



## Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:58 AM UTC

PDB ID : 9FXO / pdb\_00009fxo  
EMDB ID : EMD-50852  
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME  
WITH A/P/E-SITE TRNA AND MRNA : LM32CS1C1 M2 OE MUTANT  
Authors : Rajan, K.S.; Yonath, A.  
Deposited on : 2024-07-02  
Resolution : 2.25 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:

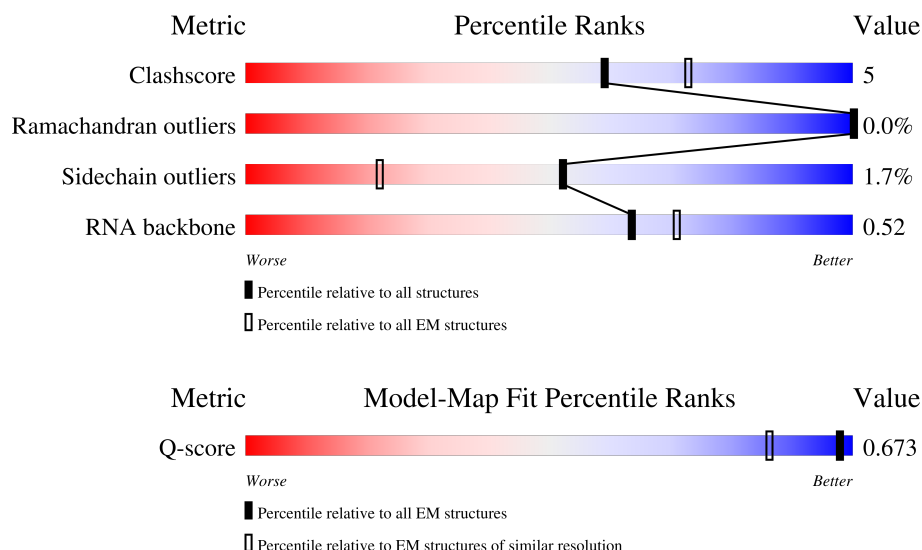
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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

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

The reported resolution of this entry is 2.25 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                       | 3458 ( 1.75 - 2.75 )                                     |

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   | L1    | 1782   |                  |
| 2   | L2    | 1526   |                  |
| 3   | L3    | 216    |                  |













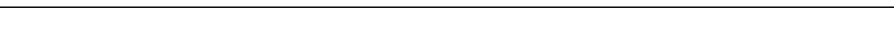

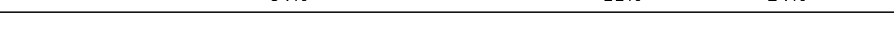

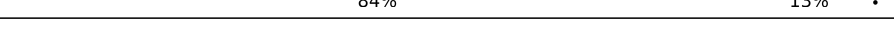








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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | L4    | 184    |    |
| 5   | L5    | 135    |    |
| 6   | L6    | 73     |    |
| 7   | L7    | 171    |    |
| 8   | L8    | 124    |    |
| 9   | LA    | 260    |    |
| 10  | LB    | 419    |    |
| 11  | LC    | 373    |    |
| 12  | LD    | 188    |    |
| 13  | LE    | 190    |    |
| 14  | LF    | 195    |    |
| 15  | LG    | 264    |   |
| 16  | LH    | 222    |  |
| 17  | LI    | 220    |  |
| 18  | LJ    | 139    |  |
| 19  | LK    | 175    |  |
| 20  | LL    | 145    |  |
| 21  | LM    | 204    |  |
| 22  | LN    | 213    |  |
| 23  | LO    | 305    |  |
| 24  | LP    | 198    |  |
| 25  | LQ    | 254    |  |
| 26  | LR    | 179    |  |
| 27  | LS    | 159    |  |
| 28  | LT    | 166    |  |









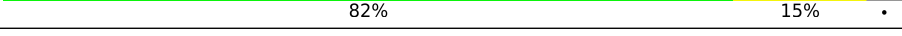

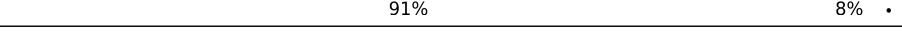
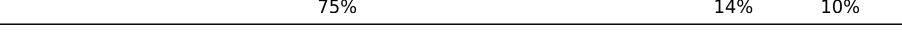

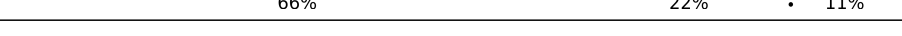


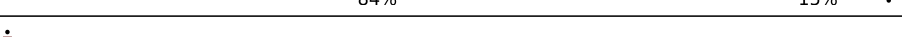

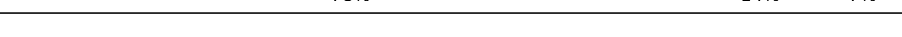






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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 29  | LU    | 129    |  78%17%5%       |
| 30  | LV    | 145    |  77%5%18%       |
| 31  | LW    | 143    |  71%14%15%      |
| 32  | LX    | 124    |  62%6%31%       |
| 33  | LY    | 134    |  90%10%.        |
| 34  | LZ    | 147    |  81%17%..       |
| 35  | La    | 127    |  85%13%..       |
| 36  | Lb    | 70     |  84%13%.        |
| 37  | Lc    | 252    |  81%10%9%       |
| 38  | Ld    | 104    |  75%15%.8%      |
| 39  | Le    | 188    |  87%12%.        |
| 40  | Lf    | 133    |  89%7%.         |
| 41  | Lg    | 144    |  85%14%..     |
| 42  | Lh    | 168    |  64%11%.24%   |
| 43  | Li    | 105    |  90%7%.       |
| 44  | Lj    | 83     |  84%13%.      |
| 45  | Lk    | 83     |  84%10%6%     |
| 46  | Ll    | 51     |  86%12%.      |
| 47  | Lm    | 128    |  34%7%59%     |
| 48  | Ln    | 34     |  85%12%.      |
| 49  | Lo    | 92     |  86%11%.      |
| 50  | Lp    | 106    |  75%15%.8%    |
| 51  | S1    | 2204   |  55%23%6%16%  |
| 52  | S2    | 76     |  11%8%.80%    |
| 52  | S4    | 76     |  39%38%12%11% |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 53  | S3    | 77     |    |
| 54  | SA    | 264    |    |
| 55  | SB    | 246    |    |
| 56  | SC    | 219    |    |
| 57  | SD    | 190    |    |
| 58  | SE    | 273    |    |
| 59  | SF    | 265    |    |
| 60  | SG    | 249    |    |
| 61  | SH    | 190    |    |
| 62  | SI    | 200    |    |
| 63  | SJ    | 130    |    |
| 64  | SK    | 220    |   |
| 65  | SL    | 149    |  |
| 66  | SM    | 116    |  |
| 67  | SN    | 168    |  |
| 68  | SO    | 144    |  |
| 69  | SP    | 143    |  |
| 70  | SQ    | 141    |  |
| 71  | SR    | 153    |  |
| 72  | SS    | 57     |  |
| 73  | ST    | 151    |  |
| 74  | SU    | 173    |  |
| 75  | SV    | 143    |  |
| 76  | SW    | 152    |  |
| 77  | SX    | 161    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 78  | SY    | 164    |  |
| 79  | SZ    | 137    |  |
| 80  | Sa    | 120    |  |
| 81  | Sb    | 112    |  |
| 82  | Sc    | 86     |  |
| 83  | Sd    | 87     |  |
| 84  | Se    | 66     |  |
| 85  | Sf    | 152    |  |
| 86  | Sg    | 312    |  |
| 87  | Sh    | 235    |  |
| 88  | S5    | 13     |  |

## 2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 218491 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 LSUa\_rRNA\_chain\_1.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | L1    | 1684     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36117 | 16147 | 6602 | 11684 | 1684 |         |       |

- Molecule 2 is a RNA chain called LSUb\_rRNA\_chain\_2.

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 2   | L2    | 1160     | Total | C     | N    | O    | P    | 0       | 0     |
|     |       |          | 24815 | 11110 | 4470 | 8075 | 1160 |         |       |

- Molecule 3 is a RNA chain called SR1\_chain\_3.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3   | L3    | 183      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3880  | 1736 | 672 | 1289 | 183 |         |       |

- Molecule 4 is a RNA chain called SR2\_chain\_4.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 4   | L4    | 184      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3937  | 1756 | 712 | 1285 | 184 |         |       |

- Molecule 5 is a RNA chain called SR4\_chain\_5.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5   | L5    | 121      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2578  | 1150 | 460 | 847 | 121 |         |       |

- Molecule 6 is a RNA chain called SR6\_chain\_6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | L6    | 71       | Total | C   | N   | O   | P  | 1       | 0     |
|     |       |          | 1526  | 684 | 274 | 496 | 72 |         |       |

- Molecule 7 is a RNA chain called 5.8S\_rRNA\_chain\_7.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 7   | L7    | 166      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3534  | 1584 | 626 | 1159 | 165 |         |       |

- Molecule 8 is a RNA chain called 5S\_rRNA\_chain\_8.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 8   | L8    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2551  | 1141 | 454 | 836 | 120 |         |       |

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | LA    | 258      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1972  | 1229 | 403 | 330 | 10 |         |       |

- Molecule 10 is a protein called Putative ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | LB    | 404      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3216  | 2024 | 638 | 541 | 13 |         |       |

- Molecule 11 is a protein called Putative ribosomal protein L1a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | LC    | 366      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2826  | 1765 | 562 | 484 | 15 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | LD    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1391  | 878 | 262 | 243 | 8 |         |       |

- Molecule 13 is a protein called Putative 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | LE    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 936 | 273 | 262 | 6 |         |       |

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | LF    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1169  | 743 | 220 | 204 | 2 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | LG    | 241      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1895  | 1190 | 376 | 322 | 7 |         |       |

- Molecule 16 is a protein called Putative 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | LH    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 1123 | 353 | 284 | 7 |         |       |

- Molecule 17 is a protein called Putative 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | LI    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1056 | 342 | 289 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| LI    | 203     | ARG      | ASN    | conflict | UNP E9AEA8 |

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | LJ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1012  | 638 | 191 | 177 | 6 |         |       |

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LK    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1329  | 827 | 263 | 231 | 8 |         |       |

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | LL    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 707 | 226 | 185 | 6 |         |       |

- Molecule 21 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | LM    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1711  | 1079 | 362 | 262 | 8 |         |       |

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | LN    | 200      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1626  | 1025 | 323 | 264 | 14 |         |       |

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | LO    | 298      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 2339  | 1486 | 440 | 407 | 6 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LP    | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1539  | 968 | 307 | 258 | 6 |         |       |

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25  | LQ    | 201      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1692  | 1041 | 370 | 275 | 6 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LR    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1455  | 925 | 279 | 246 | 5 |         |       |

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LS    | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1261  | 803 | 245 | 209 | 4 |         |       |

- Molecule 28 is a protein called Putative 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 28  | LT    | 152      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1221  | 762 | 241 | 207 | 11 |         |       |

- Molecule 29 is a protein called Putative 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | LU    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 624 | 176 | 157 | 3 |         |       |

- Molecule 30 is a protein called Putative 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | LV    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 953   | 604 | 181 | 166 | 2 |         |       |

- Molecule 31 is a protein called Putative 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | LW    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 603 | 200 | 160 | 4 |         |       |

- Molecule 32 is a protein called Putative ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | LX    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 461 | 140 | 109 | 4 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | LY    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 683 | 215 | 164 | 3 |         |       |

- Molecule 34 is a protein called Putative 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | LZ    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1117  | 685 | 238 | 189 | 5 |         |       |

- Molecule 35 is a protein called Putative 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | La    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1043  | 650 | 217 | 172 | 4 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36  | Lb    | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 546   | 335 | 125 | 86 |   |         |       |

- Molecule 37 is a protein called Putative 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | Lc    | 229      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1862  | 1185 | 358 | 308 | 11 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Ld    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 730   | 455 | 133 | 137 | 5 |         |       |

- Molecule 39 is a protein called Putative 60S ribosomal subunit protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Le    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1469  | 922 | 296 | 247 | 4 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | Lf    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1046  | 658 | 210 | 174 | 4 |         |       |

- Molecule 41 is a protein called Putative ribosomal protein l35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | Lg    | 143      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1159  | 720 | 243 | 191 | 5 |         |       |

- Molecule 42 is a protein called Putative 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | Lh    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1029  | 633 | 224 | 166 | 6 |         |       |

- Molecule 43 is a protein called Putative 60S Ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | Li    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 798   | 503 | 162 | 131 | 2 |         |       |

- Molecule 44 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Lj    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 406 | 153 | 103 | 6 |         |       |

- Molecule 45 is a protein called Putative ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Lk    | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 608   | 383 | 119 | 103 | 3 |         |       |

- Molecule 46 is a protein called Putative 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46  | Ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 450   | 291 | 95 | 63 | 1 |         |       |

- Molecule 47 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47  | Lm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 416   | 263 | 85 | 64 | 4 |         |       |

- Molecule 48 is a protein called Ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48  | Ln    | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 292   | 178 | 75 | 37 | 2 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | Lo    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 431 | 143 | 113 | 6 |         |       |

- Molecule 50 is a protein called Putative 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | Lp    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 496 | 158 | 125 | 5 |         |       |

- Molecule 51 is a RNA chain called SSU\_rRNA\_chain\_S1.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 51  | S1    | 1852     | Total | C     | N    | O     | P    | 1       | 0     |
|     |       |          | 39635 | 17733 | 7147 | 12902 | 1853 |         |       |

- Molecule 52 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 52  | S2    | 15       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 325   | 149 | 58  | 102 | 15 |         |       |
| 52  | S4    | 68       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1446  | 646 | 258 | 475 | 67 |         |       |

- Molecule 53 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 53  | S3    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1599  | 713 | 290 | 521 | 75 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 54  | SA    | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1909  | 1194 | 366 | 338 | 11 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | SB    | 211      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1662  | 1055 | 303 | 292 | 12 |         |       |

- Molecule 56 is a protein called Putative 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | SC    | 212      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1646  | 1040 | 302 | 291 | 13 |         |       |

- Molecule 57 is a protein called Putative 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | SD    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 949 | 305 | 246 | 8 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 58  | SE    | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2054  | 1301 | 393 | 351 | 9 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 59  | SF    | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1708  | 1088 | 301 | 309 | 10 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | SG    | 234      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1866  | 1163 | 383 | 317 | 3 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SH    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1441  | 896 | 276 | 262 | 7 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 62  | SI    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 1050 | 320 | 271 | 8 |         |       |

- Molecule 63 is a protein called Putative 40S ribosomal protein S15A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | SJ    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 646 | 188 | 179 | 8 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | SK    | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1582  | 986 | 326 | 268 | 2 |         |       |

- Molecule 65 is a protein called Putative 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | SL    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1140  | 731 | 210 | 196 | 3 |         |       |

- Molecule 66 is a protein called Putative ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | SM    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 503 | 146 | 154 | 2 |         |       |

- Molecule 67 is a protein called Putative 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | SN    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 874   | 560 | 152 | 155 | 7 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | SO    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1024  | 633 | 200 | 183 | 8 |         |       |

- Molecule 69 is a protein called Putative 40S ribosomal protein S23.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | SP    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1100  | 694 | 217 | 186 | 3 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 70  | SQ    | 97       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 480   | 286 | 97 | 97 |         |       |

- Molecule 71 is a protein called Putative 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | SR    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 715 | 226 | 192 | 5 |         |       |

- Molecule 72 is a protein called Putative ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 72  | SS    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 279 | 94 | 73 | 6 |         |       |

- Molecule 73 is a protein called Putative 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | ST    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1167  | 736 | 231 | 191 | 9 |         |       |

