | 1901 | OMG  | CM2-O2'-C2' | -2.20 | 108.76      | 114.52   |
| 45  | LF    | 1815 | A2M  | C4-N9-C8    | 2.20  | 108.11      | 105.73   |
| 48  | LI    | 3546 | OMC  | N4-C4-N3    | -2.19 | 114.12      | 117.97   |
| 47  | LH    | 2242 | OMC  | C4-N3-C2    | -2.19 | 116.71      | 120.25   |
| 45  | LF    | 1662 | OMG  | N1-C2-N3    | 2.19  | 127.42      | 123.32   |
| 1   | S1    | 1549 | A2M  | C4-C5-N7    | -2.19 | 107.95      | 110.62   |
| 41  | LB    | 206  | OMU  | C4-N3-C2    | -2.19 | 123.69      | 126.58   |
| 44  | LE    | 1217 | OMG  | C2-N1-C6    | -2.19 | 121.10      | 125.10   |
| 1   | S1    | 32   | PSU  | O2-C2-N1    | -2.19 | 120.38      | 122.79   |
| 41  | LB    | 281  | PSU  | O2-C2-N1    | -2.19 | 120.38      | 122.79   |
| 1   | S1    | 1601 | B8N  | C31-N3-C2   | -2.19 | 114.39      | 117.67   |
| 47  | LH    | 2879 | OMG  | N1-C2-N3    | 2.19  | 127.41      | 123.32   |
| 47  | LH    | 2899 | PSU  | O2-C2-N1    | -2.19 | 120.38      | 122.79   |
| 1   | S1    | 180  | OMG  | C6-C5-N7    | -2.19 | 126.18      | 130.25   |
| 1   | S1    | 57   | OMG  | C2-N1-C6    | -2.19 | 121.11      | 125.10   |
| 48  | LI    | 3518 | 5MC  | C5-C4-N4    | -2.19 | 118.21      | 121.48   |
| 42  | LC    | 541  | OMG  | O6-C6-N1    | -2.19 | 115.93      | 120.12   |
| 44  | LE    | 938  | 7MG  | O6-C6-N1    | -2.19 | 115.93      | 120.12   |
| 47  | LH    | 2925 | OMG  | N1-C2-N3    | 2.19  | 127.40      | 123.32   |
| 1   | S1    | 1371 | A2M  | C4-N9-C8    | 2.19  | 108.10      | 105.73   |
| 1   | S1    | 1705 | OMG  | N1-C2-N3    | 2.18  | 127.40      | 123.32   |
| 42  | LC    | 491  | OMU  | C4-N3-C2    | -2.18 | 123.70      | 126.58   |
| 51  | LL    | 3906 | A2M  | C6-C5-C4    | 2.18  | 120.12      | 117.18   |
| 1   | S1    | 645  | A2M  | O4'-C4'-C3' | -2.18 | 100.80      | 105.11   |
| 1   | S1    | 2142 | OMC  | C4-N3-C2    | -2.18 | 116.73      | 120.25   |
| 45  | LF    | 1815 | A2M  | C2'-C1'-N9  | -2.18 | 109.87      | 113.53   |
| 45  | LF    | 1568 | PSU  | O2-C2-N1    | -2.18 | 120.39      | 122.79   |
| 40  | LA    | 74   | OMG  | N1-C2-N3    | 2.18  | 127.38      | 123.32   |
| 45  | LF    | 1568 | PSU  | C6-C5-C4    | 2.17  | 119.72      | 118.20   |
| 48  | LI    | 3191 | OMG  | N1-C2-N3    | 2.17  | 127.38      | 123.32   |
| 47  | LH    | 2313 | OMC  | N4-C4-N3    | -2.17 | 114.16      | 117.97   |
| 44  | LE    | 1217 | OMG  | CM2-O2'-C2' | -2.17 | 108.83      | 114.52   |
| 46  | LG    | 2009 | OMG  | N2-C2-N3    | -2.17 | 115.51      | 119.73   |
| 42  | LC    | 594  | A2M  | C4-N9-C8    | 2.17  | 108.08      | 105.73   |
| 48  | LI    | 3187 | OMG  | N2-C2-N3    | -2.17 | 115.51      | 119.73   |
| 44  | LE    | 1452 | OMU  | CM2-O2'-C2' | -2.17 | 108.84      | 114.52   |
| 41  | LB    | 247  | OMU  | C4-N3-C2    | -2.17 | 123.72      | 126.58   |
| 46  | LG    | 1999 | OMU  | C4-N3-C2    | -2.17 | 123.72      | 126.58   |
| 48  | LI    | 3465 | OMC  | N4-C4-N3    | -2.17 | 114.17      | 117.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | S1    | 110  | A2M  | C5-C4-N9    | 2.16  | 108.30      | 105.78   |
| 48  | LI    | 3542 | PSU  | O2-C2-N1    | -2.16 | 120.41      | 122.79   |
| 44  | LE    | 1204 | A2M  | C4-C5-N7    | -2.16 | 107.98      | 110.62   |
| 45  | LF    | 1888 | A2M  | C4-N9-C8    | 2.16  | 108.07      | 105.73   |
| 1   | S1    | 407  | A2M  | C5'-C4'-C3' | -2.16 | 107.08      | 115.18   |
| 47  | LH    | 2768 | A2M  | C6-C5-C4    | 2.16  | 120.09      | 117.18   |
| 1   | S1    | 110  | A2M  | C4-N9-C8    | 2.16  | 108.07      | 105.73   |
| 47  | LH    | 2776 | OMG  | C2-N1-C6    | -2.16 | 121.16      | 125.10   |
| 47  | LH    | 2610 | OMG  | N1-C2-N3    | 2.16  | 127.36      | 123.32   |
| 1   | S1    | 1625 | OMC  | C4-N3-C2    | -2.16 | 116.77      | 120.25   |
| 45  | LF    | 1826 | OMG  | N2-C2-N3    | -2.16 | 115.53      | 119.73   |
| 1   | S1    | 103  | OMC  | C4-N3-C2    | -2.16 | 116.77      | 120.25   |
| 1   | S1    | 645  | A2M  | C6-C5-C4    | 2.16  | 120.09      | 117.18   |
| 45  | LF    | 1681 | OMU  | CM2-O2'-C2' | -2.16 | 108.86      | 114.52   |
| 48  | LI    | 3531 | PSU  | O2-C2-N1    | -2.16 | 120.42      | 122.79   |
| 44  | LE    | 1204 | A2M  | C6-C5-C4    | 2.16  | 120.08      | 117.18   |
| 45  | LF    | 1819 | OMG  | N1-C2-N3    | 2.16  | 127.35      | 123.32   |
| 45  | LF    | 1856 | OMG  | N2-C2-N3    | -2.16 | 115.53      | 119.73   |
| 44  | LE    | 1104 | OMG  | CM2-O2'-C2' | -2.16 | 108.86      | 114.52   |
| 1   | S1    | 1063 | A2M  | C4'-O4'-C1' | -2.16 | 104.71      | 109.47   |
| 47  | LH    | 2812 | A2M  | C5-C4-N9    | 2.16  | 108.29      | 105.78   |
| 48  | LI    | 3223 | OMG  | CM2-O2'-C2' | -2.16 | 108.87      | 114.52   |
| 48  | LI    | 3167 | PSU  | C6-C5-C4    | 2.15  | 119.70      | 118.20   |
| 1   | S1    | 1096 | A2M  | C6-C5-C4    | 2.15  | 120.08      | 117.18   |
| 1   | S1    | 179  | OMU  | CM2-O2'-C2' | -2.15 | 108.88      | 114.52   |
| 48  | LI    | 3191 | OMG  | N2-C2-N3    | -2.15 | 115.55      | 119.73   |
| 44  | LE    | 1217 | OMG  | N1-C2-N3    | 2.15  | 127.34      | 123.32   |
| 1   | S1    | 1744 | OMU  | C4-N3-C2    | -2.15 | 123.75      | 126.58   |
| 48  | LI    | 3509 | OMG  | N2-C2-N3    | -2.15 | 115.55      | 119.73   |
| 41  | LB    | 234  | PSU  | O2-C2-N1    | -2.15 | 120.42      | 122.79   |
| 47  | LH    | 2870 | OMG  | CM2-O2'-C2' | -2.15 | 108.89      | 114.52   |
| 44  | LE    | 1104 | OMG  | C2'-C1'-N9  | -2.15 | 110.05      | 114.22   |
| 45  | LF    | 1824 | OMU  | C4-N3-C2    | -2.15 | 123.75      | 126.58   |
| 44  | LE    | 1039 | A2M  | C4-N9-C8    | 2.15  | 108.06      | 105.73   |
| 1   | S1    | 1592 | PSU  | O2-C2-N1    | -2.15 | 120.43      | 122.79   |
| 48  | LI    | 3518 | 5MC  | N1-C2-N3    | -2.15 | 114.90      | 118.81   |
| 47  | LH    | 2812 | A2M  | C4-C5-N7    | -2.14 | 108.01      | 110.62   |
| 47  | LH    | 2776 | OMG  | CM2-O2'-C2' | -2.14 | 108.90      | 114.52   |
| 49  | LJ    | 3680 | PSU  | O2-C2-N1    | -2.14 | 120.43      | 122.79   |
| 45  | LF    | 1815 | A2M  | C6-C5-C4    | 2.14  | 120.06      | 117.18   |
| 44  | LE    | 1260 | PSU  | O4'-C1'-C2' | 2.14  | 108.17      | 105.14   |
| 45  | LF    | 1573 | OMC  | C4-N3-C2    | -2.14 | 116.80      | 120.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 44  | LE    | 1185 | OMU  | C4-N3-C2    | -2.14 | 123.76      | 126.58   |
| 44  | LE    | 949  | OMC  | C4-N3-C2    | -2.14 | 116.81      | 120.25   |
| 48  | LI    | 3535 | OMC  | C4-N3-C2    | -2.14 | 116.81      | 120.25   |
| 47  | LH    | 2887 | A2M  | C4-C5-N7    | -2.13 | 108.02      | 110.62   |
| 47  | LH    | 2642 | PSU  | O2-C2-N1    | -2.13 | 120.44      | 122.79   |
| 1   | S1    | 565  | A2M  | C5'-C4'-C3' | -2.13 | 107.18      | 115.18   |
| 48  | LI    | 3434 | OMG  | C2-N1-C6    | -2.13 | 121.21      | 125.10   |
| 48  | LI    | 3434 | OMG  | N2-C2-N3    | -2.13 | 115.58      | 119.73   |
| 1   | S1    | 641  | OMG  | N1-C2-N3    | 2.13  | 127.30      | 123.32   |
| 47  | LH    | 2897 | OMG  | N1-C2-N3    | 2.13  | 127.30      | 123.32   |
| 47  | LH    | 2769 | A2M  | C4-C5-N7    | -2.13 | 108.02      | 110.62   |
| 44  | LE    | 1104 | OMG  | N1-C2-N3    | 2.13  | 127.29      | 123.32   |
| 47  | LH    | 2920 | A2M  | C6-C5-C4    | 2.13  | 120.04      | 117.18   |
| 44  | LE    | 1312 | OMC  | CM2-O2'-C2' | -2.13 | 108.94      | 114.52   |
| 47  | LH    | 2806 | OMU  | CM2-O2'-C2' | -2.12 | 108.95      | 114.52   |
| 1   | S1    | 2075 | OMG  | N2-C2-N3    | -2.12 | 115.60      | 119.73   |
| 48  | LI    | 3401 | OMG  | CM2-O2'-C2' | -2.12 | 108.96      | 114.52   |
| 1   | S1    | 28   | A2M  | C4-N9-C8    | 2.12  | 108.03      | 105.73   |
| 1   | S1    | 1705 | OMG  | C2-N1-C6    | -2.12 | 121.23      | 125.10   |
| 48  | LI    | 3379 | OMG  | C2-N1-C6    | -2.11 | 121.25      | 125.10   |
| 1   | S1    | 1681 | OMG  | N1-C2-N3    | 2.11  | 127.26      | 123.32   |
| 47  | LH    | 2842 | PSU  | O4'-C1'-C2' | 2.11  | 108.12      | 105.14   |
| 1   | S1    | 1536 | OMG  | C2-N1-C6    | -2.11 | 121.25      | 125.10   |
| 45  | LF    | 1502 | A2M  | C4-C5-N7    | -2.11 | 108.05      | 110.62   |
| 1   | S1    | 1549 | A2M  | C2'-C1'-N9  | -2.11 | 109.98      | 113.53   |
| 45  | LF    | 1819 | OMG  | C2-N1-C6    | -2.11 | 121.25      | 125.10   |
| 44  | LE    | 1208 | OMG  | C2'-C3'-C4' | 2.11  | 106.57      | 101.99   |
| 47  | LH    | 2809 | A2M  | C5-C4-N9    | 2.11  | 108.23      | 105.78   |
| 47  | LH    | 2605 | OMU  | C4-N3-C2    | -2.11 | 123.80      | 126.58   |
| 1   | S1    | 403  | PSU  | O2-C2-N1    | -2.10 | 120.47      | 122.79   |
| 48  | LI    | 3379 | OMG  | CM2-O2'-C2' | -2.10 | 109.01      | 114.52   |
| 1   | S1    | 1900 | A2M  | C6-C5-C4    | 2.10  | 120.00      | 117.18   |
| 44  | LE    | 1081 | OMU  | C4-N3-C2    | -2.10 | 123.81      | 126.58   |