- Molecule 74 is a protein called Putative 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | SU    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1260  | 796 | 251 | 208 | 5 |         |       |

- Molecule 75 is a protein called Putative 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | SV    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 992   | 619 | 193 | 175 | 5 |         |       |

- Molecule 76 is a protein called Putative 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | SW    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 928   | 591 | 176 | 157 | 4 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S19-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | SX    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 766 | 237 | 199 | 4 |         |       |

- Molecule 78 is a protein called Putative 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | SY    | 88       | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 673   | 415 | 124 | 130 | 4 |         |       |

- Molecule 79 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | SZ    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1051  | 675 | 204 | 169 | 3 |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | Sa    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 650   | 412 | 118 | 117 | 3 |         |       |

- Molecule 81 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | Sb    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 511 | 177 | 130 | 7 |         |       |

- Molecule 82 is a protein called Putative 40S ribosomal protein S27-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | Sc    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 661   | 410 | 127 | 119 | 5 |         |       |

- Molecule 83 is a protein called Putative 40S ribosomal protein S33.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 83  | Sd    | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 496   | 301 | 100 | 91 | 4 |         |       |

- Molecule 84 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 84  | Se    | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 95 | 72 | 1 |         |       |

- Molecule 85 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 85  | Sf    | 75       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 293 | 88 | 81 | 3 |         |       |

- Molecule 86 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 86  | Sg    | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2343  | 1469 | 418 | 443 | 13 |         |       |

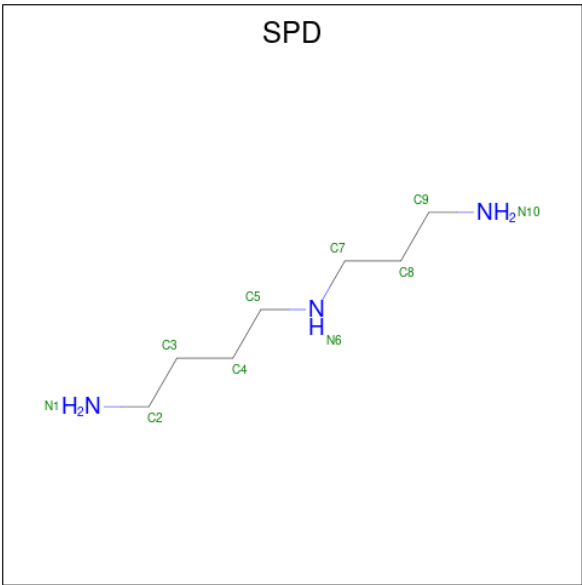
- Molecule 87 is a protein called Putative RNA binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 87  | Sh    | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1212  | 769 | 224 | 216 | 3 |         |       |

- Molecule 88 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 88  | S5    | 12       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 251   | 113 | 43 | 83 | 12 |         |       |

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

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| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 89  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L2    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L2    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | LM    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | S1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | S1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | S1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 90  | L1    | 120      | Total | Mg  | 0       |
|     |       |          | 120   | 120 |         |
| 90  | L2    | 94       | Total | Mg  | 0       |
|     |       |          | 94    | 94  |         |
| 90  | L3    | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 90  | L4    | 10       | Total | Mg  | 0       |
|     |       |          | 10    | 10  |         |
| 90  | L5    | 6        | Total | Mg  | 0       |
|     |       |          | 6     | 6   |         |
| 90  | L6    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 90  | L7    | 4        | Total | Mg  | 0       |
|     |       |          | 4     | 4   |         |
| 90  | L8    | 6        | Total | Mg  | 0       |
|     |       |          | 6     | 6   |         |
| 90  | LA    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 90  | LG    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 90  | LJ    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 90  | LN    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

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| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 90  | LS    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | LT    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | Lf    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | Lh    | 2        | Total<br>2   | Mg<br>2   | 0       |
| 90  | S1    | 109      | Total<br>109 | Mg<br>109 | 0       |
| 90  | S3    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | SG    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | SO    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | ST    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | SX    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 90  | Sb    | 1        | Total<br>1   | Mg<br>1   | 0       |

- Molecule 91 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 91  | L1    | 15       | Total<br>15 | Na<br>15 | 0       |
| 91  | L2    | 12       | Total<br>12 | Na<br>12 | 0       |
| 91  | L3    | 1        | Total<br>1  | Na<br>1  | 0       |
| 91  | L4    | 3        | Total<br>3  | Na<br>3  | 0       |
| 91  | L7    | 2        | Total<br>2  | Na<br>2  | 0       |
| 91  | LN    | 1        | Total<br>1  | Na<br>1  | 0       |
| 91  | Lf    | 1        | Total<br>1  | Na<br>1  | 0       |
| 91  | S1    | 12       | Total<br>12 | Na<br>12 | 0       |

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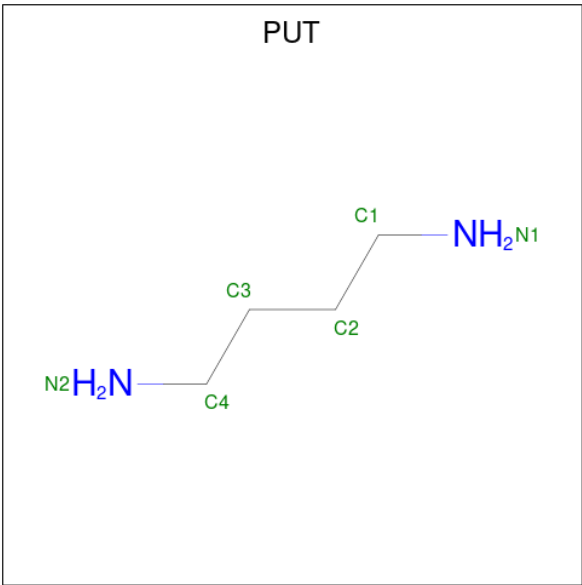
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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 91  | SS    | 1        | Total<br>1 | Na<br>1 | 0       |

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 92  | L1    | 20       | Total<br>20 | K<br>20 | 0       |
| 92  | L2    | 14       | Total<br>14 | K<br>14 | 0       |
| 92  | L4    | 4        | Total<br>4  | K<br>4  | 0       |
| 92  | L7    | 1        | Total<br>1  | K<br>1  | 0       |
| 92  | LB    | 1        | Total<br>1  | K<br>1  | 0       |
| 92  | LC    | 2        | Total<br>2  | K<br>2  | 0       |
| 92  | LM    | 1        | Total<br>1  | K<br>1  | 0       |
| 92  | LV    | 1        | Total<br>1  | K<br>1  | 0       |
| 92  | Le    | 1        | Total<br>1  | K<br>1  | 0       |
| 92  | Ll    | 1        | Total<br>1  | K<br>1  | 0       |
| 92  | S1    | 19       | Total<br>19 | K<br>19 | 0       |

- Molecule 93 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 93  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L2    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L2    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L2    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L2    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L4    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

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| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 93  | S1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 93  | S1    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

- # PAR

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 95  | LK    | 1        | Total Zn<br>1 1 | 0       |



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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 95  | Lj    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 95  | Lm    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 95  | Lo    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 95  | Lp    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 95  | SS    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 95  | Sb    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 96 is water.

| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 96  | L1    | 762      | Total<br>762 | O<br>762 | 0       |
| 96  | L2    | 787      | Total<br>787 | O<br>787 | 0       |
| 96  | L3    | 49       | Total<br>49  | O<br>49  | 0       |
| 96  | L4    | 55       | Total<br>55  | O<br>55  | 0       |
| 96  | L5    | 22       | Total<br>22  | O<br>22  | 0       |
| 96  | L7    | 24       | Total<br>24  | O<br>24  | 0       |
| 96  | LA    | 46       | Total<br>46  | O<br>46  | 0       |
| 96  | LB    | 42       | Total<br>42  | O<br>42  | 0       |
| 96  | LC    | 27       | Total<br>27  | O<br>27  | 0       |
| 96  | LD    | 1        | Total<br>1   | O<br>1   | 0       |
| 96  | LG    | 1        | Total<br>1   | O<br>1   | 0       |
| 96  | LH    | 6        | Total<br>6   | O<br>6   | 0       |
| 96  | LI    | 11       | Total<br>11  | O<br>11  | 0       |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 96  | LJ    | 5        | Total<br>5  | O<br>5  | 0       |
| 96  | LL    | 15       | Total<br>15 | O<br>15 | 0       |
| 96  | LM    | 26       | Total<br>26 | O<br>26 | 0       |
| 96  | LN    | 2        | Total<br>2  | O<br>2  | 0       |
| 96  | LO    | 1        | Total<br>1  | O<br>1  | 0       |
| 96  | LP    | 9        | Total<br>9  | O<br>9  | 0       |
| 96  | LQ    | 11       | Total<br>11 | O<br>11 | 0       |
| 96  | LS    | 4        | Total<br>4  | O<br>4  | 0       |
| 96  | LT    | 15       | Total<br>15 | O<br>15 | 0       |
| 96  | LU    | 1        | Total<br>1  | O<br>1  | 0       |
| 96  | LV    | 2        | Total<br>2  | O<br>2  | 0       |
| 96  | LW    | 5        | Total<br>5  | O<br>5  | 0       |
| 96  | LX    | 2        | Total<br>2  | O<br>2  | 0       |
| 96  | LY    | 2        | Total<br>2  | O<br>2  | 0       |
| 96  | La    | 1        | Total<br>1  | O<br>1  | 0       |
| 96  | Lb    | 5        | Total<br>5  | O<br>5  | 0       |
| 96  | Lc    | 2        | Total<br>2  | O<br>2  | 0       |
| 96  | Ld    | 4        | Total<br>4  | O<br>4  | 0       |
| 96  | Le    | 6        | Total<br>6  | O<br>6  | 0       |
| 96  | Lf    | 3        | Total<br>3  | O<br>3  | 0       |
| 96  | Lg    | 3        | Total<br>3  | O<br>3  | 0       |

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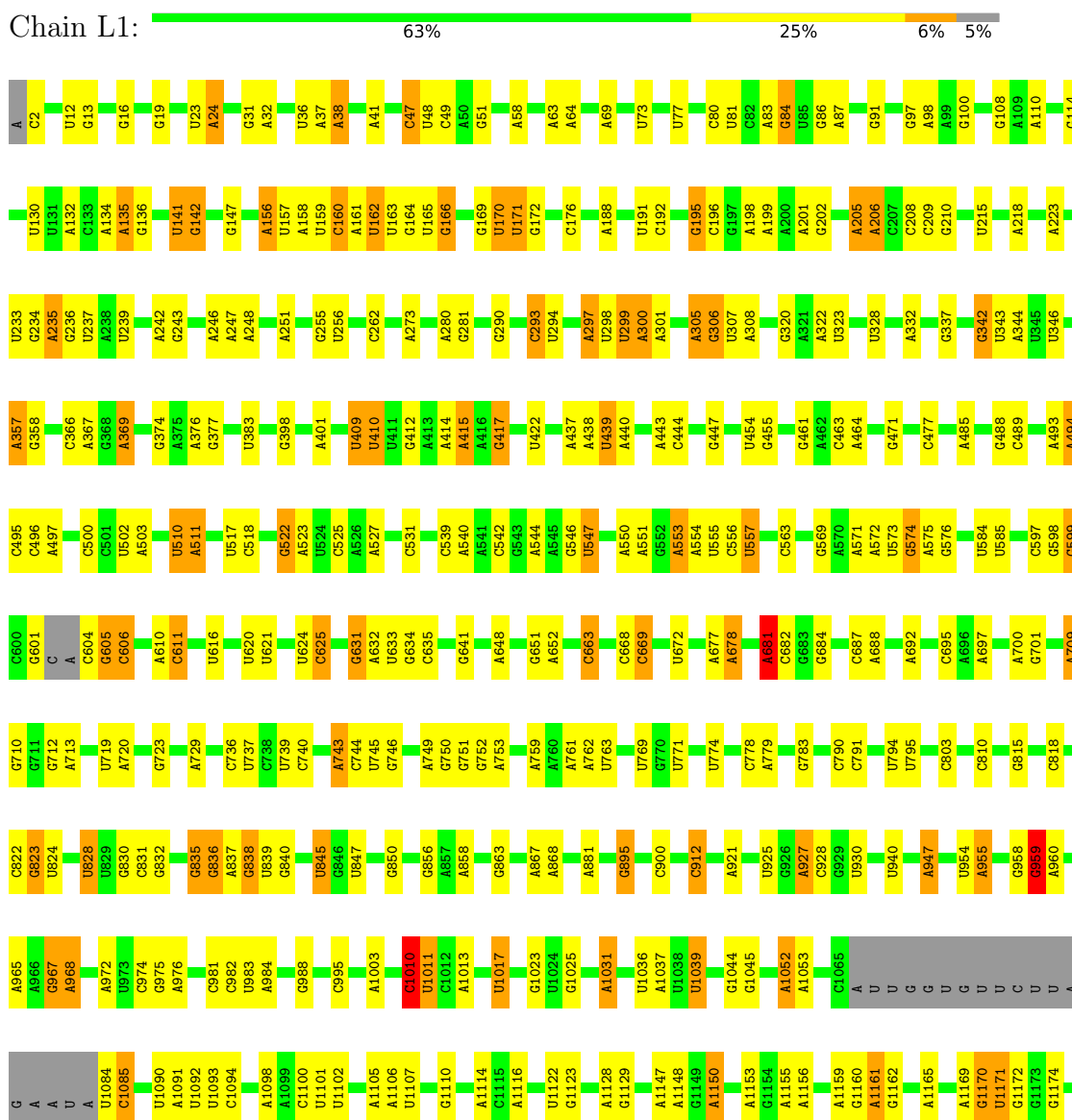
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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 96  | Lh    | 12       | Total<br>12  | O<br>12  | 0       |
| 96  | Lj    | 18       | Total<br>18  | O<br>18  | 0       |
| 96  | Ln    | 9        | Total<br>9   | O<br>9   | 0       |
| 96  | Lo    | 23       | Total<br>23  | O<br>23  | 0       |
| 96  | Lp    | 14       | Total<br>14  | O<br>14  | 0       |
| 96  | S1    | 595      | Total<br>595 | O<br>595 | 0       |
| 96  | S2    | 1        | Total<br>1   | O<br>1   | 0       |
| 96  | S3    | 6        | Total<br>6   | O<br>6   | 0       |
| 96  | S4    | 15       | Total<br>15  | O<br>15  | 0       |
| 96  | SA    | 6        | Total<br>6   | O<br>6   | 0       |
| 96  | SF    | 1        | Total<br>1   | O<br>1   | 0       |
| 96  | SJ    | 1        | Total<br>1   | O<br>1   | 0       |
| 96  | SK    | 19       | Total<br>19  | O<br>19  | 0       |
| 96  | SO    | 9        | Total<br>9   | O<br>9   | 0       |
| 96  | SP    | 4        | Total<br>4   | O<br>4   | 0       |
| 96  | ST    | 14       | Total<br>14  | O<br>14  | 0       |
| 96  | SU    | 9        | Total<br>9   | O<br>9   | 0       |
| 96  | Sb    | 9        | Total<br>9   | O<br>9   | 0       |
| 96  | Sc    | 1        | Total<br>1   | O<br>1   | 0       |
| 96  | Sg    | 1        | Total<br>1   | O<br>1   | 0       |

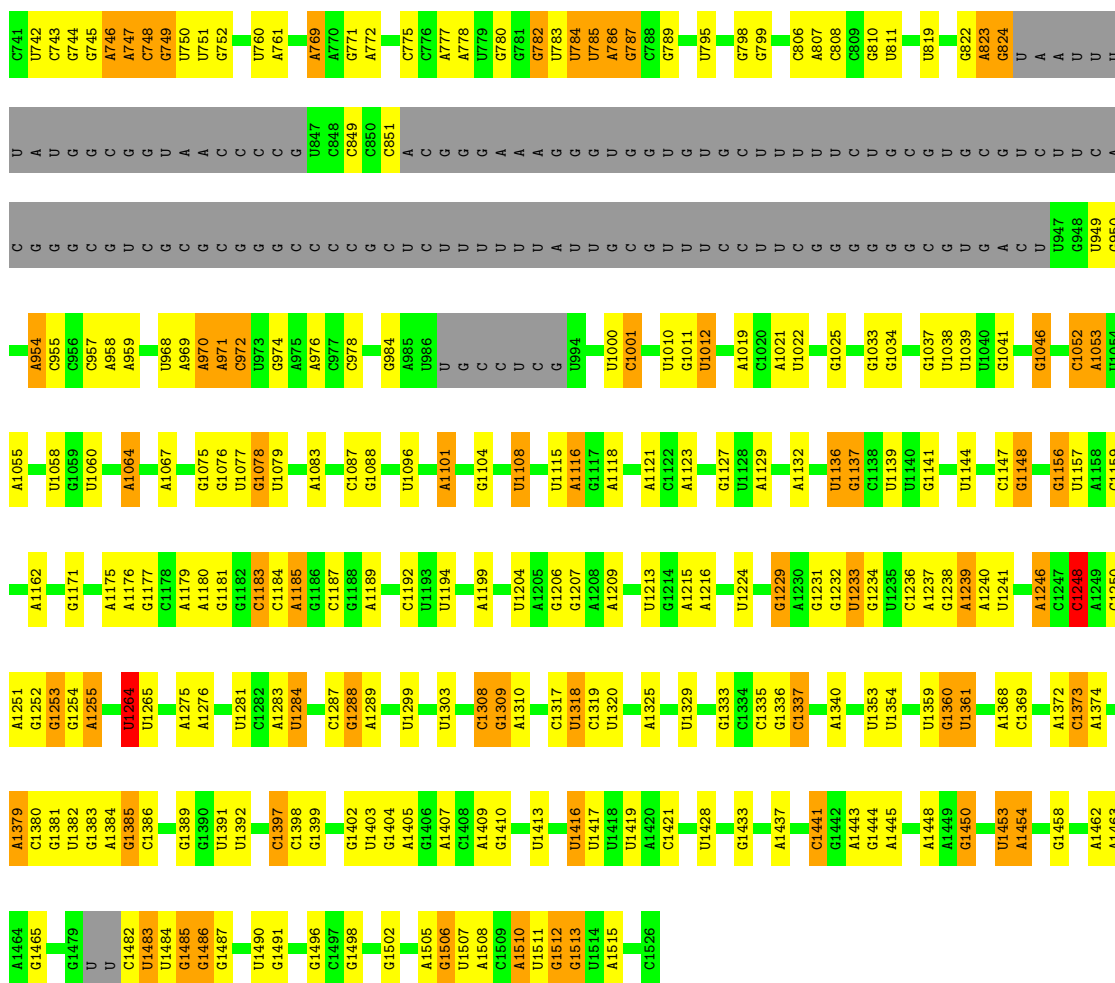
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: LSUa\_rRNA\_chain\_1

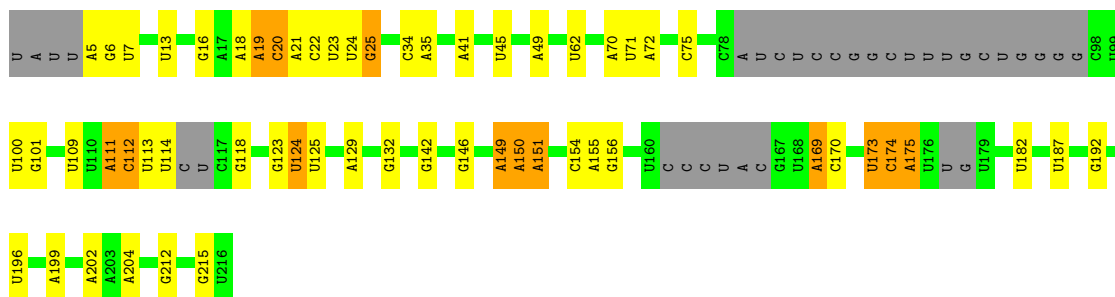






• Molecule 3: SR1\_chain\_3

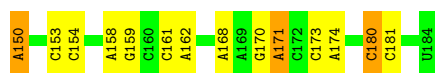
Chain L3: 58% 21% 6% 15%



• Molecule 4: SR2\_chain\_4

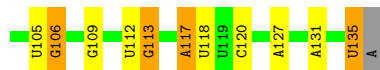
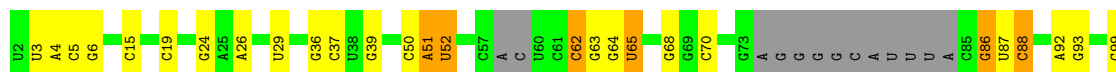
Chain L4: 73% 23% 4%





• Molecule 5: SR4\_chain\_5

Chain L5: 61% 21% 7% 10%



• Molecule 6: SR6\_chain\_6

Chain L6: 49% 37% 11%



• Molecule 7: 5.8S\_rRNA\_chain\_7

Chain L7: 69% 21% 7%



• Molecule 8: 5S\_rRNA\_chain\_8

Chain L8: 76% 20%



• Molecule 9: Putative 60S ribosomal protein L2

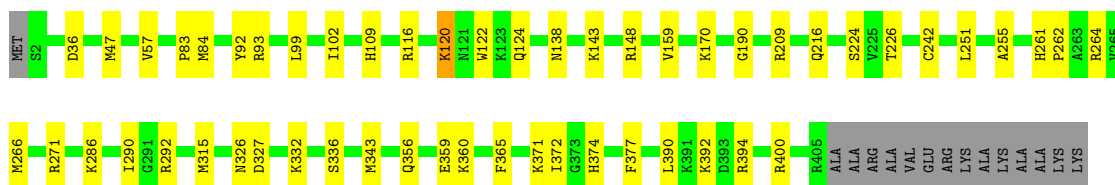
Chain LA: 89% 10%



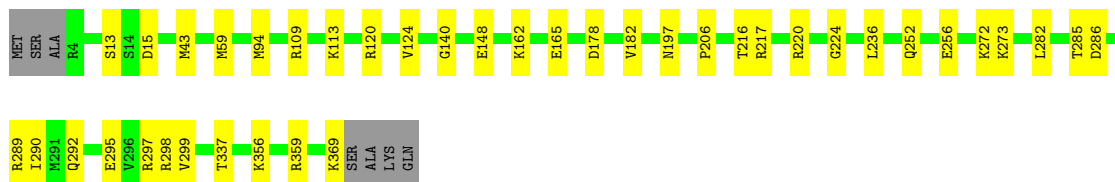
• Molecule 10: Putative ribosomal protein L3

Chain LB: 84% 12%

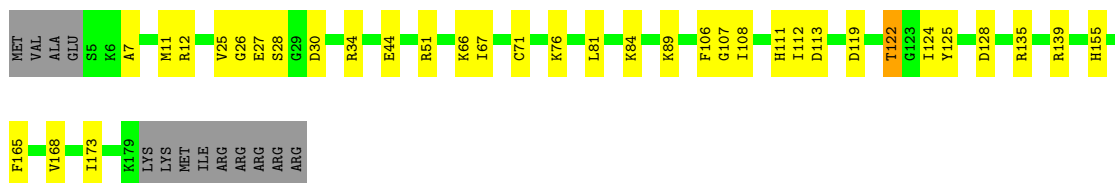
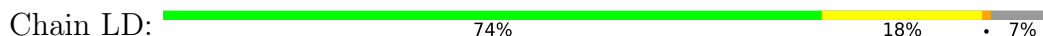




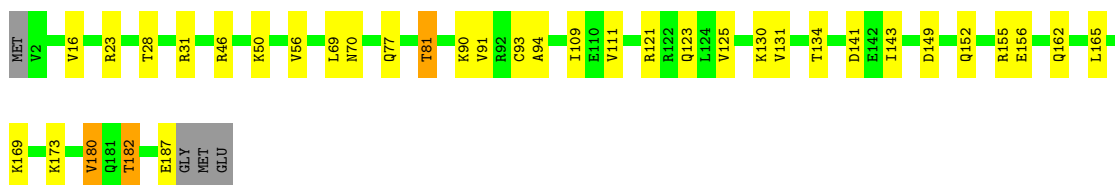
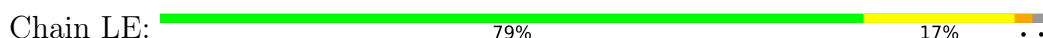
- Molecule 11: Putative ribosomal protein L1a



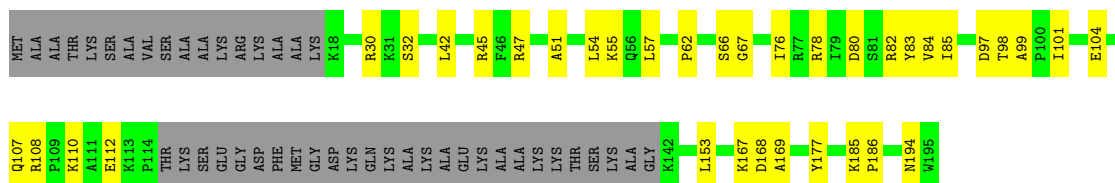
- Molecule 12: 60S ribosomal protein L11



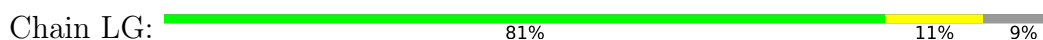
- Molecule 13: Putative 60S ribosomal protein L9



- Molecule 14: Putative 60S ribosomal protein L6



- Molecule 15: 60S ribosomal protein L7a





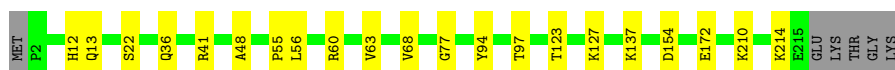
- Molecule 16: Putative 60S ribosomal protein L13a

Chain LH: 86% 14%



- Molecule 17: Putative 60S ribosomal protein L13

Chain LI: 88% 10% .



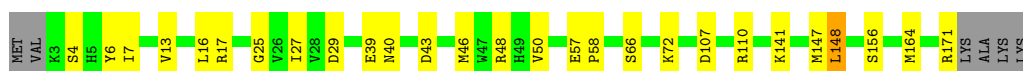
- Molecule 18: Putative 60S ribosomal protein L23

Chain LJ: 83% 14% .



- Molecule 19: Putative 40S ribosomal protein L14

Chain LK: 81% 15% ..



- Molecule 20: Putative 60S ribosomal protein L27A/L29

Chain LL: 81% 18% .




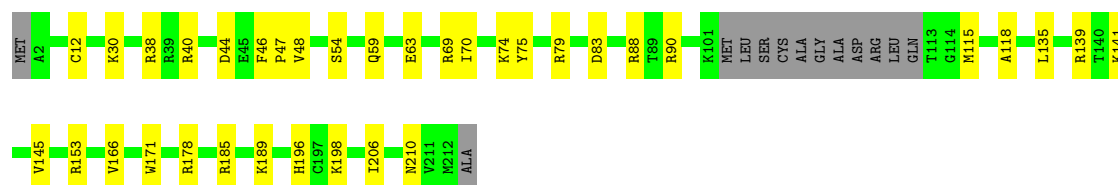
- Molecule 21: Ribosomal protein L15

Chain LM: 89% 10%




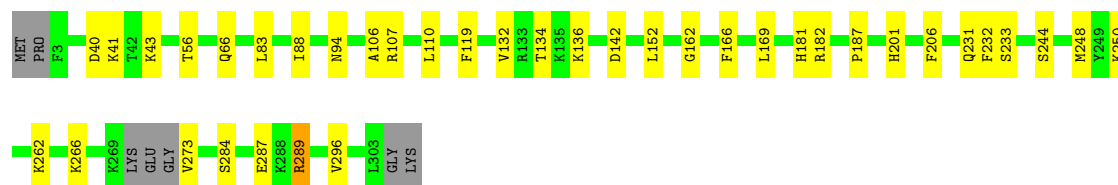
- Molecule 22: Putative 60S ribosomal protein L10

Chain LN:  77% 16% 6%




- Molecule 23: Putative 60S ribosomal protein L5

Chain LO:  85% 12% .



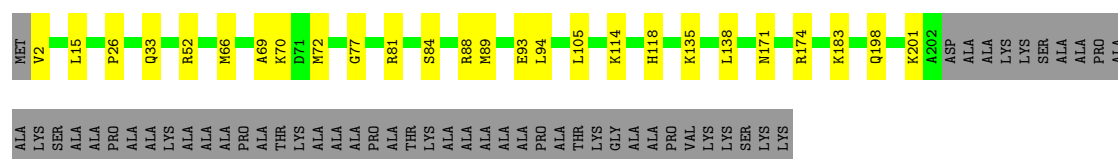
- Molecule 24: 60S ribosomal protein L18

Chain LP:  88% 12% .



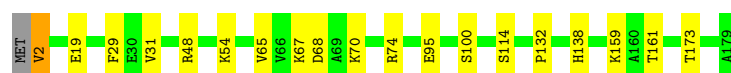
- Molecule 25: Putative 60S ribosomal protein L19

Chain LQ:  69% 10% 21%



- Molecule 26: 60S ribosomal protein L18a

Chain LR:  89% 10% ..




- Molecule 27: Putative 60S ribosomal protein L21

Chain LS:  89% 10% .




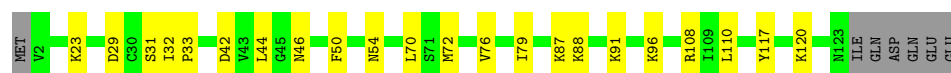
- Molecule 28: Putative 60S ribosomal protein L17

Chain LT:  83% 9% 8%




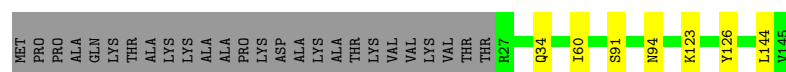
- Molecule 29: Putative 60S ribosomal protein L22

Chain LU:  78% 17% 5%



- Molecule 30: Putative 60S ribosomal protein L23a

Chain LV:  77% 5% 18%



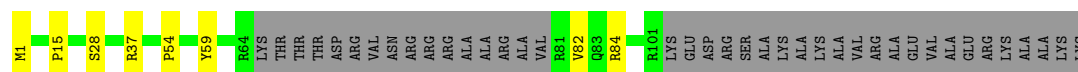
- Molecule 31: Putative 60S ribosomal protein L26

Chain LW:  71% 14% 15%



- Molecule 32: Putative ribosomal protein L24

Chain LX:  62% 6% 31%




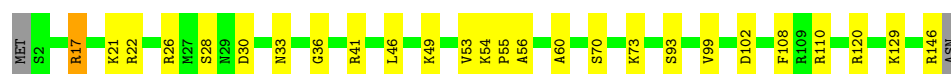
- Molecule 33: 60S ribosomal protein L27

Chain LY:  90% 10% 0%




- Molecule 34: Putative 60S ribosomal protein L28

Chain LZ:  81% 17% 0%




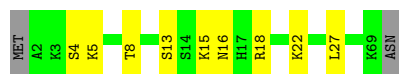
- Molecule 35: Putative 60S ribosomal protein L35

Chain La:  85% 13% ..