| 45  | LF    | 1662 | OMG  | C2-N1-C6    | -2.10 | 121.28      | 125.10   |
| 1   | S1    | 723  | A2M  | C4-C5-N7    | -2.10 | 108.06      | 110.62   |
| 1   | S1    | 649  | A2M  | C4-C5-N7    | -2.10 | 108.07      | 110.62   |
| 1   | S1    | 99   | OMC  | N4-C4-N3    | -2.10 | 114.29      | 117.97   |
| 44  | LE    | 1324 | OMG  | N1-C2-N3    | 2.09  | 127.23      | 123.32   |
| 1   | S1    | 40   | A2M  | C4-C5-N7    | -2.09 | 108.07      | 110.62   |
| 48  | LI    | 3518 | 5MC  | C1'-N1-C6   | 2.09  | 124.61      | 121.12   |
| 44  | LE    | 931  | 1MA  | C6-C5-N7    | 2.09  | 136.00      | 132.20   |
| 47  | LH    | 2920 | A2M  | C4-N9-C8    | 2.09  | 107.99      | 105.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 49  | LJ    | 3694 | OMU  | C4-N3-C2    | -2.09 | 123.83      | 126.58   |
| 47  | LH    | 2814 | A2M  | C4-C5-N7    | -2.09 | 108.07      | 110.62   |
| 45  | LF    | 1883 | OMG  | C2-N1-C6    | -2.09 | 121.29      | 125.10   |
| 47  | LH    | 2602 | OMC  | C4-N3-C2    | -2.09 | 116.89      | 120.25   |
| 45  | LF    | 1929 | A2M  | C6-C5-C4    | 2.08  | 119.99      | 117.18   |
| 45  | LF    | 1553 | OMU  | CM2-O2'-C2' | -2.08 | 109.06      | 114.52   |
| 48  | LI    | 3214 | 6MZ  | C4-N9-C8    | 2.08  | 107.98      | 105.73   |
| 44  | LE    | 1208 | OMG  | C2'-C1'-N9  | -2.08 | 110.19      | 114.22   |
| 47  | LH    | 2776 | OMG  | N1-C2-N3    | 2.08  | 127.20      | 123.32   |
| 47  | LH    | 2636 | JMH  | C31-N3-C2   | 2.08  | 120.95      | 117.31   |
| 45  | LF    | 1683 | OMG  | CM2-O2'-C2' | -2.08 | 109.07      | 114.52   |
| 45  | LF    | 1891 | A2M  | C6-C5-C4    | 2.08  | 119.98      | 117.18   |
| 48  | LI    | 3348 | A2M  | C4-C5-N7    | -2.08 | 108.09      | 110.62   |
| 45  | LF    | 1888 | A2M  | C6-C5-C4    | 2.08  | 119.97      | 117.18   |
| 44  | LE    | 1171 | PSU  | O2-C2-N1    | -2.07 | 120.51      | 122.79   |
| 47  | LH    | 2708 | A2M  | C6-C5-C4    | 2.07  | 119.97      | 117.18   |
| 47  | LH    | 2879 | OMG  | C2-N1-C6    | -2.07 | 121.32      | 125.10   |
| 2   | S2    | 37   | MIA  | C12-N6-C6   | -2.07 | 119.48      | 122.55   |
| 48  | LI    | 3315 | A2M  | C4-C5-N7    | -2.07 | 108.10      | 110.62   |
| 42  | LC    | 541  | OMG  | N1-C2-N3    | 2.07  | 127.19      | 123.32   |
| 47  | LH    | 2809 | A2M  | C4-N9-C8    | 2.07  | 107.97      | 105.73   |
| 1   | S1    | 42   | OMG  | N1-C2-N3    | 2.07  | 127.19      | 123.32   |
| 42  | LC    | 541  | OMG  | C2-N1-C6    | -2.07 | 121.33      | 125.10   |
| 46  | LG    | 2154 | PSU  | O4'-C1'-C2' | 2.07  | 108.06      | 105.14   |
| 1   | S1    | 565  | A2M  | C6-C5-C4    | 2.07  | 119.96      | 117.18   |
| 48  | LI    | 3504 | OMG  | CM2-O2'-C2' | -2.07 | 109.10      | 114.52   |
| 48  | LI    | 3187 | OMG  | N1-C2-N3    | 2.06  | 127.18      | 123.32   |
| 48  | LI    | 3434 | OMG  | CM2-O2'-C2' | -2.06 | 109.11      | 114.52   |
| 1   | S1    | 621  | OMC  | N4-C4-N3    | -2.06 | 114.35      | 117.97   |
| 42  | LC    | 628  | OMG  | N2-C2-N3    | -2.06 | 115.72      | 119.73   |
| 40  | LA    | 97   | A2M  | C4-C5-N7    | -2.06 | 108.11      | 110.62   |
| 47  | LH    | 2883 | OMG  | N1-C2-N3    | 2.06  | 127.16      | 123.32   |
| 48  | LI    | 3379 | OMG  | N1-C2-N3    | 2.06  | 127.16      | 123.32   |
| 2   | S2    | 37   | MIA  | C4-C5-N7    | -2.06 | 108.11      | 110.62   |
| 47  | LH    | 2897 | OMG  | C2-N1-C6    | -2.06 | 121.35      | 125.10   |
| 47  | LH    | 2768 | A2M  | C4-N9-C8    | 2.05  | 107.95      | 105.73   |
| 42  | LC    | 631  | OMG  | C2-N1-C6    | -2.05 | 121.35      | 125.10   |
| 47  | LH    | 2870 | OMG  | N1-C2-N3    | 2.05  | 127.16      | 123.32   |
| 47  | LH    | 2769 | A2M  | C6-C5-C4    | 2.05  | 119.94      | 117.18   |
| 40  | LA    | 41   | OMG  | N2-C2-N3    | -2.05 | 115.74      | 119.73   |
| 46  | LG    | 2146 | OMG  | N1-C2-N3    | 2.05  | 127.15      | 123.32   |
| 42  | LC    | 628  | OMG  | C2-N1-C6    | -2.05 | 121.36      | 125.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | LG    | 2009 | OMG  | C2-N1-C6    | -2.05 | 121.36      | 125.10   |
| 1   | S1    | 2116 | PSU  | O2-C2-N1    | -2.05 | 120.53      | 122.79   |
| 48  | LI    | 3348 | A2M  | C6-C5-C4    | 2.05  | 119.94      | 117.18   |
| 48  | LI    | 3535 | OMC  | CM2-O2'-C2' | -2.05 | 109.15      | 114.52   |
| 1   | S1    | 1681 | OMG  | C2-N1-C6    | -2.05 | 121.36      | 125.10   |
| 1   | S1    | 649  | A2M  | C6-C5-C4    | 2.05  | 119.94      | 117.18   |
| 48  | LI    | 3208 | OMC  | N4-C4-N3    | -2.05 | 114.38      | 117.97   |
| 1   | S1    | 2144 | 5MC  | C1'-N1-C2   | -2.05 | 113.86      | 118.42   |
| 1   | S1    | 42   | OMG  | N2-C2-N3    | -2.05 | 115.75      | 119.73   |
| 44  | LE    | 1218 | OMC  | N4-C4-N3    | -2.04 | 114.38      | 117.97   |
| 44  | LE    | 1165 | OMC  | C4-N3-C2    | -2.04 | 116.95      | 120.25   |
| 1   | S1    | 1966 | OMU  | CM2-O2'-C2' | -2.04 | 109.16      | 114.52   |
| 47  | LH    | 2358 | A2M  | C4-C5-N7    | -2.04 | 108.13      | 110.62   |
| 47  | LH    | 2242 | OMC  | N4-C4-N3    | -2.04 | 114.38      | 117.97   |
| 1   | S1    | 390  | OMG  | N2-C2-N3    | -2.04 | 115.76      | 119.73   |
| 47  | LH    | 2708 | A2M  | C4-C5-N7    | -2.04 | 108.13      | 110.62   |
| 47  | LH    | 2685 | OMC  | C1'-N1-C6   | -2.04 | 116.39      | 120.84   |
| 48  | LI    | 3377 | OMG  | C2-N1-C6    | -2.04 | 121.38      | 125.10   |
| 48  | LI    | 3223 | OMG  | N1-C2-N3    | 2.04  | 127.13      | 123.32   |
| 47  | LH    | 2679 | PSU  | O2-C2-N1    | -2.04 | 120.55      | 122.79   |
| 44  | LE    | 1106 | A2M  | C6-C5-C4    | 2.04  | 119.92      | 117.18   |
| 48  | LI    | 3504 | OMG  | N2-C2-N3    | -2.04 | 115.77      | 119.73   |
| 44  | LE    | 1121 | A2M  | C6-C5-C4    | 2.04  | 119.92      | 117.18   |
| 1   | S1    | 2123 | OMC  | N4-C4-N3    | -2.04 | 114.39      | 117.97   |
| 45  | LF    | 1683 | OMG  | N1-C2-N3    | 2.04  | 127.12      | 123.32   |
| 42  | LC    | 537  | OMC  | N4-C4-N3    | -2.04 | 114.39      | 117.97   |
| 47  | LH    | 2610 | OMG  | N2-C2-N3    | -2.04 | 115.77      | 119.73   |
| 47  | LH    | 2870 | OMG  | N2-C2-N3    | -2.03 | 115.77      | 119.73   |
| 46  | LG    | 2022 | A2M  | C4-C5-N7    | -2.03 | 108.14      | 110.62   |
| 45  | LF    | 1662 | OMG  | CM2-O2'-C2' | -2.03 | 109.19      | 114.52   |
| 48  | LI    | 3315 | A2M  | C6-C5-C4    | 2.03  | 119.92      | 117.18   |
| 1   | S1    | 2078 | 7MG  | C5-C4-N3    | -2.03 | 124.26      | 128.13   |
| 42  | LC    | 631  | OMG  | N1-C2-N3    | 2.03  | 127.12      | 123.32   |
| 48  | LI    | 3315 | A2M  | C5'-C4'-C3' | -2.03 | 107.57      | 115.18   |
| 47  | LH    | 2349 | A2M  | C4-C5-N7    | -2.03 | 108.15      | 110.62   |
| 44  | LE    | 1165 | OMC  | C1'-N1-C2   | 2.03  | 122.95      | 118.42   |
| 1   | S1    | 2078 | 7MG  | C6-C5-N7    | -2.03 | 128.72      | 131.91   |
| 48  | LI    | 3367 | A2M  | C4-N9-C8    | 2.03  | 107.93      | 105.73   |
| 1   | S1    | 390  | OMG  | C2-N1-C6    | -2.03 | 121.40      | 125.10   |
| 45  | LF    | 1573 | OMC  | N4-C4-N3    | -2.03 | 114.41      | 117.97   |
| 40  | LA    | 39   | A2M  | C5'-C4'-C3' | -2.02 | 107.60      | 115.18   |
| 45  | LF    | 1957 | OMU  | CM2-O2'-C2' | -2.02 | 109.22      | 114.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | LH    | 2883 | OMG  | N2-C2-N3    | -2.02 | 115.80      | 119.73   |
| 48  | LI    | 3401 | OMG  | O6-C6-N1    | -2.02 | 116.24      | 120.12   |
| 41  | LB    | 215  | OMG  | N2-C2-N3    | -2.02 | 115.80      | 119.73   |
| 1   | S1    | 1371 | A2M  | C6-C5-C4    | 2.02  | 119.89      | 117.18   |
| 45  | LF    | 1835 | OMG  | O6-C6-N1    | -2.02 | 116.25      | 120.12   |
| 1   | S1    | 390  | OMG  | N1-C2-N3    | 2.02  | 127.09      | 123.32   |
| 44  | LE    | 1118 | PSU  | C5-C4-N3    | 2.01  | 121.14      | 116.58   |
| 47  | LH    | 2825 | OMC  | C4-N3-C2    | -2.01 | 117.00      | 120.25   |
| 47  | LH    | 2814 | A2M  | C5-C4-N9    | 2.01  | 108.12      | 105.78   |
| 46  | LG    | 2125 | PSU  | O4'-C1'-C2' | 2.01  | 107.98      | 105.14   |
| 48  | LI    | 3568 | PSU  | O4'-C1'-C2' | 2.01  | 107.98      | 105.14   |
| 48  | LI    | 3187 | OMG  | C2-N1-C6    | -2.01 | 121.44      | 125.10   |
| 1   | S1    | 640  | PSU  | C6-C5-C4    | 2.01  | 119.60      | 118.20   |
| 42  | LC    | 483  | OMC  | N4-C4-N3    | -2.01 | 114.44      | 117.97   |
| 48  | LI    | 3521 | A2M  | C4-C5-N7    | -2.01 | 108.18      | 110.62   |
| 48  | LI    | 3451 | PSU  | O4'-C1'-C2' | 2.00  | 107.97      | 105.14   |
| 49  | LJ    | 3644 | PSU  | O4'-C1'-C2' | 2.00  | 107.97      | 105.14   |
| 1   | S1    | 1625 | OMC  | N4-C4-N3    | -2.00 | 114.45      | 117.97   |
| 1   | S1    | 1536 | OMG  | O6-C6-N1    | -2.00 | 116.28      | 120.12   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | S1    | 1601 | B8N  | C33  |