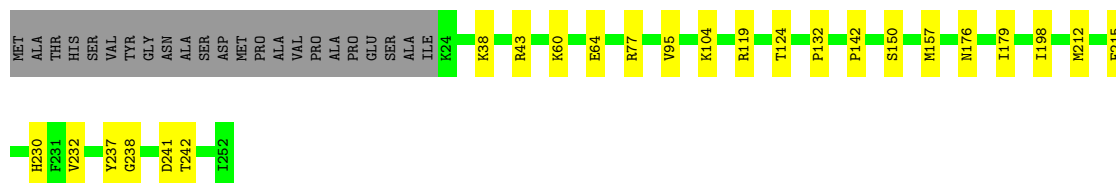
- Molecule 36: 60S ribosomal protein L29

Chain Lb:  84% 13% .




- Molecule 37: Putative 60S ribosomal protein L7

Chain Lc:  81% 10% 9%




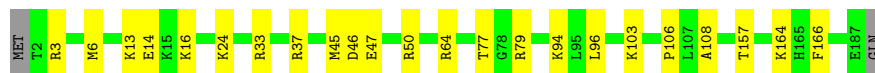
- Molecule 38: 60S ribosomal protein L30

Chain Ld:  75% 15% 8%




- Molecule 39: Putative 60S ribosomal subunit protein L31

Chain Le:  87% 12% .




- Molecule 40: 60S ribosomal protein L32

Chain Lf:  89% 7% .

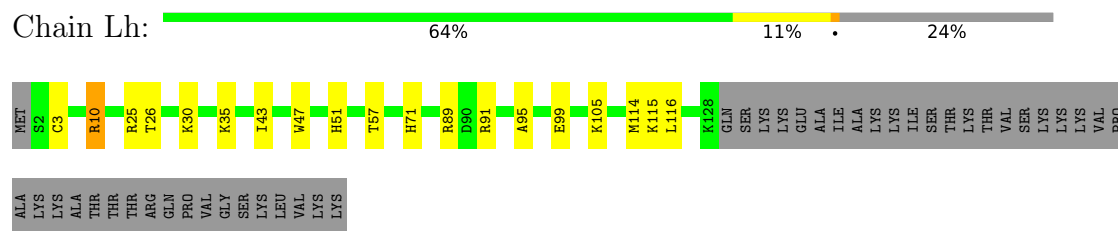


- Molecule 41: Putative ribosomal protein l35a

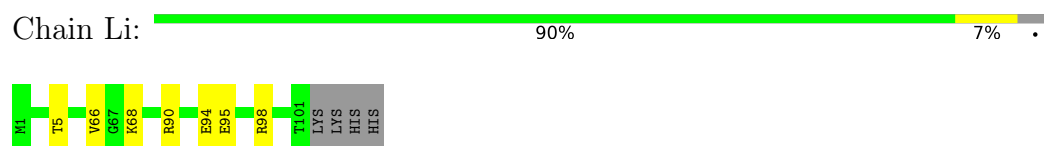
Chain Lg:  85% 14% ..



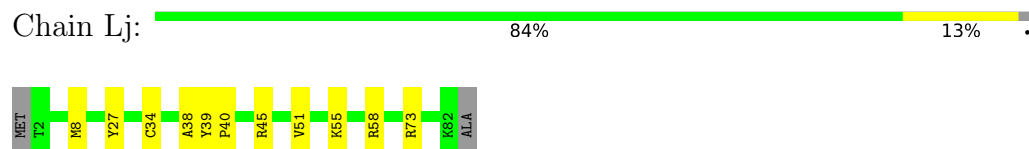
## ● Molecule 42: Putative 60S ribosomal protein L34



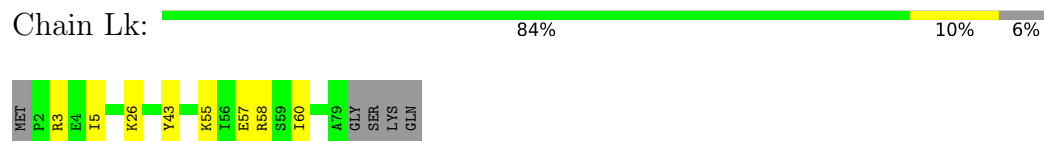
## ● Molecule 43: Putative 60S Ribosomal protein L36



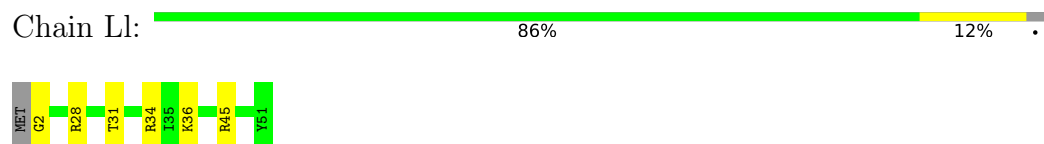
## ● Molecule 44: Ribosomal protein L37



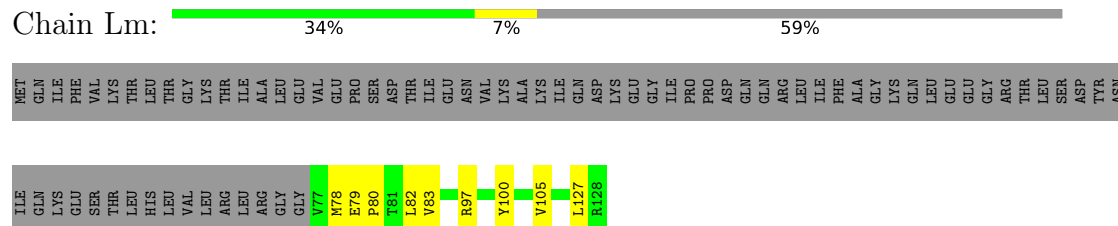
## ● Molecule 45: Putative ribosomal protein L38



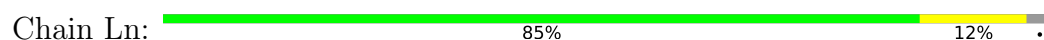
## ● Molecule 46: Putative 60S ribosomal protein L39

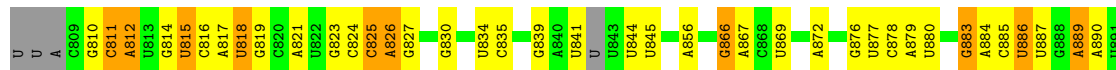


## ● Molecule 47: Ubiquitin-60S ribosomal protein L40



## ● Molecule 48: Ribosomal protein L41

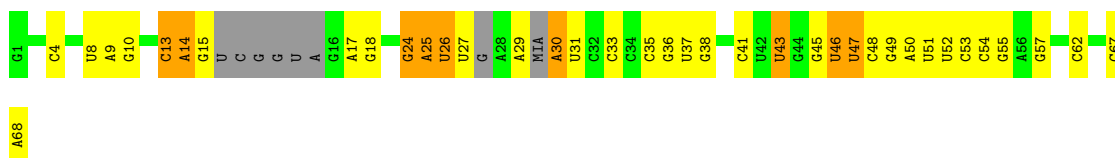








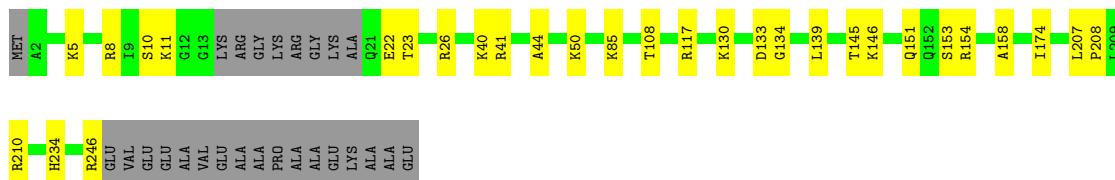
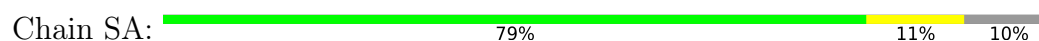
- Molecule 52: tRNA



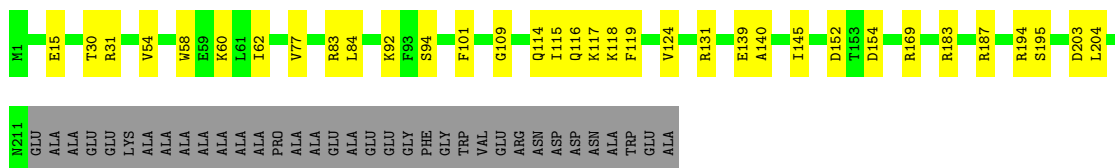
- Molecule 53: tRNA



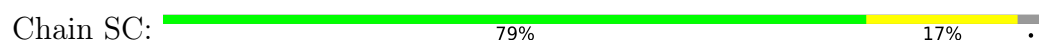
- Molecule 54: 40S ribosomal protein S3a

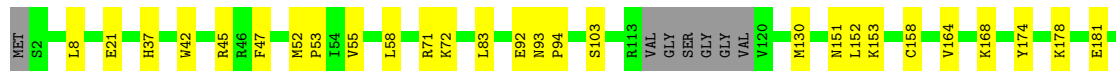


- Molecule 55: 40S ribosomal protein SA




- Molecule 56: Putative 40S ribosomal protein S3








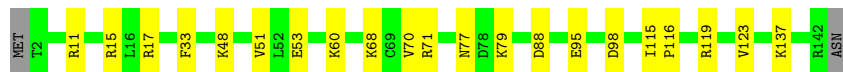
- Molecule 68: 40S ribosomal protein S14

Chain SO:  83% 12% 5%



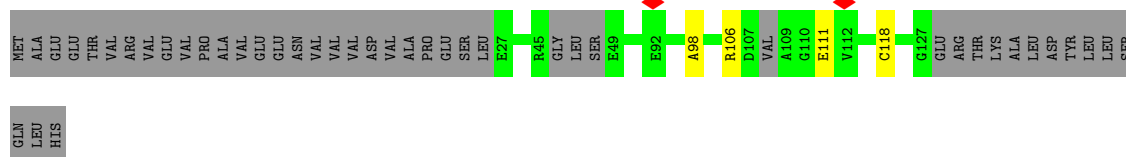
- Molecule 69: Putative 40S ribosomal protein S23

Chain SP:  84% 15% 1%




- Molecule 70: 40S ribosomal protein S12

Chain SQ:  66% 31% 3%




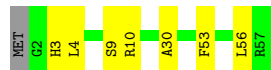
- Molecule 71: Putative 40S ribosomal protein S18

Chain SR:  78% 14% 7%



- Molecule 72: Putative ribosomal protein S29

Chain SS:  86% 12% 2%




- Molecule 73: Putative 40S ribosomal protein S13

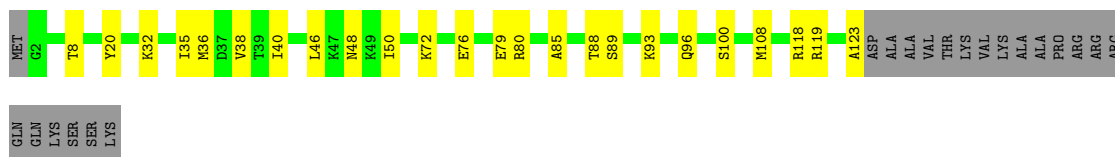
Chain ST:  87% 8% 5%



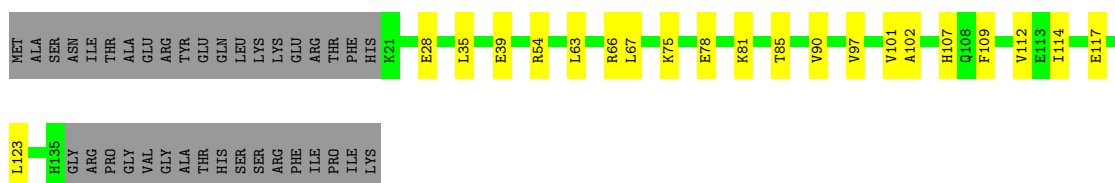
- Molecule 74: Putative 40S ribosomal protein S11

Chain SU:  81% 7% 12%

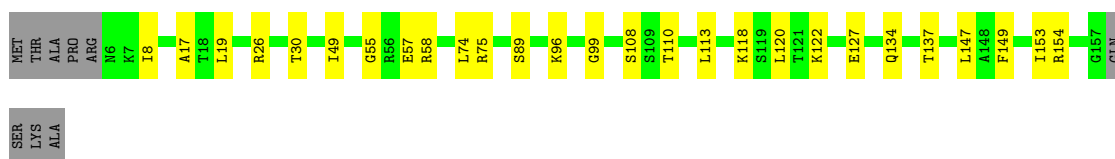
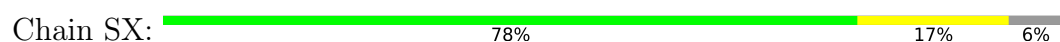
- Molecule 75: Putative 40S ribosomal protein S17



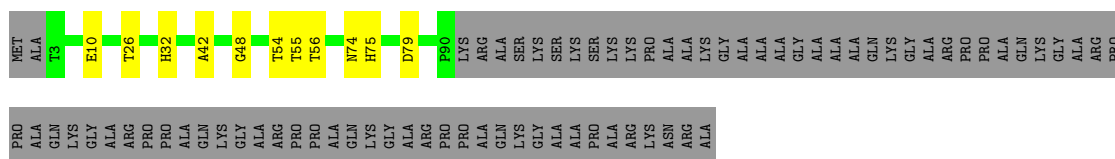
- Molecule 76: Putative 40S ribosomal protein S15



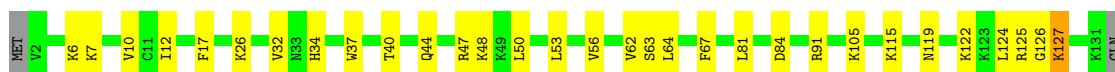
- Molecule 77: 40S ribosomal protein S19-like protein



- Molecule 78: Putative 40S ribosomal protein S21



- Molecule 79: 40S ribosomal protein S24





- 
- Diagram illustrating a 4x4 grid structure with columns labeled C1, C4, U8, U9, A12, and A. The grid is divided into four quadrants by a horizontal line. The top-left quadrant contains C1 and C4. The top-right quadrant contains U8 and U9. The bottom-left quadrant contains A12 and A. The bottom-right quadrant is empty.