All (333) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | S1    | 57  | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 57  | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 110 | A2M  | C1'-C2'-O2'-CM' |
| 1   | S1    | 180 | OMG  | C1'-C2'-O2'-CM2 |
| 1   | S1    | 280 | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 403 | PSU  | C2'-C1'-C5-C4   |
| 1   | S1    | 403 | PSU  | O4'-C1'-C5-C4   |
| 1   | S1    | 403 | PSU  | O4'-C1'-C5-C6   |
| 1   | S1    | 565 | A2M  | C3'-C4'-C5'-O5' |
| 1   | S1    | 621 | OMC  | C3'-C4'-C5'-O5' |
| 1   | S1    | 621 | OMC  | O4'-C4'-C5'-O5' |
| 1   | S1    | 640 | PSU  | C2'-C1'-C5-C4   |
| 1   | S1    | 649 | A2M  | C3'-C4'-C5'-O5' |
| 1   | S1    | 704 | OMU  | C1'-C2'-O2'-CM2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | S1    | 1063 | A2M  | C1'-C2'-O2'-CM' |
| 1   | S1    | 1371 | A2M  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1371 | A2M  | C3'-C4'-C5'-O5' |
| 1   | S1    | 1536 | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1536 | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 1549 | A2M  | C3'-C4'-C5'-O5' |
| 1   | S1    | 1601 | B8N  | C32-C31-N3-C2   |
| 1   | S1    | 1601 | B8N  | C32-C31-N3-C4   |
| 1   | S1    | 1624 | PSU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 1624 | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1966 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | S1    | 2041 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | S1    | 2101 | PSU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2101 | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 2180 | A2M  | O4'-C1'-N9-C8   |
| 1   | S1    | 2180 | A2M  | O4'-C1'-N9-C4   |
| 1   | S1    | 2288 | MA6  | O4'-C4'-C5'-O5' |
| 1   | S1    | 2305 | PSU  | O4'-C1'-C5-C6   |
| 2   | S2    | 37   | MIA  | N1-C2-S10-C11   |
| 2   | S2    | 37   | MIA  | N3-C2-S10-C11   |
| 2   | S2    | 37   | MIA  | C12-C13-C14-C15 |
| 2   | S2    | 37   | MIA  | C12-C13-C14-C16 |
| 40  | LA    | 74   | OMG  | C1'-C2'-O2'-CM2 |
| 40  | LA    | 97   | A2M  | O4'-C4'-C5'-O5' |
| 40  | LA    | 97   | A2M  | C3'-C4'-C5'-O5' |
| 41  | LB    | 215  | OMG  | C1'-C2'-O2'-CM2 |
| 41  | LB    | 247  | OMU  | C3'-C4'-C5'-O5' |
| 41  | LB    | 247  | OMU  | O4'-C4'-C5'-O5' |
| 41  | LB    | 281  | PSU  | C2'-C1'-C5-C4   |
| 42  | LC    | 302  | PSU  | C3'-C4'-C5'-O5' |
| 42  | LC    | 302  | PSU  | O4'-C4'-C5'-O5' |
| 42  | LC    | 537  | OMC  | C3'-C4'-C5'-O5' |
| 42  | LC    | 537  | OMC  | O4'-C4'-C5'-O5' |
| 42  | LC    | 541  | OMG  | C1'-C2'-O2'-CM2 |
| 42  | LC    | 577  | OMC  | C1'-C2'-O2'-CM2 |
| 44  | LE    | 935  | A2M  | O4'-C4'-C5'-O5' |
| 44  | LE    | 936  | OMC  | C3'-C4'-C5'-O5' |
| 44  | LE    | 936  | OMC  | O4'-C4'-C5'-O5' |
| 44  | LE    | 1075 | PSU  | C2'-C1'-C5-C4   |
| 44  | LE    | 1075 | PSU  | C2'-C1'-C5-C6   |
| 44  | LE    | 1075 | PSU  | O4'-C4'-C5'-O5' |
| 44  | LE    | 1081 | OMU  | C1'-C2'-O2'-CM2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 44  | LE    | 1118 | PSU  | O4'-C1'-C5-C4   |
| 44  | LE    | 1118 | PSU  | O4'-C1'-C5-C6   |
| 44  | LE    | 1126 | PSU  | C2'-C1'-C5-C4   |
| 44  | LE    | 1126 | PSU  | O4'-C1'-C5-C4   |
| 44  | LE    | 1126 | PSU  | O4'-C1'-C5-C6   |
| 44  | LE    | 1165 | OMC  | O4'-C1'-N1-C2   |
| 44  | LE    | 1165 | OMC  | O4'-C1'-N1-C6   |
| 44  | LE    | 1185 | OMU  | C1'-C2'-O2'-CM2 |
| 45  | LF    | 1573 | OMC  | O4'-C1'-N1-C2   |
| 45  | LF    | 1573 | OMC  | O4'-C1'-N1-C6   |
| 45  | LF    | 1573 | OMC  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1662 | OMG  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1667 | OMG  | C1'-C2'-O2'-CM2 |
| 45  | LF    | 1681 | OMU  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1819 | OMG  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1819 | OMG  | C1'-C2'-O2'-CM2 |
| 45  | LF    | 1835 | OMG  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1835 | OMG  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1856 | OMG  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1976 | OMC  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1976 | OMC  | O4'-C4'-C5'-O5' |
| 46  | LG    | 2022 | A2M  | O4'-C4'-C5'-O5' |
| 46  | LG    | 2022 | A2M  | C3'-C4'-C5'-O5' |
| 46  | LG    | 2129 | OMU  | C1'-C2'-O2'-CM2 |
| 46  | LG    | 2146 | OMG  | O4'-C4'-C5'-O5' |
| 46  | LG    | 2171 | PSU  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2242 | OMC  | C1'-C2'-O2'-CM2 |
| 47  | LH    | 2349 | A2M  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2358 | A2M  | C1'-C2'-O2'-CM' |
| 47  | LH    | 2602 | OMC  | C2'-C1'-N1-C2   |
| 47  | LH    | 2602 | OMC  | C2'-C1'-N1-C6   |
| 47  | LH    | 2636 | JMH  | O4'-C1'-N1-C2   |
| 47  | LH    | 2636 | JMH  | O4'-C1'-N1-C6   |
| 47  | LH    | 2685 | OMC  | C2'-C1'-N1-C2   |
| 47  | LH    | 2685 | OMC  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2713 | OMU  | C1'-C2'-O2'-CM2 |
| 47  | LH    | 2713 | OMU  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2742 | PSU  | O4'-C1'-C5-C4   |
| 47  | LH    | 2742 | PSU  | O4'-C1'-C5-C6   |
| 47  | LH    | 2746 | PSU  | C2'-C1'-C5-C4   |
| 47  | LH    | 2746 | PSU  | O4'-C1'-C5-C4   |
| 47  | LH    | 2746 | PSU  | O4'-C1'-C5-C6   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | LH    | 2769 | A2M  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2776 | OMG  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2802 | PSU  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2812 | A2M  | C1'-C2'-O2'-CM' |
| 47  | LH    | 2835 | OMU  | C1'-C2'-O2'-CM2 |
| 47  | LH    | 2835 | OMU  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2849 | A2M  | C1'-C2'-O2'-CM' |
| 47  | LH    | 2853 | OMC  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2853 | OMC  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2879 | OMG  | C1'-C2'-O2'-CM2 |
| 47  | LH    | 2887 | A2M  | C1'-C2'-O2'-CM' |
| 47  | LH    | 2899 | PSU  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2920 | A2M  | C1'-C2'-O2'-CM' |
| 47  | LH    | 2925 | OMG  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2925 | OMG  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2925 | OMG  | C1'-C2'-O2'-CM2 |
| 48  | LI    | 3167 | PSU  | C2'-C1'-C5-C4   |
| 48  | LI    | 3167 | PSU  | O4'-C1'-C5-C4   |
| 48  | LI    | 3167 | PSU  | O4'-C1'-C5-C6   |
| 48  | LI    | 3191 | OMG  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3191 | OMG  | C1'-C2'-O2'-CM2 |
| 48  | LI    | 3208 | OMC  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3208 | OMC  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3214 | 6MZ  | N1-C6-N6-C9     |
| 48  | LI    | 3315 | A2M  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3377 | OMG  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3446 | PSU  | C2'-C1'-C5-C4   |
| 48  | LI    | 3446 | PSU  | C2'-C1'-C5-C6   |
| 49  | LJ    | 3636 | OMU  | C1'-C2'-O2'-CM2 |
| 49  | LJ    | 3718 | OMU  | C1'-C2'-O2'-CM2 |
| 51  | LL    | 3906 | A2M  | O4'-C4'-C5'-O5' |
| 51  | LL    | 3906 | A2M  | C3'-C4'-C5'-O5' |
| 52  | LM    | 3957 | OMC  | O4'-C4'-C5'-O5' |
| 1   | S1    | 8    | OMU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 176  | PSU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 176  | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 280  | PSU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 485  | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 723  | A2M  | O4'-C4'-C5'-O5' |
| 1   | S1    | 723  | A2M  | C3'-C4'-C5'-O5' |
| 1   | S1    | 1068 | PSU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 1068 | PSU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | S1    | 1096 | A2M  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2075 | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 2078 | 7MG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2142 | OMC  | O4'-C4'-C5'-O5' |
| 1   | S1    | 2288 | MA6  | C3'-C4'-C5'-O5' |
| 42  | LC    | 483  | OMC  | C3'-C4'-C5'-O5' |
| 42  | LC    | 483  | OMC  | O4'-C4'-C5'-O5' |
| 44  | LE    | 935  | A2M  | C3'-C4'-C5'-O5' |
| 44  | LE    | 1075 | PSU  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1504 | OMU  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1856 | OMG  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1929 | A2M  | O4'-C4'-C5'-O5' |
| 46  | LG    | 2146 | OMG  | C3'-C4'-C5'-O5' |
| 46  | LG    | 2171 | PSU  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2349 | A2M  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2713 | OMU  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2768 | A2M  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2768 | A2M  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2776 | OMG  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3042 | PSU  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3167 | PSU  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3191 | OMG  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3214 | 6MZ  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3214 | 6MZ  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3315 | A2M  | O4'-C4'-C5'-O5' |
| 49  | LJ    | 3697 | PSU  | C3'-C4'-C5'-O5' |
| 52  | LM    | 3957 | OMC  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2685 | OMC  | C2'-C1'-N1-C6   |
| 1   | S1    | 390  | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 565  | A2M  | O4'-C4'-C5'-O5' |
| 1   | S1    | 649  | A2M  | O4'-C4'-C5'-O5' |
| 1   | S1    | 682  | OMU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 682  | OMU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1549 | A2M  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1711 | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 2075 | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2078 | 7MG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 2305 | PSU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2305 | PSU  | O4'-C4'-C5'-O5' |
| 44  | LE    | 1260 | PSU  | C3'-C4'-C5'-O5' |
| 44  | LE    | 1260 | PSU  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1662 | OMG  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 45  | LF    | 1819 | OMG  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1929 | A2M  | C3'-C4'-C5'-O5' |
| 46  | LG    | 2005 | A2M  | O4'-C4'-C5'-O5' |
| 46  | LG    | 2005 | A2M  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2685 | OMC  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2744 | A2M  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2744 | A2M  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2769 | A2M  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2802 | PSU  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3167 | PSU  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3377 | OMG  | O4'-C4'-C5'-O5' |
| 49  | LJ    | 3697 | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 8    | OMU  | C2'-C1'-N1-C6   |
| 1   | S1    | 485  | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2142 | OMC  | C3'-C4'-C5'-O5' |
| 1   | S1    | 180  | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 180  | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 390  | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 640  | PSU  | C3'-C4'-C5'-O5' |
| 42  | LC    | 308  | PSU  | C3'-C4'-C5'-O5' |
| 49  | LJ    | 3694 | OMU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 1096 | A2M  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1554 | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1711 | PSU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2116 | PSU  | C3'-C4'-C5'-O5' |
| 40  | LA    | 74   | OMG  | O4'-C4'-C5'-O5' |
| 42  | LC    | 491  | OMU  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1504 | OMU  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1573 | OMC  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1667 | OMG  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1681 | OMU  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1926 | PSU  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1957 | OMU  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2242 | OMC  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2835 | OMU  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2899 | PSU  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3456 | 5MC  | C2'-C1'-N1-C6   |
| 42  | LC    | 491  | OMU  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1667 | OMG  | C3'-C4'-C5'-O5' |
| 42  | LC    | 308  | PSU  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3446 | PSU  | O4'-C4'-C5'-O5' |
| 42  | LC    | 577  | OMC  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | LH    | 2242 | OMC  | C3'-C4'-C5'-O5' |
| 1   | S1    | 640  | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 641  | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1900 | A2M  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1900 | A2M  | C3'-C4'-C5'-O5' |
| 40  | LA    | 74   | OMG  | C3'-C4'-C5'-O5' |
| 44  | LE    | 949  | OMC  | C1'-C2'-O2'-CM2 |
| 1   | S1    | 8    | OMU  | O4'-C1'-N1-C6   |
| 1   | S1    | 8    | OMU  | C2'-C1'-N1-C2   |
| 1   | S1    | 407  | A2M  | C2'-C1'-N9-C4   |
| 1   | S1    | 723  | A2M  | C2'-C1'-N9-C8   |
| 47  | LH    | 2812 | A2M  | C2'-C1'-N9-C8   |
| 48  | LI    | 3456 | 5MC  | O4'-C1'-N1-C6   |
| 1   | S1    | 1096 | A2M  | C4'-C5'-O5'-P   |
| 1   | S1    | 1705 | OMG  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1705 | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 2116 | PSU  | O4'-C4'-C5'-O5' |
| 41  | LB    | 280  | PSU  | C3'-C4'-C5'-O5' |
| 41  | LB    | 280  | PSU  | O4'-C4'-C5'-O5' |
| 45  | LF    | 1926 | PSU  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3042 | PSU  | C3'-C4'-C5'-O5' |
| 49  | LJ    | 3694 | OMU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 103  | OMC  | O4'-C1'-N1-C6   |
| 1   | S1    | 407  | A2M  | C2'-C1'-N9-C8   |
| 1   | S1    | 57   | OMG  | C4'-C5'-O5'-P   |
| 1   | S1    | 1063 | A2M  | C4'-C5'-O5'-P   |
| 48  | LI    | 3042 | PSU  | C4'-C5'-O5'-P   |
| 48  | LI    | 3214 | 6MZ  | C4'-C5'-O5'-P   |
| 48  | LI    | 3510 | PSU  | C4'-C5'-O5'-P   |
| 1   | S1    | 99   | OMC  | O4'-C4'-C5'-O5' |
| 41  | LB    | 281  | PSU  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2610 | OMG  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3456 | 5MC  | C2'-C1'-N1-C2   |
| 1   | S1    | 8    | OMU  | O4'-C1'-N1-C2   |
| 1   | S1    | 1068 | PSU  | C4'-C5'-O5'-P   |
| 41  | LB    | 247  | OMU  | C4'-C5'-O5'-P   |
| 46  | LG    | 2022 | A2M  | C4'-C5'-O5'-P   |
| 44  | LE    | 1222 | OMU  | O4'-C1'-N1-C6   |
| 47  | LH    | 2602 | OMC  | O4'-C1'-N1-C6   |
| 45  | LF    | 1819 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | LI    | 3355 | OMC  | C3'-C2'-O2'-CM2 |
| 47  | LH    | 2602 | OMC  | O4'-C1'-N1-C2   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 48  | LI    | 3456 | 5MC  | O4'-C1'-N1-C2   |
| 44  | LE    | 931  | 1MA  | C2'-C1'-N9-C8   |
| 1   | S1    | 280  | PSU  | C4'-C5'-O5'-P   |
| 41  | LB    | 234  | PSU  | C4'-C5'-O5'-P   |
| 42  | LC    | 567  | PSU  | C4'-C5'-O5'-P   |
| 45  | LF    | 1957 | OMU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 641  | OMG  | C3'-C4'-C5'-O5' |
| 1   | S1    | 103  | OMC  | O4'-C1'-N1-C2   |
| 41  | LB    | 247  | OMU  | C2'-C1'-N1-C6   |
| 1   | S1    | 280  | PSU  | O4'-C1'-C5-C4   |
| 1   | S1    | 1715 | PSU  | O4'-C1'-C5-C4   |
| 47  | LH    | 2802 | PSU  | O4'-C1'-C5-C4   |
| 48  | LI    | 2999 | PSU  | O4'-C1'-C5-C4   |
| 48  | LI    | 3206 | PSU  | O4'-C1'-C5-C4   |
| 48  | LI    | 3531 | PSU  | O4'-C1'-C5-C4   |
| 1   | S1    | 8    | OMU  | C3'-C2'-O2'-CM2 |
| 1   | S1    | 645  | A2M  | C3'-C2'-O2'-CM' |
| 45  | LF    | 1573 | OMC  | C3'-C2'-O2'-CM2 |
| 47  | LH    | 2602 | OMC  | C3'-C2'-O2'-CM2 |
| 48  | LI    | 3223 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | LI    | 3504 | OMG  | C3'-C2'-O2'-CM2 |
| 49  | LJ    | 3688 | OMG  | C3'-C2'-O2'-CM2 |
| 44  | LE    | 1222 | OMU  | C2'-C1'-N1-C6   |
| 47  | LH    | 2812 | A2M  | O4'-C1'-N9-C8   |
| 1   | S1    | 1601 | B8N  | N34-C33-C34-O35 |
| 47  | LH    | 2685 | OMC  | O4'-C1'-N1-C6   |
| 44  | LE    | 931  | 1MA  | C2'-C1'-N9-C4   |
| 1   | S1    | 110  | A2M  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3171 | OMU  | C3'-C4'-C5'-O5' |
| 1   | S1    | 645  | A2M  | O4'-C1'-N9-C8   |
| 47  | LH    | 2769 | A2M  | C4'-C5'-O5'-P   |
| 47  | LH    | 2776 | OMG  | C4'-C5'-O5'-P   |
| 1   | S1    | 186  | OMU  | O4'-C4'-C5'-O5' |
| 42  | LC    | 577  | OMC  | C3'-C4'-C5'-O5' |
| 47  | LH    | 2586 | PSU  | O4'-C4'-C5'-O5' |
| 1   | S1    | 1625 | OMC  | C1'-C2'-O2'-CM2 |
| 46  | LG    | 2009 | OMG  | C1'-C2'-O2'-CM2 |
| 48  | LI    | 3367 | A2M  | C1'-C2'-O2'-CM' |
| 48  | LI    | 3500 | A2M  | C1'-C2'-O2'-CM' |
| 49  | LJ    | 3688 | OMG  | C1'-C2'-O2'-CM2 |
| 48  | LI    | 3208 | OMC  | O4'-C1'-N1-C6   |
| 1   | S1    | 103  | OMC  | C2'-C1'-N1-C2   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | S1    | 407  | A2M  | O4'-C1'-N9-C8   |
| 1   | S1    | 723  | A2M  | O4'-C1'-N9-C8   |
| 44  | LE    | 1106 | A2M  | O4'-C1'-N9-C8   |
| 46  | LG    | 2125 | PSU  | C3'-C4'-C5'-O5' |
| 48  | LI    | 3171 | OMU  | O4'-C4'-C5'-O5' |
| 48  | LI    | 3208 | OMC  | C2'-C1'-N1-C6   |
| 44  | LE    | 1260 | PSU  | O4'-C1'-C5-C6   |
| 47  | LH    | 2802 | PSU  | O4'-C1'-C5-C6   |
| 44  | LE    | 1222 | OMU  | C2'-C1'-N1-C2   |
| 45  | LF    | 1822 | OMC  | C2'-C1'-N1-C2   |
| 44  | LE    | 1222 | OMU  | O4'-C1'-N1-C2   |
| 45  | LF    | 1819 | OMG  | C4'-C5'-O5'-P   |
| 1   | S1    | 1554 | PSU  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1568 | PSU  | O4'-C4'-C5'-O5' |
| 41  | LB    | 247  | OMU  | C2'-C1'-N1-C2   |
| 48  | LI    | 3500 | A2M  | C3'-C2'-O2'-CM' |
| 41  | LB    | 281  | PSU  | C3'-C4'-C5'-O5' |
| 44  | LE    | 1106 | A2M  | C3'-C4'-C5'-O5' |
| 45  | LF    | 1822 | OMC  | O4'-C4'-C5'-O5' |
| 47  | LH    | 2766 | 5MC  | O4'-C4'-C5'-O5' |
| 49  | LJ    | 3680 | PSU  | O4'-C4'-C5'-O5' |
| 42  | LC    | 483  | OMC  | C2'-C1'-N1-C2   |
| 1   | S1    | 1371 | A2M  | C4'-C5'-O5'-P   |
| 1   | S1    | 723  | A2M  | C2'-C1'-N9-C4   |
| 47  | LH    | 2812 | A2M  | C2'-C1'-N9-C4   |