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 150124                                  | 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 ( $e^-/\text{\AA}^2$ ) | 0.92                                    | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.201                                   | Depositor |
| Minimum map value                    | -0.079                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.005                                   | Depositor |
| Map size (Å)                         | 395.76, 395.76, 395.76                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.8245, 0.8245, 0.8245                  | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, A2M, B8N, NA, 7MG, 1MA, K, PUT, MA6, PAR, ZN, 5MC, OMC, PSU, SPD, OMU, MG, MIA

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   | L1    | 0.15         | 2/39379 (0.0%) | 0.24        | 0/61402 |
| 2   | L2    | 0.17         | 5/26133 (0.0%) | 0.25        | 0/40729 |
| 3   | L3    | 0.13         | 0/4306         | 0.24        | 0/6694  |
| 4   | L4    | 0.09         | 0/4376         | 0.22        | 0/6822  |
| 5   | L5    | 0.10         | 0/2878         | 0.25        | 0/4479  |
| 6   | L6    | 0.10         | 0/1705         | 0.24        | 0/2652  |
| 7   | L7    | 0.17         | 0/3804         | 0.26        | 0/5923  |
| 8   | L8    | 0.08         | 0/2851         | 0.18        | 0/4439  |
| 9   | LA    | 0.11         | 0/2018         | 0.30        | 0/2712  |
| 10  | LB    | 0.11         | 0/3283         | 0.27        | 0/4412  |
| 11  | LC    | 0.09         | 0/2876         | 0.26        | 0/3868  |
| 12  | LD    | 0.09         | 0/1414         | 0.25        | 0/1888  |
| 13  | LE    | 0.09         | 0/1497         | 0.24        | 0/2017  |
| 14  | LF    | 0.11         | 0/1191         | 0.31        | 0/1608  |
| 15  | LG    | 0.08         | 0/1921         | 0.24        | 0/2588  |
| 16  | LH    | 0.08         | 0/1803         | 0.25        | 0/2422  |
| 17  | LI    | 0.09         | 0/1728         | 0.26        | 0/2313  |
| 18  | LJ    | 0.10         | 0/1029         | 0.30        | 0/1388  |
| 19  | LK    | 0.08         | 0/1348         | 0.22        | 0/1808  |
| 20  | LL    | 0.10         | 0/1151         | 0.28        | 0/1538  |
| 21  | LM    | 0.09         | 0/1751         | 0.24        | 0/2338  |
| 22  | LN    | 0.08         | 0/1658         | 0.26        | 0/2217  |
| 23  | LO    | 0.09         | 0/2381         | 0.26        | 0/3187  |
| 24  | LP    | 0.08         | 0/1564         | 0.24        | 0/2092  |
| 25  | LQ    | 0.08         | 0/1712         | 0.22        | 0/2265  |
| 26  | LR    | 0.09         | 0/1489         | 0.24        | 0/2008  |
| 27  | LS    | 0.10         | 0/1290         | 0.26        | 0/1736  |
| 28  | LT    | 0.10         | 0/1245         | 0.29        | 0/1670  |
| 29  | LU    | 0.08         | 0/976          | 0.24        | 0/1303  |
| 30  | LV    | 0.09         | 0/968          | 0.26        | 0/1302  |
| 31  | LW    | 0.08         | 0/981          | 0.26        | 0/1310  |

| Mol | Chain | Bond lengths |                | Bond angles |               |
|-----|-------|--------------|----------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5       |
| 32  | LX    | 0.09         | 0/735          | 0.25        | 0/989         |
| 33  | LY    | 0.07         | 0/1086         | 0.21        | 0/1452        |
| 34  | LZ    | 0.09         | 0/1133         | 0.22        | 0/1516        |
| 35  | La    | 0.09         | 0/1054         | 0.24        | 0/1399        |
| 36  | Lb    | 0.08         | 0/557          | 0.23        | 0/743         |
| 37  | Lc    | 0.09         | 0/1896         | 0.25        | 0/2540        |
| 38  | Ld    | 0.10         | 0/740          | 0.26        | 0/1003        |
| 39  | Le    | 0.08         | 0/1488         | 0.22        | 0/1979        |
| 40  | Lf    | 0.08         | 0/1066         | 0.26        | 0/1424        |
| 41  | Lg    | 0.09         | 0/1183         | 0.25        | 0/1588        |
| 42  | Lh    | 0.10         | 0/1045         | 0.28        | 0/1390        |
| 43  | Li    | 0.11         | 0/813          | 0.29        | 0/1088        |
| 44  | Lj    | 0.10         | 0/682          | 0.30        | 0/911         |
| 45  | Lk    | 0.09         | 0/617          | 0.26        | 0/828         |
| 46  | Ll    | 0.08         | 0/463          | 0.23        | 0/617         |
| 47  | Lm    | 0.09         | 0/422          | 0.28        | 0/562         |
| 48  | Ln    | 0.11         | 0/296          | 0.29        | 0/386         |
| 49  | Lo    | 0.11         | 0/705          | 0.33        | 0/940         |
| 50  | Lp    | 0.10         | 0/797          | 0.25        | 0/1053        |
| 51  | S1    | 0.13         | 2/43029 (0.0%) | 0.23        | 0/67033       |
| 52  | S2    | 0.09         | 0/328          | 0.25        | 0/503         |
| 52  | S4    | 0.11         | 0/1613         | 0.27        | 0/2508        |
| 53  | S3    | 0.08         | 0/1785         | 0.18        | 0/2778        |
| 54  | SA    | 0.10         | 0/1933         | 0.28        | 0/2596        |
| 55  | SB    | 0.10         | 0/1696         | 0.28        | 0/2293        |
| 56  | SC    | 0.08         | 0/1674         | 0.22        | 0/2240        |
| 57  | SD    | 0.09         | 0/1536         | 0.24        | 0/2059        |
| 58  | SE    | 0.09         | 0/2092         | 0.27        | 0/2819        |
| 59  | SF    | 0.09         | 0/1744         | 0.25        | 0/2362        |
| 60  | SG    | 0.09         | 0/1889         | 0.24        | 0/2523        |
| 61  | SH    | 0.08         | 0/1463         | 0.23        | 0/1963        |
| 62  | SI    | 0.10         | 0/1679         | 0.28        | 0/2255        |
| 63  | SJ    | 0.09         | 0/1038         | 0.25        | 0/1391        |
| 64  | SK    | 0.09         | 0/1605         | 0.25        | 0/2150        |
| 65  | SL    | 0.08         | 0/1161         | 0.24        | 0/1559        |
| 66  | SM    | 0.09         | 0/815          | 0.24        | 0/1105        |
| 67  | SN    | 0.46         | 2/899 (0.2%)   | 0.89        | 5/1217 (0.4%) |
| 68  | SO    | 0.10         | 0/1039         | 0.30        | 0/1395        |
| 69  | SP    | 0.09         | 0/1120         | 0.25        | 0/1500        |
| 70  | SQ    | 0.08         | 0/477          | 0.24        | 0/660         |
| 71  | SR    | 0.08         | 0/1158         | 0.23        | 0/1553        |
| 72  | SS    | 0.08         | 0/458          | 0.25        | 0/607         |
| 73  | ST    | 0.09         | 0/1190         | 0.27        | 0/1594        |

| Mol | Chain | Bond lengths |                  | Bond angles |                 |
|-----|-------|--------------|------------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5         |
| 74  | SU    | 0.09         | 0/1289           | 0.27        | 0/1731          |
| 75  | SV    | 0.08         | 0/1002           | 0.22        | 0/1334          |
| 76  | SW    | 0.09         | 0/948            | 0.22        | 0/1275          |
| 77  | SX    | 0.08         | 0/1237           | 0.24        | 0/1661          |
| 78  | SY    | 0.09         | 0/684            | 0.25        | 0/928           |
| 79  | SZ    | 0.09         | 0/1071           | 0.27        | 0/1425          |
| 80  | Sa    | 0.08         | 0/657            | 0.24        | 0/882           |
| 81  | Sb    | 0.09         | 0/842            | 0.25        | 0/1127          |
| 82  | Sc    | 0.08         | 0/675            | 0.23        | 0/907           |
| 83  | Sd    | 0.08         | 0/498            | 0.31        | 0/668           |
| 84  | Se    | 0.09         | 0/457            | 0.26        | 0/609           |
| 85  | Sf    | 0.07         | 0/472            | 0.25        | 0/640           |
| 86  | Sg    | 0.08         | 0/2400           | 0.26        | 0/3260          |
| 87  | Sh    | 0.09         | 0/1231           | 0.27        | 0/1671          |
| 88  | S5    | 0.08         | 0/279            | 0.21        | 0/431           |
| All | All   | 0.13         | 11/226647 (0.0%) | 0.25        | 5/332750 (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 |
|-----|-------|---------------------|---------------------|
| 28  | LT    | 0                   | 1                   |

All (11) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 67  | SN    | 100  | PRO  | CG-CD | -11.35 | 1.12        | 1.50     |
| 67  | SN    | 100  | PRO  | CB-CG | -5.79  | 1.20        | 1.49     |
| 2   | L2    | 527  | A2M  | O3'-P | 5.36   | 1.61        | 1.56     |
| 2   | L2    | 1384 | A2M  | O3'-P | 5.20   | 1.61        | 1.56     |
| 51  | S1    | 668  | A2M  | O3'-P | 5.17   | 1.61        | 1.56     |
| 1   | L1    | 1253 | OMU  | O3'-P | 5.12   | 1.61        | 1.56     |
| 2   | L2    | 604  | A2M  | O3'-P | 5.11   | 1.61        | 1.56     |
| 2   | L2    | 1372 | A2M  | O3'-P | 5.11   | 1.61        | 1.56     |
| 1   | L1    | 1039 | OMU  | O3'-P | 5.08   | 1.61        | 1.56     |
| 51  | S1    | 98   | A2M  | O3'-P | 5.05   | 1.61        | 1.56     |
| 2   | L2    | 572  | A2M  | O3'-P | 5.05   | 1.61        | 1.56     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 67  | SN    | 100 | PRO  | N-CD-CG  | -19.68 | 73.69       | 103.20   |
| 67  | SN    | 100 | PRO  | CA-CB-CG | -17.99 | 70.31       | 104.50   |
| 67  | SN    | 100 | PRO  | CB-CG-CD | 8.34   | 132.79      | 106.10   |
| 67  | SN    | 100 | PRO  | N-CA-CB  | -6.44  | 97.40       | 103.19   |
| 67  | SN    | 100 | PRO  | CA-N-CD  | -6.41  | 103.03      | 112.00   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 28  | LT    | 135 | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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   | L1    | 36117 | 0        | 18210    | 264     | 0            |
| 2   | L2    | 24815 | 0        | 12579    | 193     | 0            |
| 3   | L3    | 3880  | 0        | 1967     | 29      | 0            |
| 4   | L4    | 3937  | 0        | 1989     | 19      | 0            |
| 5   | L5    | 2578  | 0        | 1309     | 23      | 0            |
| 6   | L6    | 1526  | 0        | 779      | 23      | 0            |
| 7   | L7    | 3534  | 0        | 1793     | 30      | 0            |
| 8   | L8    | 2551  | 0        | 1293     | 14      | 0            |
| 9   | LA    | 1972  | 0        | 2018     | 21      | 0            |
| 10  | LB    | 3216  | 0        | 3334     | 47      | 0            |
| 11  | LC    | 2826  | 0        | 2942     | 24      | 0            |
| 12  | LD    | 1391  | 0        | 1436     | 21      | 0            |
| 13  | LE    | 1477  | 0        | 1558     | 22      | 0            |
| 14  | LF    | 1169  | 0        | 1242     | 26      | 0            |
| 15  | LG    | 1895  | 0        | 1993     | 18      | 0            |
| 16  | LH    | 1767  | 0        | 1872     | 20      | 0            |
| 17  | LI    | 1695  | 0        | 1764     | 15      | 0            |
| 18  | LJ    | 1012  | 0        | 1057     | 12      | 0            |
| 19  | LK    | 1329  | 0        | 1381     | 17      | 0            |
| 20  | LL    | 1124  | 0        | 1151     | 22      | 0            |
| 21  | LM    | 1711  | 0        | 1790     | 20      | 0            |
| 22  | LN    | 1626  | 0        | 1696     | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | LO    | 2339  | 0        | 2424     | 25      | 0            |
| 24  | LP    | 1539  | 0        | 1648     | 21      | 0            |
| 25  | LQ    | 1692  | 0        | 1807     | 16      | 0            |
| 26  | LR    | 1455  | 0        | 1492     | 13      | 0            |
| 27  | LS    | 1261  | 0        | 1311     | 13      | 0            |
| 28  | LT    | 1221  | 0        | 1256     | 11      | 0            |
| 29  | LU    | 960   | 0        | 987      | 15      | 0            |
| 30  | LV    | 953   | 0        | 1016     | 5       | 0            |
| 31  | LW    | 967   | 0        | 1040     | 15      | 0            |
| 32  | LX    | 714   | 0        | 727      | 6       | 0            |
| 33  | LY    | 1065  | 0        | 1135     | 8       | 0            |
| 34  | LZ    | 1117  | 0        | 1165     | 18      | 0            |
| 35  | La    | 1043  | 0        | 1142     | 11      | 0            |
| 36  | Lb    | 546   | 0        | 575      | 5       | 0            |
| 37  | Lc    | 1862  | 0        | 1959     | 16      | 0            |
| 38  | Ld    | 730   | 0        | 743      | 10      | 0            |
| 39  | Le    | 1469  | 0        | 1599     | 17      | 0            |
| 40  | Lf    | 1046  | 0        | 1106     | 6       | 0            |
| 41  | Lg    | 1159  | 0        | 1209     | 16      | 0            |
| 42  | Lh    | 1029  | 0        | 1084     | 17      | 0            |
| 43  | Li    | 798   | 0        | 853      | 3       | 0            |
| 44  | Lj    | 668   | 0        | 672      | 8       | 0            |
| 45  | Lk    | 608   | 0        | 641      | 5       | 0            |
| 46  | Ll    | 450   | 0        | 483      | 6       | 0            |
| 47  | Lm    | 416   | 0        | 446      | 7       | 0            |
| 48  | Ln    | 292   | 0        | 331      | 4       | 0            |
| 49  | Lo    | 693   | 0        | 712      | 7       | 0            |
| 50  | Lp    | 784   | 0        | 841      | 13      | 0            |
| 51  | S1    | 39635 | 0        | 20030    | 303     | 0            |
| 52  | S2    | 325   | 0        | 175      | 3       | 0            |
| 52  | S4    | 1446  | 0        | 738      | 16      | 0            |
| 53  | S3    | 1599  | 0        | 816      | 9       | 0            |
| 54  | SA    | 1909  | 0        | 1999     | 18      | 0            |
| 55  | SB    | 1662  | 0        | 1692     | 22      | 0            |
| 56  | SC    | 1646  | 0        | 1716     | 26      | 0            |
| 57  | SD    | 1508  | 0        | 1582     | 29      | 0            |
| 58  | SE    | 2054  | 0        | 2148     | 19      | 0            |
| 59  | SF    | 1708  | 0        | 1754     | 17      | 0            |
| 60  | SG    | 1866  | 0        | 1990     | 32      | 0            |
| 61  | SH    | 1441  | 0        | 1469     | 19      | 0            |
| 62  | SI    | 1649  | 0        | 1752     | 26      | 0            |
| 63  | SJ    | 1021  | 0        | 1050     | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 64  | SK    | 1582  | 0        | 1652     | 21      | 0            |
| 65  | SL    | 1140  | 0        | 1197     | 16      | 0            |
| 66  | SM    | 805   | 0        | 844      | 16      | 0            |
| 67  | SN    | 874   | 0        | 860      | 13      | 0            |
| 68  | SO    | 1024  | 0        | 1052     | 13      | 0            |
| 69  | SP    | 1100  | 0        | 1146     | 15      | 0            |
| 70  | SQ    | 480   | 0        | 229      | 2       | 0            |
| 71  | SR    | 1138  | 0        | 1186     | 12      | 0            |
| 72  | SS    | 452   | 0        | 459      | 5       | 0            |
| 73  | ST    | 1167  | 0        | 1243     | 9       | 0            |
| 74  | SU    | 1260  | 0        | 1301     | 7       | 0            |
| 75  | SV    | 992   | 0        | 1065     | 20      | 0            |
| 76  | SW    | 928   | 0        | 955      | 13      | 0            |
| 77  | SX    | 1206  | 0        | 1231     | 16      | 0            |
| 78  | SY    | 673   | 0        | 664      | 8       | 0            |
| 79  | SZ    | 1051  | 0        | 1130     | 17      | 0            |
| 80  | Sa    | 650   | 0        | 688      | 12      | 0            |
| 81  | Sb    | 825   | 0        | 859      | 7       | 0            |
| 82  | Sc    | 661   | 0        | 647      | 10      | 0            |
| 83  | Sd    | 496   | 0        | 511      | 4       | 0            |
| 84  | Se    | 449   | 0        | 475      | 8       | 0            |
| 85  | Sf    | 465   | 0        | 353      | 14      | 0            |
| 86  | Sg    | 2343  | 0        | 2256     | 41      | 0            |
| 87  | Sh    | 1212  | 0        | 1139     | 29      | 0            |
| 88  | S5    | 251   | 0        | 130      | 1       | 0            |
| 89  | L1    | 150   | 0        | 285      | 14      | 0            |
| 89  | L2    | 20    | 0        | 36       | 1       | 0            |
| 89  | LM    | 10    | 0        | 19       | 3       | 0            |
| 89  | S1    | 30    | 0        | 57       | 5       | 0            |
| 90  | L1    | 120   | 0        | 0        | 0       | 0            |
| 90  | L2    | 94    | 0        | 0        | 0       | 0            |
| 90  | L3    | 5     | 0        | 0        | 0       | 0            |
| 90  | L4    | 10    | 0        | 0        | 0       | 0            |
| 90  | L5    | 6     | 0        | 0        | 0       | 0            |
| 90  | L6    | 2     | 0        | 0        | 0       | 0            |
| 90  | L7    | 4     | 0        | 0        | 0       | 0            |
| 90  | L8    | 6     | 0        | 0        | 0       | 0            |
| 90  | LA    | 2     | 0        | 0        | 0       | 0            |
| 90  | LG    | 1     | 0        | 0        | 0       | 0            |
| 90  | LJ    | 1     | 0        | 0        | 0       | 0            |
| 90  | LN    | 1     | 0        | 0        | 0       | 0            |
| 90  | LS    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 90  | LT    | 1     | 0        | 0        | 0       | 0            |
| 90  | Lf    | 1     | 0        | 0        | 0       | 0            |
| 90  | Lh    | 2     | 0        | 0        | 0       | 0            |
| 90  | S1    | 109   | 0        | 0        | 0       | 0            |
| 90  | S3    | 1     | 0        | 0        | 0       | 0            |
| 90  | SG    | 1     | 0        | 0        | 0       | 0            |
| 90  | SO    | 1     | 0        | 0        | 0       | 0            |
| 90  | ST    | 1     | 0        | 0        | 0       | 0            |
| 90  | SX    | 1     | 0        | 0        | 0       | 0            |
| 90  | Sb    | 1     | 0        | 0        | 0       | 0            |
| 91  | L1    | 15    | 0        | 0        | 0       | 0            |
| 91  | L2    | 12    | 0        | 0        | 0       | 0            |
| 91  | L3    | 1     | 0        | 0        | 0       | 0            |
| 91  | L4    | 3     | 0        | 0        | 0       | 0            |
| 91  | L7    | 2     | 0        | 0        | 0       | 0            |
| 91  | LN    | 1     | 0        | 0        | 0       | 0            |
| 91  | Lf    | 1     | 0        | 0        | 0       | 0            |
| 91  | S1    | 12    | 0        | 0        | 0       | 0            |
| 91  | SS    | 1     | 0        | 0        | 0       | 0            |
| 92  | L1    | 20    | 0        | 0        | 0       | 0            |
| 92  | L2    | 14    | 0        | 0        | 0       | 0            |
| 92  | L4    | 4     | 0        | 0        | 0       | 0            |
| 92  | L7    | 1     | 0        | 0        | 0       | 0            |
| 92  | LB    | 1     | 0        | 0        | 0       | 0            |
| 92  | LC    | 2     | 0        | 0        | 0       | 0            |
| 92  | LM    | 1     | 0        | 0        | 0       | 0            |
| 92  | LV    | 1     | 0        | 0        | 0       | 0            |
| 92  | Le    | 1     | 0        | 0        | 0       | 0            |
| 92  | Ll    | 1     | 0        | 0        | 0       | 0            |
| 92  | S1    | 19    | 0        | 0        | 0       | 0            |
| 93  | L1    | 42    | 0        | 82       | 1       | 0            |
| 93  | L2    | 30    | 0        | 60       | 1       | 0            |
| 93  | L4    | 6     | 0        | 12       | 0       | 0            |
| 93  | L5    | 6     | 0        | 12       | 0       | 0            |
| 93  | S1    | 12    | 0        | 24       | 0       | 0            |
| 94  | L1    | 42    | 0        | 45       | 3       | 0            |
| 94  | L2    | 84    | 0        | 90       | 6       | 0            |
| 94  | L7    | 42    | 0        | 45       | 4       | 0            |
| 94  | S1    | 84    | 0        | 89       | 5       | 0            |
| 95  | LK    | 1     | 0        | 0        | 0       | 0            |
| 95  | Lj    | 1     | 0        | 0        | 0       | 0            |
| 95  | Lm    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 95  | Lo    | 1     | 0        | 0        | 0       | 0            |
| 95  | Lp    | 1     | 0        | 0        | 0       | 0            |
| 95  | SS    | 1     | 0        | 0        | 0       | 0            |
| 95  | Sb    | 1     | 0        | 0        | 0       | 0            |
| 96  | L1    | 762   | 0        | 0        | 4       | 0            |
| 96  | L2    | 787   | 0        | 0        | 4       | 0            |
| 96  | L3    | 49    | 0        | 0        | 0       | 0            |
| 96  | L4    | 55    | 0        | 0        | 1       | 0            |
| 96  | L5    | 22    | 0        | 0        | 0       | 0            |
| 96  | L7    | 24    | 0        | 0        | 0       | 0            |
| 96  | LA    | 46    | 0        | 0        | 1       | 0            |
| 96  | LB    | 42    | 0        | 0        | 0       | 0            |
| 96  | LC    | 27    | 0        | 0        | 0       | 0            |
| 96  | LD    | 1     | 0        | 0        | 0       | 0            |
| 96  | LG    | 1     | 0        | 0        | 0       | 0            |
| 96  | LH    | 6     | 0        | 0        | 0       | 0            |
| 96  | LI    | 11    | 0        | 0        | 0       | 0            |
| 96  | LJ    | 5     | 0        | 0        | 0       | 0            |
| 96  | LL    | 15    | 0        | 0        | 0       | 0            |
| 96  | LM    | 26    | 0        | 0        | 0       | 0            |
| 96  | LN    | 2     | 0        | 0        | 0       | 0            |
| 96  | LO    | 1     | 0        | 0        | 0       | 0            |
| 96  | LP    | 9     | 0        | 0        | 0       | 0            |
| 96  | LQ    | 11    | 0        | 0        | 0       | 0            |
| 96  | LS    | 4     | 0        | 0        | 0       | 0            |
| 96  | LT    | 15    | 0        | 0        | 0       | 0            |
| 96  | LU    | 1     | 0        | 0        | 0       | 0            |
| 96  | LV    | 2     | 0        | 0        | 0       | 0            |
| 96  | LW    | 5     | 0        | 0        | 1       | 0            |
| 96  | LX    | 2     | 0        | 0        | 0       | 0            |
| 96  | LY    | 2     | 0        | 0        | 0       | 0            |
| 96  | La    | 1     | 0        | 0        | 0       | 0            |
| 96  | Lb    | 5     | 0        | 0        | 0       | 0            |
| 96  | Lc    | 2     | 0        | 0        | 0       | 0            |
| 96  | Ld    | 4     | 0        | 0        | 0       | 0            |
| 96  | Le    | 6     | 0        | 0        | 0       | 0            |
| 96  | Lf    | 3     | 0        | 0        | 0       | 0            |
| 96  | Lg    | 3     | 0        | 0        | 0       | 0            |
| 96  | Lh    | 12    | 0        | 0        | 0       | 0            |
| 96  | Lj    | 18    | 0        | 0        | 0       | 0            |
| 96  | Ln    | 9     | 0        | 0        | 0       | 0            |
| 96  | Lo    | 23    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 96  | Lp    | 14     | 0        | 0        | 0       | 0            |
| 96  | S1    | 595    | 0        | 0        | 3       | 0            |
| 96  | S2    | 1      | 0        | 0        | 0       | 0            |
| 96  | S3    | 6      | 0        | 0        | 0       | 0            |
| 96  | S4    | 15     | 0        | 0        | 0       | 0            |
| 96  | SA    | 6      | 0        | 0        | 0       | 0            |
| 96  | SF    | 1      | 0        | 0        | 0       | 0            |
| 96  | SJ    | 1      | 0        | 0        | 0       | 0            |
| 96  | SK    | 19     | 0        | 0        | 0       | 0            |
| 96  | SO    | 9      | 0        | 0        | 0       | 0            |
| 96  | SP    | 4      | 0        | 0        | 0       | 0            |
| 96  | ST    | 14     | 0        | 0        | 0       | 0            |
| 96  | SU    | 9      | 0        | 0        | 0       | 0            |
| 96  | Sb    | 9      | 0        | 0        | 0       | 0            |
| 96  | Sc    | 1      | 0        | 0        | 0       | 0            |
| 96  | Sg    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 218491 | 0        | 158596   | 1688    | 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 5.