There are no ring outliers.

174 monomers are involved in 259 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 47  | LH    | 2879 | OMG  | 1       | 0            |
| 47  | LH    | 2617 | PSU  | 1       | 0            |
| 40  | LA    | 16   | PSU  | 1       | 0            |
| 47  | LH    | 2361 | PSU  | 1       | 0            |
| 48  | LI    | 3509 | OMG  | 3       | 0            |
| 41  | LB    | 183  | A2M  | 1       | 0            |
| 1   | S1    | 393  | OMC  | 1       | 0            |
| 44  | LE    | 938  | 7MG  | 1       | 0            |
| 44  | LE    | 949  | OMC  | 3       | 0            |
| 1   | S1    | 1705 | OMG  | 1       | 0            |
| 1   | S1    | 28   | A2M  | 3       | 0            |
| 42  | LC    | 541  | OMG  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 47  | LH    | 2348 | OMC  | 1       | 0            |
| 48  | LI    | 3546 | OMC  | 1       | 0            |
| 45  | LF    | 1856 | OMG  | 5       | 0            |
| 1   | S1    | 1966 | OMU  | 2       | 0            |
| 48  | LI    | 3500 | A2M  | 2       | 0            |
| 45  | LF    | 1929 | A2M  | 1       | 0            |
| 47  | LH    | 2909 | OMU  | 2       | 0            |
| 46  | LG    | 2129 | OMU  | 1       | 0            |
| 45  | LF    | 1502 | A2M  | 1       | 0            |
| 44  | LE    | 1185 | OMU  | 1       | 0            |
| 45  | LF    | 1859 | PSU  | 1       | 0            |
| 47  | LH    | 2610 | OMG  | 1       | 0            |
| 47  | LH    | 2605 | OMU  | 3       | 0            |
| 47  | LH    | 2812 | A2M  | 2       | 0            |
| 45  | LF    | 1976 | OMC  | 1       | 0            |
| 44  | LE    | 1204 | A2M  | 2       | 0            |
| 44  | LE    | 1104 | OMG  | 1       | 0            |
| 1   | S1    | 533  | A2M  | 1       | 0            |
| 45  | LF    | 1586 | PSU  | 2       | 0            |
| 1   | S1    | 89   | PSU  | 1       | 0            |
| 47  | LH    | 2835 | OMU  | 1       | 0            |
| 44  | LE    | 1198 | PSU  | 1       | 0            |
| 1   | S1    | 640  | PSU  | 1       | 0            |
| 48  | LI    | 3446 | PSU  | 1       | 0            |
| 47  | LH    | 2713 | OMU  | 1       | 0            |
| 48  | LI    | 3379 | OMG  | 1       | 0            |
| 45  | LF    | 1582 | PSU  | 1       | 0            |
| 48  | LI    | 3208 | OMC  | 3       | 0            |
| 49  | LJ    | 3694 | OMU  | 2       | 0            |
| 53  | LN    | 3969 | PSU  | 2       | 0            |
| 1   | S1    | 2041 | OMU  | 1       | 0            |
| 44  | LE    | 1452 | OMU  | 1       | 0            |
| 41  | LB    | 247  | OMU  | 4       | 0            |
| 47  | LH    | 2621 | PSU  | 2       | 0            |
| 1   | S1    | 704  | OMU  | 3       | 0            |
| 47  | LH    | 2754 | PSU  | 2       | 0            |
| 1   | S1    | 1601 | B8N  | 1       | 0            |
| 1   | S1    | 1660 | PSU  | 1       | 0            |
| 46  | LG    | 2154 | PSU  | 1       | 0            |
| 48  | LI    | 3542 | PSU  | 1       | 0            |
| 1   | S1    | 723  | A2M  | 2       | 0            |
| 1   | S1    | 1625 | OMC  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 40  | LA    | 97   | A2M  | 1       | 0            |
| 47  | LH    | 2642 | PSU  | 2       | 0            |
| 47  | LH    | 2870 | OMG  | 1       | 0            |
| 52  | LM    | 3963 | PSU  | 1       | 0            |
| 44  | LE    | 1121 | A2M  | 2       | 0            |
| 48  | LI    | 3374 | OMC  | 2       | 0            |
| 1   | S1    | 121  | PSU  | 1       | 0            |
| 47  | LH    | 2602 | OMC  | 3       | 0            |
| 44  | LE    | 1201 | OMG  | 2       | 0            |
| 46  | LG    | 2022 | A2M  | 2       | 0            |
| 1   | S1    | 1900 | A2M  | 1       | 0            |
| 44  | LE    | 1075 | PSU  | 1       | 0            |
| 48  | LI    | 3159 | OMU  | 1       | 0            |
| 47  | LH    | 2842 | PSU  | 1       | 0            |
| 48  | LI    | 3367 | A2M  | 1       | 0            |
| 44  | LE    | 1081 | OMU  | 1       | 0            |
| 1   | S1    | 2116 | PSU  | 1       | 0            |
| 48  | LI    | 3434 | OMG  | 1       | 0            |
| 48  | LI    | 3167 | PSU  | 1       | 0            |
| 1   | S1    | 1096 | A2M  | 2       | 0            |
| 1   | S1    | 2288 | MA6  | 1       | 0            |
| 45  | LF    | 1681 | OMU  | 1       | 0            |
| 47  | LH    | 2897 | OMG  | 1       | 0            |
| 1   | S1    | 1641 | OMU  | 2       | 0            |
| 42  | LC    | 537  | OMC  | 3       | 0            |
| 44  | LE    | 935  | A2M  | 3       | 0            |
| 1   | S1    | 2046 | A2M  | 1       | 0            |
| 48  | LI    | 3451 | PSU  | 1       | 0            |
| 48  | LI    | 3465 | OMC  | 1       | 0            |
| 1   | S1    | 180  | OMG  | 5       | 0            |
| 48  | LI    | 3377 | OMG  | 1       | 0            |
| 47  | LH    | 2920 | A2M  | 2       | 0            |
| 1   | S1    | 649  | A2M  | 2       | 0            |
| 44  | LE    | 1171 | PSU  | 1       | 0            |
| 48  | LI    | 3521 | A2M  | 2       | 0            |
| 1   | S1    | 1393 | PSU  | 1       | 0            |
| 49  | LJ    | 3636 | OMU  | 2       | 0            |
| 44  | LE    | 936  | OMC  | 1       | 0            |
| 48  | LI    | 3503 | PSU  | 1       | 0            |
| 44  | LE    | 931  | 1MA  | 1       | 0            |
| 40  | LA    | 74   | OMG  | 2       | 0            |
| 1   | S1    | 2287 | MA6  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | S1    | 403  | PSU  | 1       | 0            |
| 1   | S1    | 110  | A2M  | 2       | 0            |
| 1   | S1    | 1037 | OMC  | 1       | 0            |
| 45  | LF    | 1822 | OMC  | 2       | 0            |
| 1   | S1    | 1681 | OMG  | 1       | 0            |
| 48  | LI    | 3518 | 5MC  | 2       | 0            |
| 1   | S1    | 565  | A2M  | 1       | 0            |
| 47  | LH    | 2849 | A2M  | 5       | 0            |
| 1   | S1    | 57   | OMG  | 1       | 0            |
| 52  | LM    | 3957 | OMC  | 1       | 0            |
| 45  | LF    | 1815 | A2M  | 1       | 0            |
| 1   | S1    | 1536 | OMG  | 1       | 0            |
| 51  | LL    | 3865 | PSU  | 1       | 0            |
| 1   | S1    | 1591 | PSU  | 2       | 0            |
| 48  | LI    | 3535 | OMC  | 2       | 0            |
| 1   | S1    | 1597 | UR3  | 2       | 0            |
| 44  | LE    | 1165 | OMC  | 2       | 0            |
| 48  | LI    | 3444 | PSU  | 2       | 0            |
| 45  | LF    | 1738 | A2M  | 1       | 0            |
| 47  | LH    | 2346 | OMU  | 1       | 0            |
| 49  | LJ    | 3701 | PSU  | 1       | 0            |
| 2   | S2    | 37   | MIA  | 2       | 0            |
| 47  | LH    | 2744 | A2M  | 1       | 0            |
| 1   | S1    | 27   | PSU  | 2       | 0            |
| 48  | LI    | 3533 | A2M  | 2       | 0            |
| 44  | LE    | 1023 | PSU  | 1       | 0            |
| 48  | LI    | 3204 | PSU  | 2       | 0            |
| 49  | LJ    | 3680 | PSU  | 1       | 0            |
| 1   | S1    | 179  | OMU  | 2       | 0            |
| 1   | S1    | 1616 | OMU  | 1       | 0            |
| 48  | LI    | 3206 | PSU  | 1       | 0            |
| 47  | LH    | 2925 | OMG  | 1       | 0            |
| 48  | LI    | 3456 | 5MC  | 1       | 0            |
| 48  | LI    | 3145 | PSU  | 2       | 0            |
| 48  | LI    | 3562 | PSU  | 2       | 0            |
| 48  | LI    | 3531 | PSU  | 2       | 0            |
| 42  | LC    | 498  | PSU  | 1       | 0            |
| 48  | LI    | 3191 | OMG  | 1       | 0            |
| 42  | LC    | 594  | A2M  | 3       | 0            |
| 1   | S1    | 1960 | PSU  | 1       | 0            |
| 1   | S1    | 2180 | A2M  | 1       | 0            |
| 1   | S1    | 1371 | A2M  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | S1    | 2131 | PSU  | 1       | 0            |
| 47  | LH    | 2708 | A2M  | 2       | 0            |
| 47  | LH    | 2832 | OMC  | 2       | 0            |
| 47  | LH    | 2242 | OMC  | 1       | 0            |
| 49  | LJ    | 3718 | OMU  | 1       | 0            |
| 46  | LG    | 2125 | PSU  | 1       | 0            |
| 1   | S1    | 280  | PSU  | 1       | 0            |
| 47  | LH    | 2904 | B8H  | 1       | 0            |
| 49  | LJ    | 3644 | PSU  | 2       | 0            |
| 1   | S1    | 1549 | A2M  | 3       | 0            |
| 47  | LH    | 2358 | A2M  | 2       | 0            |
| 1   | S1    | 1624 | PSU  | 1       | 0            |
| 47  | LH    | 2887 | A2M  | 2       | 0            |
| 48  | LI    | 3214 | 6MZ  | 3       | 0            |
| 41  | LB    | 215  | OMG  | 1       | 0            |
| 40  | LA    | 41   | OMG  | 1       | 0            |
| 47  | LH    | 2802 | PSU  | 1       | 0            |
| 47  | LH    | 2899 | PSU  | 1       | 0            |
| 45  | LF    | 1891 | A2M  | 1       | 0            |
| 44  | LE    | 1363 | PSU  | 2       | 0            |
| 1   | S1    | 485  | OMG  | 2       | 0            |
| 47  | LH    | 2769 | A2M  | 2       | 0            |
| 45  | LF    | 1883 | OMG  | 1       | 0            |
| 47  | LH    | 2685 | OMC  | 2       | 0            |
| 46  | LG    | 2146 | OMG  | 1       | 0            |
| 52  | LM    | 3953 | PSU  | 1       | 0            |
| 42  | LC    | 577  | OMC  | 1       | 0            |
| 1   | S1    | 2078 | 7MG  | 1       | 0            |
| 1   | S1    | 1744 | OMU  | 2       | 0            |
| 1   | S1    | 1715 | PSU  | 1       | 0            |
| 46  | LG    | 2009 | OMG  | 1       | 0            |
| 40  | LA    | 68   | PSU  | 1       | 0            |
| 48  | LI    | 3171 | OMU  | 1       | 0            |
| 44  | LE    | 1315 | OMU  | 1       | 0            |
| 47  | LH    | 2625 | OMU  | 2       | 0            |
| 1   | S1    | 641  | OMG  | 3       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

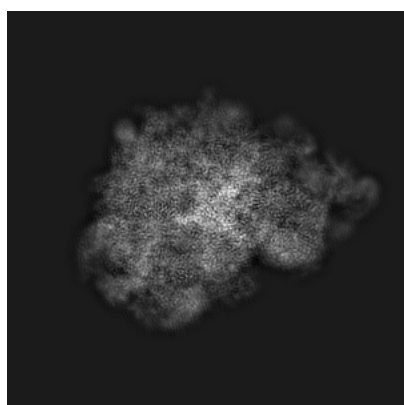
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11232. These allow visual inspection of the internal detail of the map and identification of artifacts.

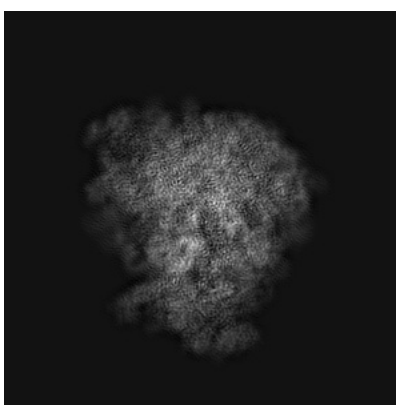
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

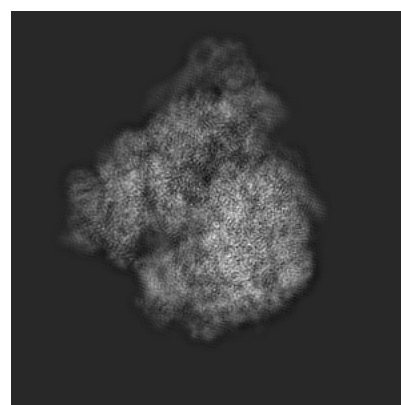
#### 6.1.1 Primary map



X



Y

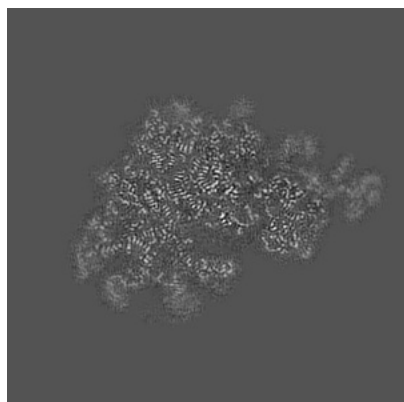


Z

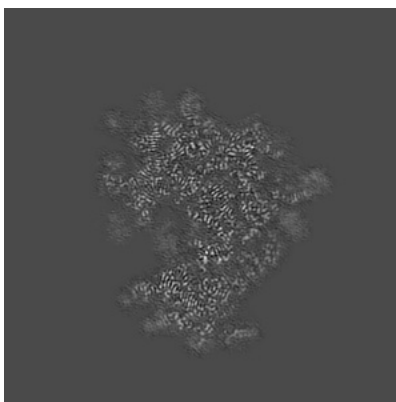
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

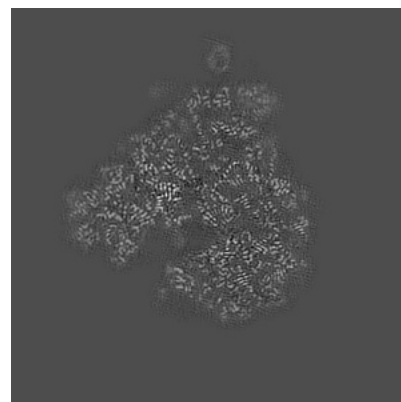
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

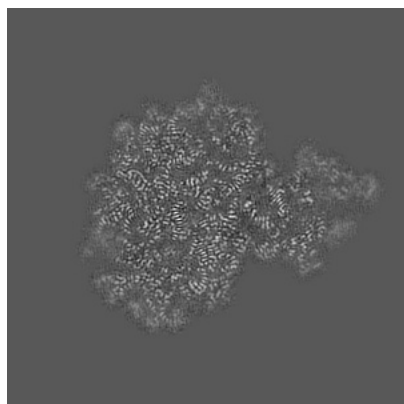


Z Index: 200

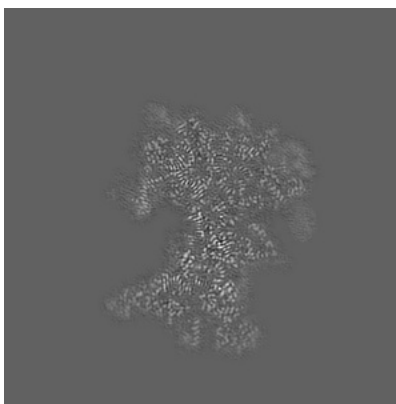
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

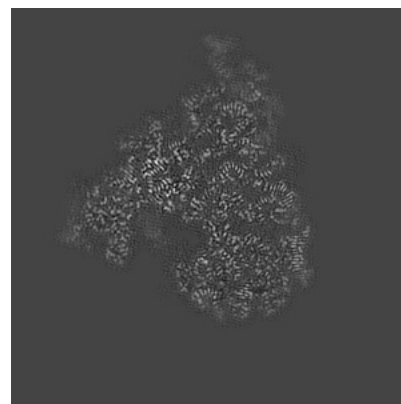
### 6.3.1 Primary map



X Index: 220



Y Index: 224

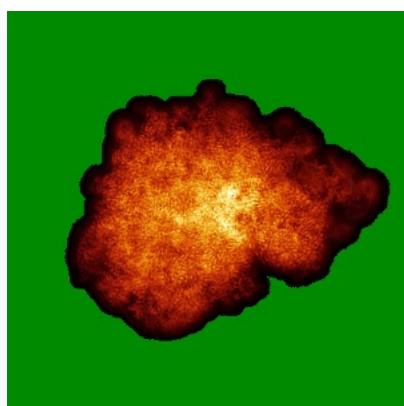


Z Index: 208

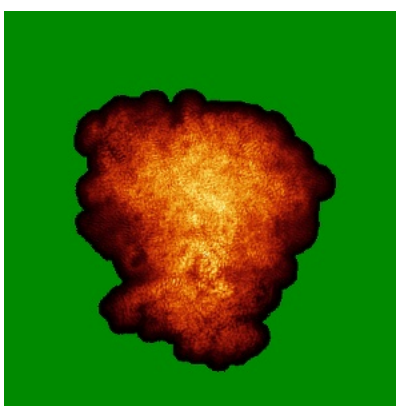
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

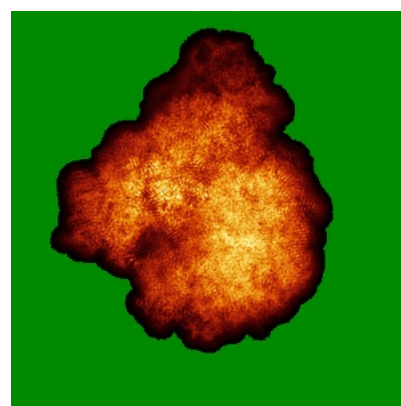
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

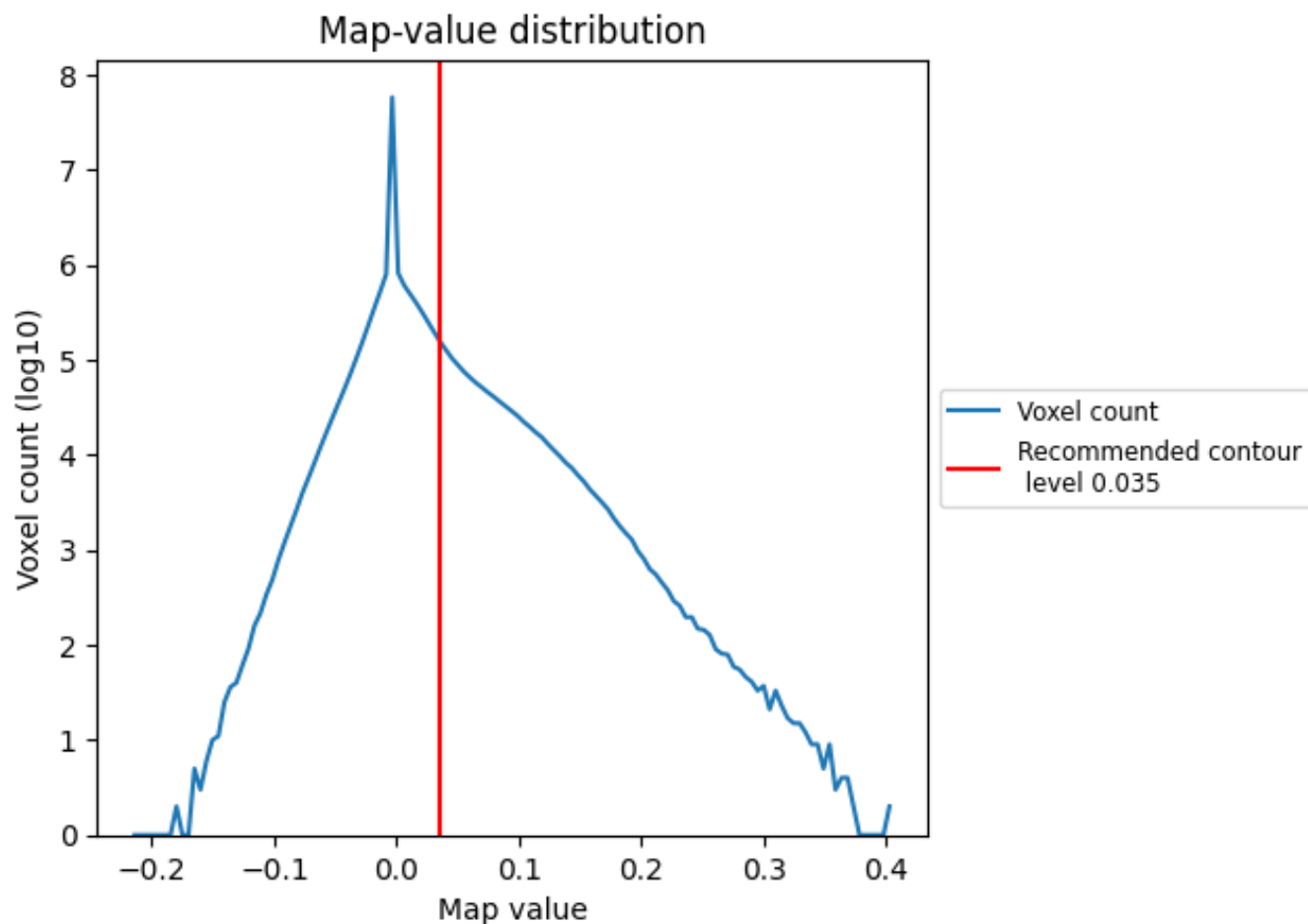
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