All (1688) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 94:L2:1729:PAR:O43 | 94:L2:1729:PAR:C13 | 1.65                     | 1.24              |
| 94:S1:2445:PAR:C13 | 94:S1:2445:PAR:O43 | 1.65                     | 1.24              |
| 94:L2:1728:PAR:O43 | 94:L2:1728:PAR:C13 | 1.65                     | 1.19              |
| 94:L7:208:PAR:O43  | 94:L7:208:PAR:C13  | 1.65                     | 1.17              |
| 94:L1:1978:PAR:O43 | 94:L1:1978:PAR:C13 | 1.65                     | 1.12              |
| 94:S1:2446:PAR:O43 | 94:S1:2446:PAR:C13 | 1.65                     | 1.12              |
| 51:S1:955:A:HO2'   | 51:S1:956:A:H8     | 1.04                     | 0.94              |
| 51:S1:1281:C:HO2'  | 63:SJ:2:THR:N      | 1.73                     | 0.86              |
| 2:L2:1441:C:H5     | 6:L6:6:G:H1        | 1.22                     | 0.86              |
| 87:Sh:163:GLN:HE21 | 87:Sh:178:ASP:HA   | 1.40                     | 0.86              |
| 2:L2:1078:OMG:N2   | 2:L2:1236:C:O2     | 2.10                     | 0.82              |
| 51:S1:264:C:O2     | 51:S1:275:A:N6     | 2.14                     | 0.81              |
| 2:L2:1139:U:HO2'   | 2:L2:1171:G:HO2'   | 1.31                     | 0.78              |
| 2:L2:1502:G:OP2    | 39:Le:33:ARG:NH1   | 2.18                     | 0.77              |
| 2:L2:134:C:H5      | 2:L2:344:G:H1      | 1.34                     | 0.76              |
| 5:L5:65:U:H3       | 5:L5:93:G:H1       | 1.33                     | 0.75              |
| 1:L1:1182:C:O2     | 1:L1:1190:OMG:N2   | 2.19                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L8:55:G:H21      | 12:LD:11:MET:HE3   | 1.52                     | 0.74              |
| 51:S1:694:U:H3     | 51:S1:751:G:H1     | 1.33                     | 0.74              |
| 2:L2:569:G:O2'     | 2:L2:571:G:OP2     | 2.05                     | 0.74              |
| 8:L8:67:C:N4       | 22:LN:210:ASN:O    | 2.21                     | 0.74              |
| 2:L2:1458:G:OP1    | 10:LB:148:ARG:NH1  | 2.21                     | 0.73              |
| 19:LK:43:ASP:HB3   | 19:LK:46:MET:HB2   | 1.71                     | 0.73              |
| 31:LW:28:MET:HB3   | 31:LW:98:PRO:HG2   | 1.69                     | 0.72              |
| 64:SK:113:TYR:OH   | 64:SK:169:HIS:NE2  | 2.18                     | 0.72              |
| 94:L2:1729:PAR:O44 | 94:L2:1729:PAR:N64 | 2.23                     | 0.72              |
| 51:S1:1114:G:H1    | 51:S1:1207:U:H3    | 1.36                     | 0.72              |
| 1:L1:599:G:H1      | 1:L1:606:C:H5      | 1.37                     | 0.72              |
| 51:S1:779:A:H62    | 51:S1:839:G:H1     | 1.37                     | 0.72              |
| 1:L1:242:A:H5''    | 34:LZ:146:ARG:HD3  | 1.71                     | 0.71              |
| 87:Sh:136:SER:OG   | 87:Sh:177:LEU:O    | 2.09                     | 0.71              |
| 1:L1:1685:G:H22    | 1:L1:1715:U:H3     | 1.37                     | 0.71              |
| 8:L8:111:A:OP1     | 23:LO:289:ARG:NH1  | 2.23                     | 0.71              |
| 52:S4:43:U:H3      | 52:S4:55:G:H1      | 1.39                     | 0.71              |
| 51:S1:1767:G:OP1   | 51:S1:1767:G:N2    | 2.23                     | 0.70              |
| 5:L5:37:C:OP2      | 10:LB:392:LYS:NZ   | 2.25                     | 0.70              |
| 1:L1:1527:OMC:HM22 | 1:L1:1528:PSU:H5'' | 1.73                     | 0.70              |
| 48:Ln:3:THR:HG22   | 51:S1:2196:G:H5''  | 1.74                     | 0.70              |
| 84:Se:25:GLU:OE2   | 84:Se:25:GLU:N     | 2.26                     | 0.69              |
| 1:L1:611:C:OP2     | 11:LC:359:ARG:NH1  | 2.26                     | 0.69              |
| 51:S1:1543:B8N:O3' | 65:SL:148:TYR:O    | 2.10                     | 0.69              |
| 85:Sf:123:PRO:HA   | 85:Sf:127:ALA:HB2  | 1.74                     | 0.69              |
| 1:L1:1588:G:O2'    | 1:L1:1590:G:OP2    | 2.10                     | 0.69              |
| 57:SD:51:MET:HE3   | 57:SD:75:ILE:HD11  | 1.75                     | 0.69              |
| 2:L2:782:G:H1      | 2:L2:807:A:H61     | 1.40                     | 0.68              |
| 11:LC:113:LYS:HG2  | 21:LM:203:LYS:HB3  | 1.75                     | 0.68              |
| 78:SY:10:GLU:OE2   | 78:SY:10:GLU:N     | 2.25                     | 0.68              |
| 1:L1:1250:U:OP2    | 16:LH:67:ARG:NH1   | 2.25                     | 0.68              |
| 51:S1:159:C:OP1    | 60:SG:2:LYS:NZ     | 2.26                     | 0.68              |
| 56:SC:207:ILE:HD13 | 75:SV:50:ILE:HD11  | 1.75                     | 0.68              |
| 87:Sh:67:VAL:HG12  | 87:Sh:70:ALA:H     | 1.58                     | 0.68              |
| 51:S1:878:C:H2'    | 51:S1:879:A:H8     | 1.58                     | 0.68              |
| 2:L2:743:C:H2'     | 2:L2:744:G:H8      | 1.59                     | 0.68              |
| 67:SN:94:MET:HE3   | 67:SN:98:GLN:HB3   | 1.76                     | 0.68              |
| 1:L1:1684:G:H22    | 1:L1:1716:G:H1     | 1.40                     | 0.68              |
| 51:S1:927:G:H1     | 51:S1:959:U:H3     | 1.40                     | 0.68              |
| 5:L5:62:C:H3'      | 5:L5:63:G:H21      | 1.59                     | 0.67              |
| 5:L5:64:G:OP2      | 5:L5:64:G:N2       | 2.22                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:S4:26:U:O2      | 52:S4:30:A:N6      | 2.27                     | 0.67              |
| 74:SU:36:PRO:HB3   | 74:SU:47:ILE:HD11  | 1.75                     | 0.67              |
| 3:L3:212:G:H5'     | 33:LY:131:ARG:HH22 | 1.60                     | 0.67              |
| 51:S1:1980:U:H4'   | 51:S1:2019:OMC:H4' | 1.75                     | 0.67              |
| 21:LM:195:ASN:O    | 89:LM:301:SPD:N10  | 2.27                     | 0.67              |
| 14:LF:42:LEU:HD11  | 14:LF:85:ILE:HG13  | 1.75                     | 0.67              |
| 58:SE:97:ARG:HB2   | 58:SE:111:LEU:HD11 | 1.76                     | 0.66              |
| 2:L2:1402:G:N2     | 2:L2:1405:A:OP2    | 2.28                     | 0.66              |
| 35:La:92:THR:HG22  | 35:La:95:ARG:H     | 1.60                     | 0.66              |
| 2:L2:67:G:O6       | 39:Le:103:LYS:NZ   | 2.28                     | 0.66              |
| 1:L1:306:G:H5''    | 21:LM:14:LYS:HE3   | 1.76                     | 0.66              |
| 51:S1:695:G:H1     | 51:S1:750:U:H3     | 1.43                     | 0.66              |
| 59:SF:138:ARG:HA   | 59:SF:141:MET:HE2  | 1.77                     | 0.66              |
| 68:SO:106:GLN:HG2  | 81:Sb:47:LEU:HD23  | 1.76                     | 0.66              |
| 1:L1:601:G:H1'     | 1:L1:604:C:H5      | 1.60                     | 0.66              |
| 1:L1:1679:G:H1     | 1:L1:1721:U:H3     | 1.42                     | 0.66              |
| 7:L7:93:C:O2'      | 7:L7:94:G:OP1      | 2.13                     | 0.66              |
| 86:Sg:123:VAL:HG22 | 86:Sg:133:VAL:HG22 | 1.78                     | 0.66              |
| 1:L1:1715:U:H2'    | 1:L1:1716:G:H8     | 1.61                     | 0.66              |
| 51:S1:255:A:H5''   | 51:S1:943:U:H1'    | 1.76                     | 0.66              |
| 54:SA:151:GLN:HE21 | 54:SA:153:SER:HB2  | 1.60                     | 0.66              |
| 1:L1:983:U:O2'     | 89:L1:1813:SPD:N1  | 2.29                     | 0.65              |
| 4:L4:126:G:O2'     | 4:L4:127:G:N2      | 2.29                     | 0.65              |
| 7:L7:71:A:H3'      | 31:LW:48:ARG:HB2   | 1.77                     | 0.65              |
| 64:SK:57:ALA:HB2   | 64:SK:196:GLY:HA2  | 1.79                     | 0.65              |
| 69:SP:60:LYS:HG3   | 69:SP:116:PRO:HG3  | 1.78                     | 0.65              |
| 76:SW:75:LYS:HE3   | 76:SW:78:GLU:HB2   | 1.78                     | 0.65              |
| 51:S1:1207:U:H5'   | 73:ST:55:ARG:HD3   | 1.78                     | 0.65              |
| 70:SQ:106:ARG:HA   | 70:SQ:111:GLU:HA   | 1.78                     | 0.65              |
| 58:SE:84:MET:HE2   | 58:SE:120:LEU:H    | 1.62                     | 0.65              |
| 14:LF:54:LEU:HD11  | 14:LF:66:SER:HB3   | 1.77                     | 0.65              |
| 15:LG:106:ARG:HG3  | 15:LG:109:ARG:HH21 | 1.62                     | 0.65              |
| 2:L2:1108:U:H5'    | 12:LD:67:ILE:HD11  | 1.76                     | 0.65              |
| 43:Li:95:GLU:OE1   | 43:Li:98:ARG:NH2   | 2.30                     | 0.65              |
| 51:S1:761:A:H62    | 51:S1:768:A:H61    | 1.42                     | 0.65              |
| 51:S1:1539:PSU:O4  | 51:S1:1550:OMG:N2  | 2.28                     | 0.65              |
| 86:Sg:38:ALA:HB3   | 86:Sg:61:LEU:HB2   | 1.78                     | 0.65              |
| 93:L2:1727:PUT:H31 | 10:LB:242:CYS:HB2  | 1.79                     | 0.65              |
| 5:L5:113:G:OP2     | 39:Le:64:ARG:N     | 2.20                     | 0.65              |
| 56:SC:177:ARG:NH1  | 84:Se:63:GLY:O     | 2.30                     | 0.64              |
| 81:Sb:48:ASP:OD1   | 81:Sb:51:SER:OG    | 2.12                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:SC:207:ILE:HD11 | 75:SV:46:LEU:HD13  | 1.77                     | 0.64              |
| 62:SI:2:GLN:HB2    | 62:SI:5:LEU:HD13   | 1.80                     | 0.64              |
| 51:S1:1724:G:OP2   | 51:S1:1724:G:N2    | 2.26                     | 0.64              |
| 2:L2:1284:PSU:H2'  | 47:Lm:97:ARG:HD3   | 1.79                     | 0.64              |
| 2:L2:1353:U:O2'    | 2:L2:1373:C:O2     | 2.15                     | 0.64              |
| 13:LE:46:ARG:NH2   | 19:LK:6:TYR:OH     | 2.27                     | 0.64              |
| 86:Sg:238:ILE:HA   | 86:Sg:254:THR:HG22 | 1.79                     | 0.64              |
| 9:LA:18:VAL:O      | 96:LA:401:HOH:O    | 2.15                     | 0.64              |
| 51:S1:689[A]:U:O2' | 51:S1:690:G:OP2    | 2.11                     | 0.64              |
| 52:S4:9:A:O2'      | 52:S4:10:G:N7      | 2.29                     | 0.64              |
| 66:SM:77:PHE:HB3   | 72:SS:53:PHE:HB3   | 1.79                     | 0.64              |
| 27:LS:51:GLY:HA3   | 27:LS:92:ARG:HG3   | 1.80                     | 0.64              |
| 51:S1:227:U:O3'    | 64:SK:164:ARG:NH2  | 2.30                     | 0.63              |
| 1:L1:684:G:H4'     | 89:L1:1806:SPD:H82 | 1.80                     | 0.63              |
| 12:LD:112:ILE:HD11 | 12:LD:124:ILE:HG12 | 1.81                     | 0.63              |
| 86:Sg:188:ARG:HH22 | 86:Sg:223:LEU:HA   | 1.62                     | 0.63              |
| 6:L6:67:C:OP1      | 41:Lg:96:ARG:NH2   | 2.31                     | 0.63              |
| 51:S1:1493:A:OP1   | 96:S1:2501:HOH:O   | 2.14                     | 0.63              |
| 54:SA:154:ARG:HG2  | 54:SA:154:ARG:HH11 | 1.62                     | 0.63              |
| 2:L2:984:G:H1      | 2:L2:1000:U:H3     | 1.45                     | 0.63              |
| 20:LL:29:GLU:CD    | 20:LL:29:GLU:H     | 2.07                     | 0.63              |
| 51:S1:171:C:OP1    | 60:SG:134:ARG:NH1  | 2.32                     | 0.63              |
| 51:S1:1589:G:H1    | 51:S1:1600:C:H5    | 1.44                     | 0.63              |
| 2:L2:1510:A:H62    | 10:LB:326:ASN:HB3  | 1.64                     | 0.62              |
| 54:SA:207:LEU:HD12 | 54:SA:208:PRO:HD2  | 1.80                     | 0.62              |
| 13:LE:90:LYS:HB2   | 13:LE:182:THR:HG23 | 1.82                     | 0.62              |
| 1:L1:1525:A:H5'    | 1:L1:1526:U:C5'    | 2.30                     | 0.62              |
| 62:SI:183:ARG:HG2  | 62:SI:183:ARG:HH11 | 1.64                     | 0.62              |
| 87:Sh:148:THR:HG23 | 87:Sh:196:ARG:HE   | 1.65                     | 0.62              |
| 4:L4:154:C:H4'     | 13:LE:155:ARG:HE   | 1.64                     | 0.62              |
| 79:SZ:34:HIS:HB2   | 79:SZ:37:TRP:HB2   | 1.82                     | 0.62              |
| 1:L1:166:G:OP1     | 17:LI:137:LYS:NZ   | 2.32                     | 0.62              |
| 2:L2:823:A:O2'     | 2:L2:824:G:N2      | 2.32                     | 0.62              |
| 1:L1:836:G:OP2     | 24:LP:98:ARG:NH2   | 2.32                     | 0.62              |
| 3:L3:5:A:N6        | 3:L3:215:G:O2'     | 2.33                     | 0.62              |
| 51:S1:886:U:H5'    | 58:SE:238:LYS:HZ1  | 1.65                     | 0.62              |
| 77:SX:74:LEU:HD12  | 77:SX:120:LEU:HD22 | 1.82                     | 0.62              |
| 2:L2:974:G:H4'     | 42:Lh:91:ARG:HG2   | 1.82                     | 0.61              |
| 51:S1:1905:C:O2'   | 51:S1:1906:G:O5'   | 2.15                     | 0.61              |
| 56:SC:174:CYS:HB2  | 56:SC:181:ILE:HB   | 1.81                     | 0.61              |
| 1:L1:927:A2M:HM'2  | 1:L1:928:C:H5'     | 1.82                     | 0.61              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:L2:771:G:N7      | 9:LA:67:TYR:OH      | 2.25                     | 0.61              |
| 7:L7:94:G:OP2      | 44:Lj:73:ARG:NH1    | 2.32                     | 0.61              |
| 51:S1:128:C:H4'    | 51:S1:129:U:O5'     | 1.99                     | 0.61              |
| 51:S1:821:A:O2'    | 60:SG:225:GLN:OE1   | 2.17                     | 0.61              |
| 79:SZ:125:ARG:HG3  | 79:SZ:126:GLY:H     | 1.64                     | 0.61              |
| 34:LZ:22:ARG:HB3   | 40:Lf:76:PRO:HG2    | 1.82                     | 0.61              |
| 38:Ld:55:ARG:O     | 38:Ld:59:GLU:HG3    | 2.01                     | 0.61              |
| 80:Sa:91:LEU:HD21  | 80:Sa:94:CYS:HB2    | 1.82                     | 0.61              |
| 12:LD:26:GLY:HA2   | 12:LD:67:ILE:HB     | 1.81                     | 0.61              |
| 55:SB:131:ARG:NH2  | 55:SB:154:ASP:O     | 2.34                     | 0.61              |
| 2:L2:335:C:H3'     | 2:L2:336:C:H5''     | 1.82                     | 0.61              |
| 3:L3:155:A:H61     | 3:L3:174:C:H42      | 1.48                     | 0.61              |
| 51:S1:689[A]:U:H4' | 51:S1:690:G:H5''    | 1.83                     | 0.61              |
| 2:L2:786:A:H4'     | 2:L2:787:G:OP1      | 2.00                     | 0.61              |
| 36:Lb:5:LYS:HE2    | 36:Lb:8:THR:HB      | 1.82                     | 0.61              |
| 7:L7:9:G:OP2       | 94:L7:208:PAR:N64   | 2.34                     | 0.60              |
| 7:L7:31:A:O2'      | 7:L7:33:U:OP2       | 2.14                     | 0.60              |
| 2:L2:1012:U:OP1    | 15:LG:49[B]:ARG:NH2 | 2.34                     | 0.60              |
| 39:Le:47:GLU:OE2   | 39:Le:50:ARG:NH1    | 2.34                     | 0.60              |
| 1:L1:77:U:H5''     | 21:LM:186:PRO:HG3   | 1.84                     | 0.60              |
| 37:Lc:60:LYS:NZ    | 37:Lc:64:GLU:OE2    | 2.34                     | 0.60              |
| 52:S4:50:A:O2'     | 52:S4:52:U:OP2      | 2.11                     | 0.60              |
| 23:LO:134:THR:HG22 | 23:LO:136:LYS:H     | 1.67                     | 0.60              |
| 52:S4:25:A:H3'     | 52:S4:26:U:H5''     | 1.82                     | 0.60              |
| 1:L1:485:A:O5'     | 14:LF:110:LYS:NZ    | 2.34                     | 0.60              |
| 5:L5:70:C:H41      | 5:L5:88:C:H42       | 1.49                     | 0.60              |
| 7:L7:93:C:H2'      | 7:L7:94:G:H5''      | 1.84                     | 0.60              |
| 51:S1:1119:U:H5'   | 51:S1:1120:U:H5'    | 1.84                     | 0.60              |