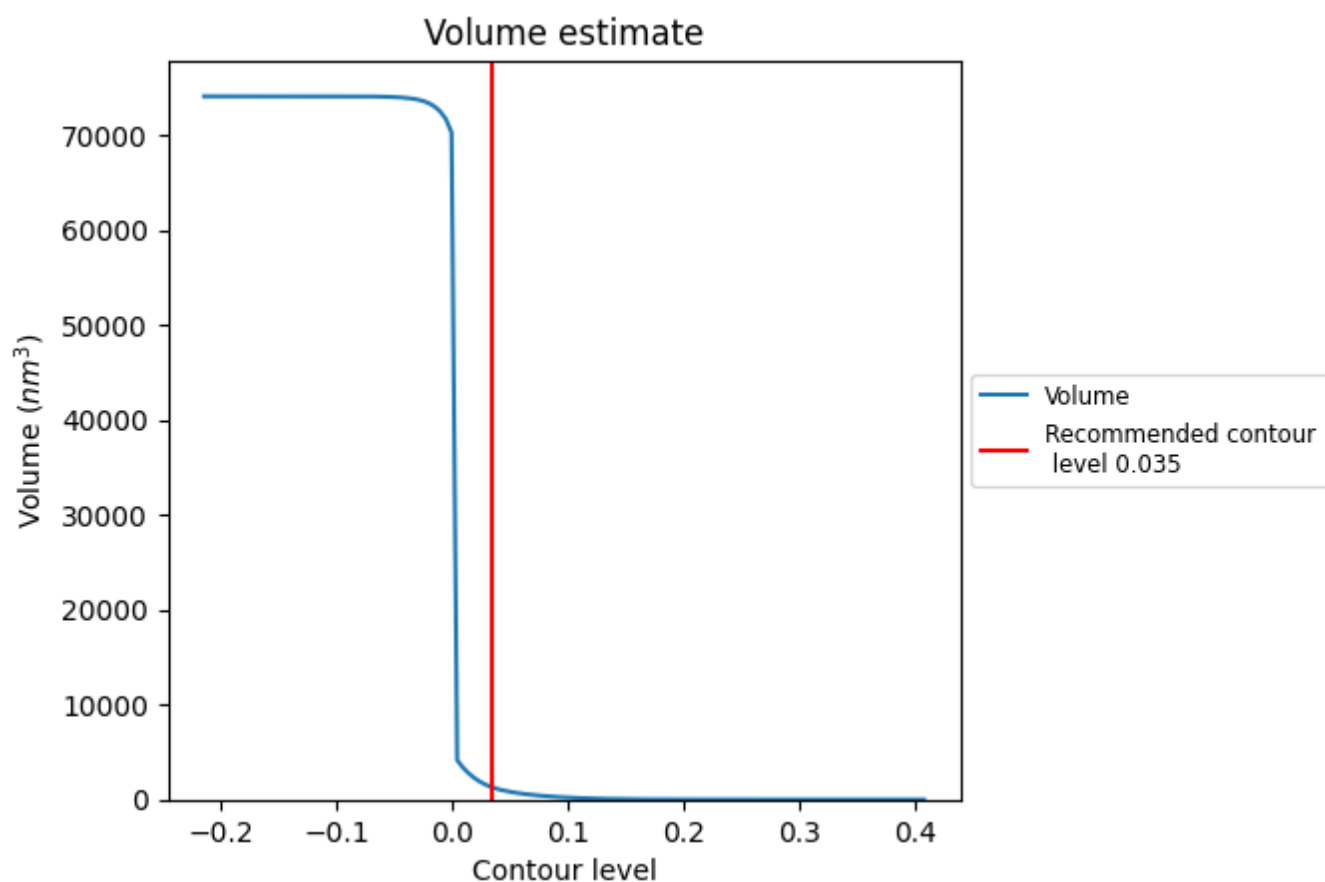
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

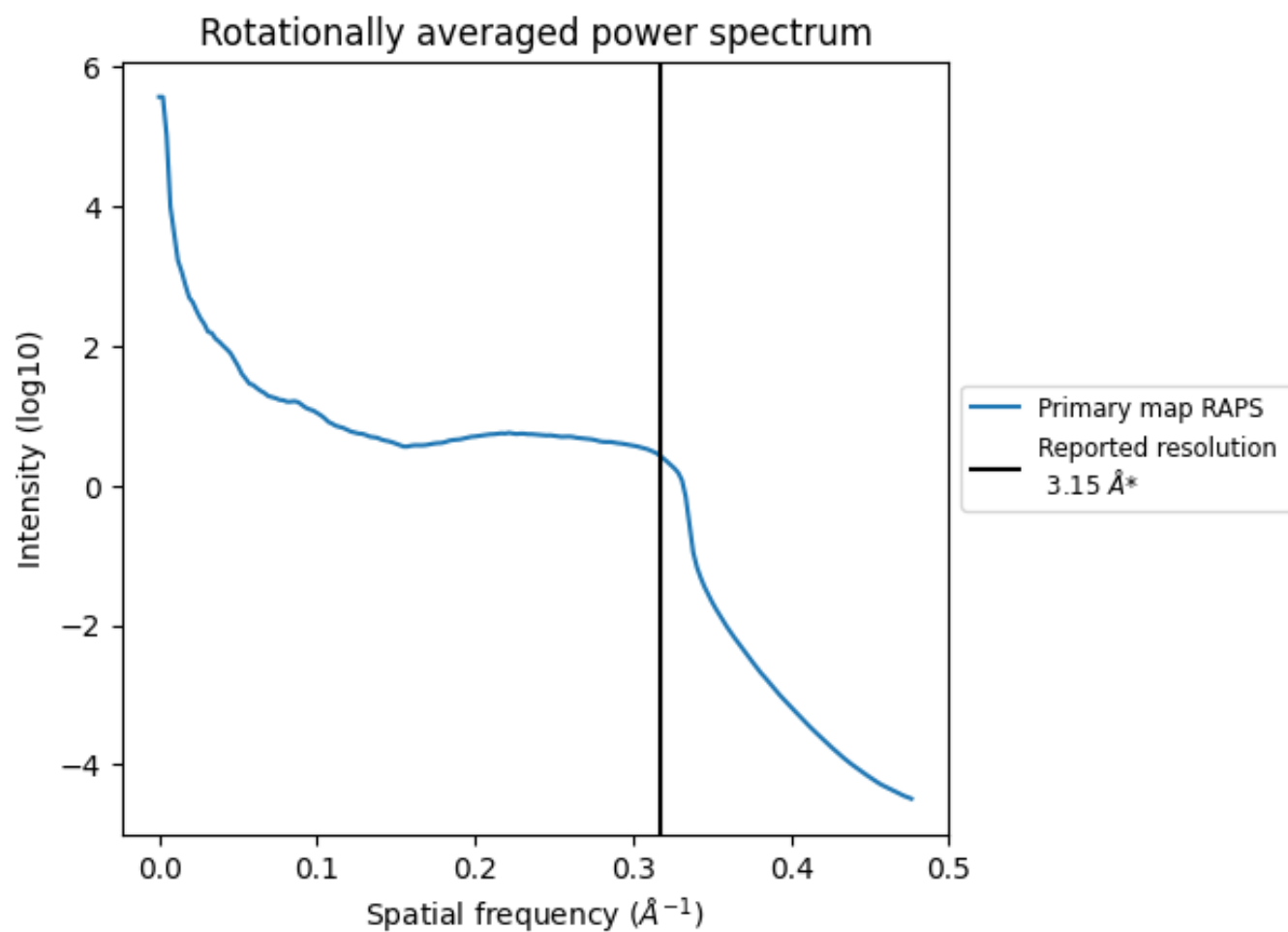
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1287 nm<sup>3</sup>; this corresponds to an approximate mass of 1163 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.317 Å<sup>-1</sup>

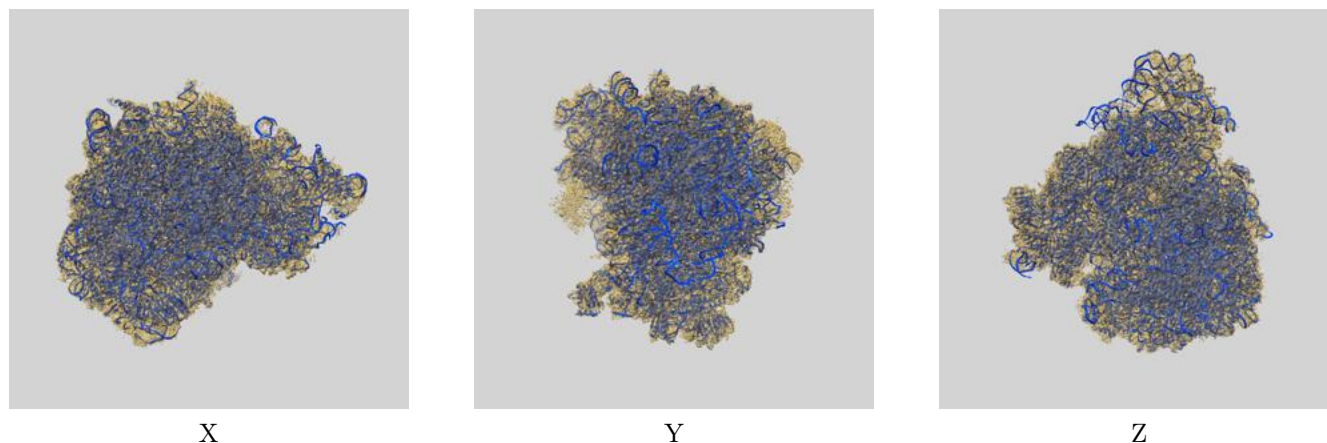
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

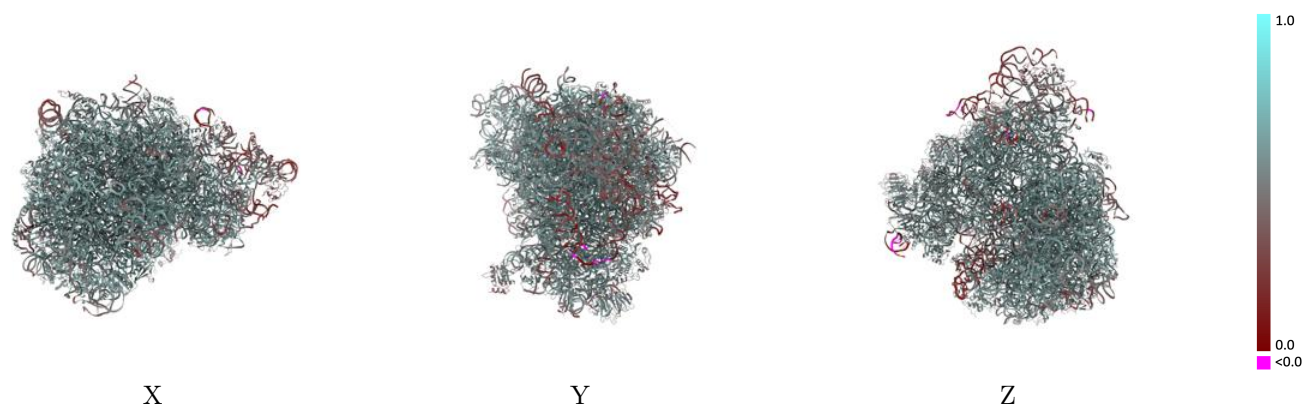
This section contains information regarding the fit between EMDB map EMD-11232 and PDB model 6ZJ3. Per-residue inclusion information can be found in section 3 on page 25.

### 9.1 Map-model overlay [i](#)



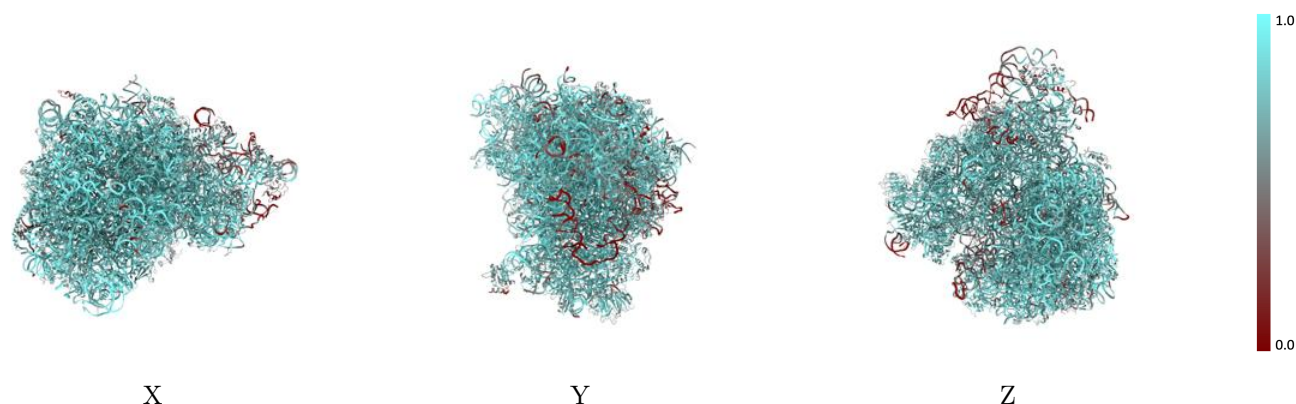
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



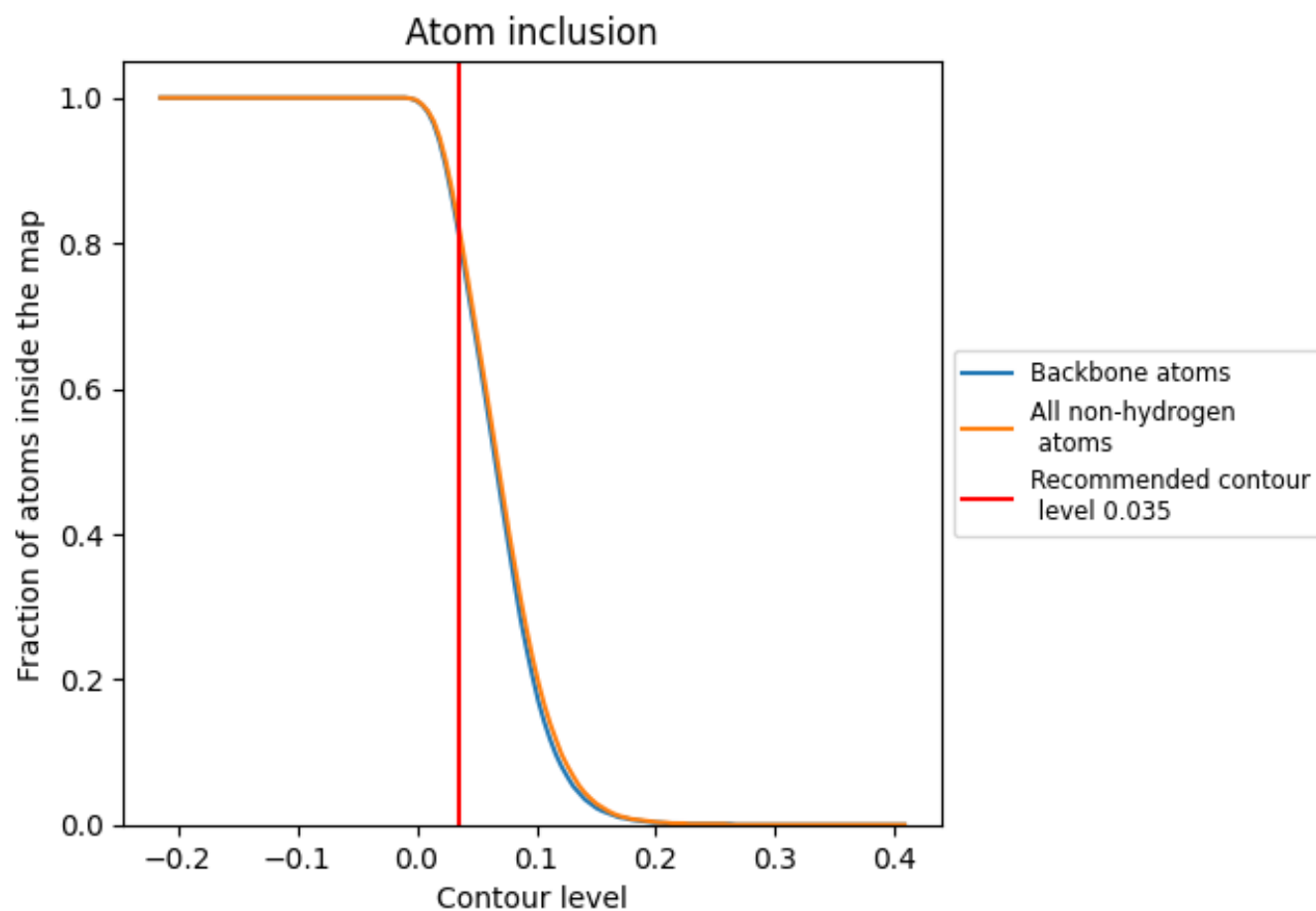
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8250   |  0.5480   |
| L1    |  0.7850   |  0.5730   |
| L2    |  0.8830   |  0.5940   |
| L3    |  0.8980   |  0.5890   |
| L4    |  0.8340   |  0.6000   |
| L5    |  0.8540   |  0.5980   |
| L6    |  0.6850   |  0.5090   |
| L7    |  0.7020   |  0.5340   |
| LA    |  0.9480   |  0.5950   |
| LB    |  0.9540   |  0.6010   |
| LC    |  0.8730   |  0.5390   |
| LD    |  0.8810   |  0.5420   |
| LE    |  0.8770   |  0.5470   |
| LF    |  0.9330   |  0.5980   |
| LG    |  0.9000  |  0.5740  |
| LH    |  0.9030 |  0.5750 |
| LI    |  0.8660 |  0.5530 |
| LJ    |  0.9540 |  0.6030 |
| LK    |  0.8830 |  0.5600 |
| LL    |  0.8450 |  0.5070 |
| LM    |  0.9470 |  0.5950 |
| LN    |  0.7320 |  0.4480 |
| LO    |  0.9600 |  0.5900 |
| LP    |  0.8590 |  0.6080 |
| LQ    |  0.8710 |  0.6000 |
| LR    |  0.8070 |  0.5750 |
| LS    |  0.7780 |  0.5390 |
| LT    |  0.8400 |  0.5800 |
| LU    |  0.6720 |  0.5130 |
| LV    |  0.7460 |  0.5500 |
| LW    |  0.8540 |  0.5900 |
| LX    |  0.8020 |  0.5650 |
| LY    |  0.8500 |  0.5950 |
| LZ    |  0.8280 |  0.5720 |
| La    |  0.8280 |  0.5970 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Lb    |  0.8880   |  0.6130   |
| Lc    |  0.7550   |  0.5610   |
| Ld    |  0.8310   |  0.5660   |
| Le    |  0.8350   |  0.5980   |
| Lf    |  0.7540   |  0.5550   |
| Lg    |  0.8630   |  0.5930   |
| Lh    |  0.8060   |  0.5860   |
| Li    |  0.8700   |  0.5970   |
| Lj    |  0.6440   |  0.5160   |
| Lk    |  0.7920   |  0.5670   |
| Ll    |  0.8210   |  0.5720   |
| Lm    |  0.8260   |  0.5920   |
| Ln    |  0.7600   |  0.5530   |
| Lo    |  0.7610   |  0.5570   |
| Lp    |  0.8020   |  0.5710   |
| Lq    |  0.7700   |  0.5490   |
| Lr    |  0.8380   |  0.5860   |
| Ls    |  0.7940   |  0.5590   |
| Lt    |  0.8640   |  0.5800   |
| Lu    |  0.8430  |  0.5960  |
| Lv    |  0.8360 |  0.6090 |
| Lw    |  0.8370 |  0.5830 |
| Lx    |  0.8090 |  0.5780 |
| Ly    |  0.8340 |  0.5860 |
| Lz    |  0.6990 |  0.5420 |
| S1    |  0.8230 |  0.5160 |
| S2    |  0.2830 |  0.2810 |
| S3    |  0.7970 |  0.4760 |
| S4    |  0.5100 |  0.2660 |
| S5    |  0.9480 |  0.5610 |
| SA    |  0.7140 |  0.5350 |
| SB    |  0.8010 |  0.5480 |
| SC    |  0.7950 |  0.5440 |
| SD    |  0.7710 |  0.5550 |
| SE    |  0.8010 |  0.5790 |
| SF    |  0.8050 |  0.5660 |
| SG    |  0.7120 |  0.5330 |
| SH    |  0.8020 |  0.5490 |
| SI    |  0.5890 |  0.4930 |
| SJ    |  0.8290 |  0.5840 |
| SK    |  0.8220 |  0.5720 |
| SL    |  0.8070 |  0.5640 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| SM    |  0.7440   |  0.5290   |
| SN    |  0.7950   |  0.5540   |
| SO    |  0.7320   |  0.5530   |
| SP    |  0.8330   |  0.5900   |
| SQ    |  0.5150   |  0.4050   |
| SR    |  0.7940   |  0.5510   |
| SS    |  0.8990   |  0.5890   |
| ST    |  0.7890   |  0.5650   |
| SU    |  0.8530   |  0.6060   |
| SV    |  0.7220   |  0.5110   |
| SW    |  0.7830   |  0.5500   |
| SX    |  0.7960   |  0.5450   |
| SY    |  0.7240   |  0.5490   |
| SZ    |  0.7990   |  0.5560   |
| Sa    |  0.7610   |  0.5440   |
| Sb    |  0.8280   |  0.5730   |
| Sc    |  0.7480   |  0.5580   |
| Sd    |  0.7100   |  0.5040   |
| Se    |  0.7210   |  0.5180   |
| Sf    |  0.6560  |  0.4920  |
| Sg    |  0.4740 |  0.3850 |
| Sh    |  0.7210 |  0.5050 |