| 61:SH:83:LEU:HD22  | 61:SH:94:PRO:HB2    | 1.83                     | 0.60              |
| 2:L2:1052:C:O2'    | 2:L2:1053:A:O5'     | 2.17                     | 0.60              |
| 15:LG:142:ARG:HG2  | 15:LG:146:LYS:HE2   | 1.82                     | 0.60              |
| 48:Ln:25:ARG:HH22  | 51:S1:2152:A:H4'    | 1.67                     | 0.60              |
| 51:S1:1108:A:H5''  | 73:ST:16:LEU:HD12   | 1.84                     | 0.60              |
| 1:L1:494:A:OP1     | 14:LF:82:ARG:NE     | 2.33                     | 0.60              |
| 2:L2:512:PSU:OP1   | 53:S3:25:U:O2'      | 2.20                     | 0.60              |
| 2:L2:695:G:H2'     | 2:L2:696:A:C8       | 2.37                     | 0.60              |
| 51:S1:913:G:OP2    | 51:S1:913:G:N2      | 2.29                     | 0.60              |
| 65:SL:100:GLN:HB2  | 65:SL:108:LYS:HE3   | 1.83                     | 0.60              |
| 86:Sg:13:TRP:HB2   | 86:Sg:34:ARG:HG3    | 1.84                     | 0.60              |
| 86:Sg:132:ARG:HG2  | 86:Sg:143:GLU:HG2   | 1.84                     | 0.60              |
| 1:L1:556:C:H5''    | 1:L1:557:U:H5''     | 1.83                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L3:23:U:O2'      | 3:L3:25:G:OP1      | 2.19                     | 0.60              |
| 20:LL:72:THR:HG22  | 20:LL:108:LYS:HB3  | 1.83                     | 0.60              |
| 2:L2:1510:A:N6     | 10:LB:327:ASP:H    | 2.00                     | 0.59              |
| 5:L5:127:A:OP1     | 39:Le:79:ARG:NH2   | 2.35                     | 0.59              |
| 54:SA:146:LYS:HB3  | 54:SA:210:ARG:HB2  | 1.84                     | 0.59              |
| 80:Sa:60:ILE:HB    | 80:Sa:101:TYR:HB2  | 1.84                     | 0.59              |
| 1:L1:663:C:OP1     | 16:LH:111:LYS:NZ   | 2.35                     | 0.59              |
| 1:L1:1105:A:H5''   | 2:L2:1064:A:H61    | 1.65                     | 0.59              |
| 1:L1:1209:G:OP2    | 1:L1:1209:G:N2     | 2.29                     | 0.59              |
| 64:SK:162:TRP:HB3  | 64:SK:166:ARG:HH21 | 1.67                     | 0.59              |
| 2:L2:28:G:H4'      | 44:Lj:8:MET:HG3    | 1.83                     | 0.59              |
| 42:Lh:10:ARG:HG2   | 42:Lh:10:ARG:HH11  | 1.66                     | 0.59              |
| 1:L1:1281:A:O2'    | 1:L1:1348:A:N6     | 2.35                     | 0.59              |
| 1:L1:1372:G:H2'    | 1:L1:1373:A2M:H8   | 1.84                     | 0.59              |
| 6:L6:67:C:N4       | 41:Lg:96:ARG:O     | 2.30                     | 0.59              |
| 13:LE:155:ARG:NH1  | 13:LE:156:GLU:OE2  | 2.34                     | 0.59              |
| 51:S1:478:C:H5''   | 69:SP:48:LYS:HE3   | 1.83                     | 0.59              |
| 53:S3:8:U:O2'      | 53:S3:22:A:N6      | 2.35                     | 0.59              |
| 85:Sf:140:CYS:SG   | 85:Sf:141:GLY:N    | 2.75                     | 0.59              |
| 1:L1:130:U:H2'     | 1:L1:132:A:H62     | 1.67                     | 0.59              |
| 1:L1:982:C:OP1     | 89:L1:1813:SPD:N10 | 2.35                     | 0.59              |
| 2:L2:1329:U:O2'    | 4:L4:42:A:OP1      | 2.18                     | 0.59              |
| 41:Lg:74:ARG:HG2   | 41:Lg:141:PRO:HD3  | 1.83                     | 0.59              |
| 1:L1:1493:G:N2     | 1:L1:1496:A:OP2    | 2.28                     | 0.59              |
| 71:SR:88:GLN:HA    | 71:SR:96:THR:HG23  | 1.83                     | 0.59              |
| 1:L1:1487:U:OP1    | 94:L7:208:PAR:N24  | 2.36                     | 0.59              |
| 6:L6:49:C:N4       | 41:Lg:29:LYS:O     | 2.36                     | 0.59              |
| 1:L1:1084:U:H3'    | 1:L1:1085:C:H5''   | 1.84                     | 0.59              |
| 3:L3:156:G:H1      | 3:L3:173:U:H3      | 1.49                     | 0.59              |
| 18:LJ:111:MET:HE1  | 18:LJ:116:ILE:HG13 | 1.85                     | 0.59              |
| 61:SH:8:LEU:HD21   | 61:SH:55:VAL:HG11  | 1.84                     | 0.59              |
| 6:L6:70:G:HO2'     | 6:L6:71:A:H8       | 1.50                     | 0.59              |
| 27:LS:82:THR:HG22  | 36:Lb:16:ASN:HA    | 1.83                     | 0.59              |
| 51:S1:2010:G:H1    | 51:S1:2026:U:H3    | 1.50                     | 0.59              |
| 67:SN:3:THR:HB     | 67:SN:51:GLN:HG3   | 1.84                     | 0.59              |
| 1:L1:1667:G:OP2    | 21:LM:34:HIS:NE2   | 2.25                     | 0.58              |
| 51:S1:672:G:N1     | 51:S1:1217:A:OP1   | 2.32                     | 0.58              |
| 2:L2:1136:U:H2'    | 2:L2:1137:G:C8     | 2.38                     | 0.58              |
| 2:L2:1253:OMG:HM21 | 2:L2:1255:A:H2'    | 1.84                     | 0.58              |
| 2:L2:1335:C:H2'    | 2:L2:1337:C:H5''   | 1.85                     | 0.58              |
| 2:L2:1510:A:N7     | 10:LB:326:ASN:ND2  | 2.51                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:LQ:105:LEU:HD13 | 25:LQ:135:LYS:HE3  | 1.85                     | 0.58              |
| 51:S1:1788:U:H5'   | 75:SV:48:ASN:HB3   | 1.84                     | 0.58              |
| 57:SD:4:TYR:O      | 58:SE:19:LYS:NZ    | 2.33                     | 0.58              |
| 14:LF:194:ASN:O    | 19:LK:110:ARG:NH2  | 2.37                     | 0.58              |
| 51:S1:1234:G:N3    | 89:S1:2301:SPD:N1  | 2.51                     | 0.58              |
| 1:L1:912:C:OP1     | 96:L1:2001:HOH:O   | 2.17                     | 0.58              |
| 2:L2:1404:G:H5''   | 9:LA:220:GLY:HA3   | 1.84                     | 0.58              |
| 3:L3:174:C:H2'     | 3:L3:175:A:C8      | 2.38                     | 0.58              |
| 60:SG:129:ASP:OD1  | 60:SG:129:ASP:N    | 2.37                     | 0.58              |
| 11:LC:178:ASP:HB3  | 11:LC:206:PRO:HD3  | 1.85                     | 0.58              |
| 20:LL:39:HIS:O     | 20:LL:40:HIS:ND1   | 2.35                     | 0.58              |
| 51:S1:1781:U:O2'   | 51:S1:1782:G:N7    | 2.33                     | 0.58              |
| 51:S1:816:C:OP1    | 87:Sh:174:TYR:OH   | 2.21                     | 0.58              |
| 61:SH:181:GLU:OE1  | 61:SH:184:ARG:NH2  | 2.37                     | 0.58              |
| 79:SZ:63:SER:HB3   | 79:SZ:81:LEU:HB2   | 1.84                     | 0.58              |
| 16:LH:79:ARG:HA    | 16:LH:88:PRO:HD2   | 1.85                     | 0.58              |
| 24:LP:23:ASN:HB3   | 24:LP:26:ILE:HB    | 1.83                     | 0.58              |
| 70:SQ:98:ALA:HB2   | 70:SQ:118:CYS:H    | 1.68                     | 0.58              |
| 13:LE:31:ARG:NH1   | 13:LE:187:GLU:OE2  | 2.37                     | 0.58              |
| 51:S1:1632:C:O2    | 51:S1:1829:OMG:N2  | 2.19                     | 0.58              |
| 3:L3:154:C:H42     | 3:L3:175:A:H61     | 1.52                     | 0.58              |
| 31:LW:71:TYR:O     | 96:LW:201:HOH:O    | 2.17                     | 0.58              |
| 32:LX:84:ARG:NH1   | 60:SG:132:ALA:O    | 2.37                     | 0.58              |
| 51:S1:1362:A:OP1   | 82:Sc:17:ARG:NH2   | 2.37                     | 0.58              |
| 1:L1:493:A:O2'     | 14:LF:80:ASP:OD2   | 2.22                     | 0.57              |
| 11:LC:282:LEU:HD11 | 24:LP:29:LEU:HG    | 1.85                     | 0.57              |
| 45:Lk:55:LYS:HD2   | 45:Lk:58:ARG:HH22  | 1.68                     | 0.57              |
| 55:SB:15:GLU:OE1   | 75:SV:118:ARG:NH2  | 2.37                     | 0.57              |
| 55:SB:60:LYS:NZ    | 78:SY:74:ASN:OD1   | 2.33                     | 0.57              |
| 56:SC:27:GLU:HG2   | 56:SC:68:LEU:HD21  | 1.86                     | 0.57              |
| 1:L1:631:G:O6      | 37:Lc:43:ARG:NE    | 2.36                     | 0.57              |
| 2:L2:623:A:H5''    | 2:L2:624:C:H5      | 1.68                     | 0.57              |
| 11:LC:43:MET:HB3   | 11:LC:236:LEU:HD21 | 1.86                     | 0.57              |
| 86:Sg:178:VAL:O    | 86:Sg:187:GLU:N    | 2.37                     | 0.57              |
| 5:L5:51:A:H1'      | 5:L5:52:U:H2'      | 1.85                     | 0.57              |
| 6:L6:68:A:N6       | 41:Lg:34:TYR:OH    | 2.37                     | 0.57              |
| 10:LB:138:ASN:HA   | 10:LB:143:LYS:HZ3  | 1.69                     | 0.57              |
| 51:S1:1572:C:H41   | 51:S1:1615:G:H1    | 1.52                     | 0.57              |
| 2:L2:558:A:OP1     | 2:L2:560:OMU:H5    | 2.05                     | 0.57              |
| 66:SM:39:ARG:NH2   | 66:SM:97:LYS:O     | 2.37                     | 0.57              |
| 1:L1:141:U:H1'     | 1:L1:142:G:H5'     | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:L2:1391:U:H2'    | 2:L2:1392:U:H6     | 1.68                     | 0.57              |
| 56:SC:56:GLU:OE1   | 56:SC:56:GLU:N     | 2.38                     | 0.57              |
| 47:Lm:78:MET:HE3   | 47:Lm:83:VAL:HA    | 1.86                     | 0.57              |
| 51:S1:479:A2M:O5'  | 51:S1:479:A2M:H8   | 2.04                     | 0.57              |
| 56:SC:123:ARG:O    | 56:SC:127:GLU:HG3  | 2.05                     | 0.57              |
| 2:L2:646:G:H5'     | 2:L2:647:A:OP2     | 2.04                     | 0.57              |
| 2:L2:1486:G:H2'    | 2:L2:1487:G:H8     | 1.70                     | 0.57              |
| 10:LB:93:ARG:HB3   | 10:LB:102:ILE:HD11 | 1.87                     | 0.57              |
| 75:SV:32:LYS:O     | 75:SV:36:MET:HG2   | 2.04                     | 0.57              |
| 1:L1:604:C:O2'     | 1:L1:605:G:O4'     | 2.23                     | 0.57              |
| 2:L2:1407:A:N7     | 9:LA:215:ASN:ND2   | 2.53                     | 0.57              |
| 4:L4:24:A:H5''     | 16:LH:7:LYS:HB2    | 1.87                     | 0.57              |
| 64:SK:76:VAL:HG12  | 64:SK:108:PRO:HG2  | 1.85                     | 0.57              |
| 69:SP:11:ARG:NH2   | 74:SU:117:LYS:O    | 2.34                     | 0.57              |
| 82:Sc:34:MET:HE2   | 82:Sc:49:SER:HA    | 1.87                     | 0.57              |
| 7:L7:60:U:O4       | 35:La:63:ASN:ND2   | 2.33                     | 0.57              |
| 51:S1:1885:A:H5'   | 65:SL:20:THR:HG21  | 1.86                     | 0.57              |
| 51:S1:1914:U:OP1   | 77:SX:134:GLN:NE2  | 2.35                     | 0.56              |
| 1:L1:1242:U:OP1    | 19:LK:17:ARG:NH2   | 2.38                     | 0.56              |
| 2:L2:421:A:N7      | 96:L2:1832:HOH:O   | 2.32                     | 0.56              |
| 5:L5:26:A:OP2      | 10:LB:116:ARG:NH2  | 2.38                     | 0.56              |
| 10:LB:216:GLN:OE1  | 10:LB:360:LYS:NZ   | 2.39                     | 0.56              |
| 13:LE:123:GLN:NE2  | 13:LE:156:GLU:OE1  | 2.32                     | 0.56              |
| 16:LH:65:GLU:OE1   | 16:LH:69:LYS:NZ    | 2.29                     | 0.56              |
| 34:LZ:21:LYS:HG2   | 34:LZ:26:ARG:HG2   | 1.87                     | 0.56              |
| 57:SD:58:LEU:HD22  | 57:SD:68:ARG:HA    | 1.86                     | 0.56              |
| 57:SD:77:ARG:NH1   | 57:SD:81:GLU:OE2   | 2.36                     | 0.56              |
| 1:L1:100:G:OP2     | 1:L1:100:G:N2      | 2.35                     | 0.56              |
| 1:L1:837:A:H4'     | 1:L1:838:G:H5'     | 1.85                     | 0.56              |
| 1:L1:1599:U:O2     | 1:L1:1626:OMG:N2   | 2.37                     | 0.56              |
| 2:L2:1379:A:H5''   | 2:L2:1381:G:H4'    | 1.86                     | 0.56              |
| 13:LE:125:VAL:HG13 | 13:LE:156:GLU:HG3  | 1.86                     | 0.56              |
| 59:SF:55:VAL:HG21  | 59:SF:78:ILE:HG23  | 1.88                     | 0.56              |
| 59:SF:182:VAL:HB   | 59:SF:209:TYR:HB2  | 1.87                     | 0.56              |
| 64:SK:68:ALA:HB2   | 64:SK:201:ILE:HD11 | 1.88                     | 0.56              |
| 87:Sh:165:LEU:O    | 87:Sh:166:ARG:NH1  | 2.38                     | 0.56              |
| 1:L1:2:C:H5'       | 7:L7:169:A:H2      | 1.71                     | 0.56              |
| 5:L5:131:A:OP1     | 28:LT:43:LYS:NZ    | 2.38                     | 0.56              |
| 8:L8:32:C:H5'      | 12:LD:139:ARG:HD3  | 1.88                     | 0.56              |
| 53:S3:1:C:H42      | 53:S3:73:A:H61     | 1.53                     | 0.56              |
| 86:Sg:262:ASP:HB2  | 86:Sg:269:ILE:HD11 | 1.86                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:S1:286:G:H1'    | 60:SG:217:ALA:HB1  | 1.87                     | 0.56              |
| 51:S1:701:G:H22    | 51:S1:745:G:H22    | 1.54                     | 0.56              |
| 94:S1:2445:PAR:N64 | 94:S1:2445:PAR:O44 | 2.38                     | 0.56              |
| 1:L1:206:A:OP2     | 34:LZ:54:LYS:NZ    | 2.38                     | 0.56              |
| 60:SG:2:LYS:HB2    | 60:SG:111:LEU:HD12 | 1.88                     | 0.56              |
| 1:L1:1238:C:H5''   | 1:L1:1239:U:H5'    | 1.86                     | 0.56              |
| 51:S1:263:G:H5'    | 87:Sh:169:ARG:HG3  | 1.87                     | 0.56              |
| 51:S1:396:G:O6     | 69:SP:15:ARG:NH2   | 2.39                     | 0.56              |
| 51:S1:994:U:H3     | 51:S1:1018:G:H1    | 1.54                     | 0.56              |
| 51:S1:2150:G:N7    | 94:S1:2446:PAR:O44 | 2.39                     | 0.56              |
| 66:SM:17:VAL:HG11  | 66:SM:95:VAL:HG11  | 1.88                     | 0.56              |
| 82:Sc:11:PRO:HB2   | 82:Sc:16:GLU:HG2   | 1.86                     | 0.56              |
| 25:LQ:15:LEU:HD13  | 25:LQ:52:ARG:HB2   | 1.87                     | 0.56              |
| 87:Sh:177:LEU:HD12 | 87:Sh:183:ALA:HA   | 1.88                     | 0.56              |
| 1:L1:1092:U:O2'    | 22:LN:196:HIS:NE2  | 2.35                     | 0.55              |
| 1:L1:1153:A:H2'    | 1:L1:1155:A:H62    | 1.70                     | 0.55              |
| 5:L5:127:A:C5      | 39:Le:13:LYS:HD3   | 2.41                     | 0.55              |
| 21:LM:198:ILE:HD13 | 89:LM:301:SPD:H81  | 1.88                     | 0.55              |
| 51:S1:1619:G:HO2'  | 51:S1:1849:G:HO2'  | 1.54                     | 0.55              |
| 51:S1:617:G:H4'    | 69:SP:88:ASP:HB3   | 1.87                     | 0.55              |
| 87:Sh:160:VAL:HG21 | 87:Sh:186:PHE:HD2  | 1.71                     | 0.55              |
| 28:LT:112:MET:HE3  | 28:LT:150:MET:HG3  | 1.88                     | 0.55              |
| 51:S1:789:G:OP1    | 58:SE:173:ARG:NH1  | 2.39                     | 0.55              |
| 51:S1:79:A:O2'     | 51:S1:501:A:N1     | 2.32                     | 0.55              |
| 86:Sg:148:GLY:HA2  | 86:Sg:179:TRP:HH2  | 1.71                     | 0.55              |
| 51:S1:1911:U:H5    | 51:S1:1928:G:H1    | 1.54                     | 0.55              |
| 51:S1:1961:G:O2'   | 51:S1:1987:G:N2    | 2.40                     | 0.55              |
| 57:SD:47:THR:O     | 57:SD:51:MET:HG3   | 2.06                     | 0.55              |
| 76:SW:35:LEU:HG    | 76:SW:39:GLU:HB2   | 1.89                     | 0.55              |
| 1:L1:97:G:N7       | 17:LI:12:HIS:NE2   | 2.54                     | 0.55              |
| 12:LD:111:HIS:HD2  | 12:LD:125:TYR:H    | 1.52                     | 0.55              |
| 2:L2:978:C:OP1     | 15:LG:33:LYS:NZ    | 2.37                     | 0.55              |
| 20:LL:80:ARG:NH2   | 20:LL:106:TYR:OH   | 2.38                     | 0.55              |
| 22:LN:88:ARG:HG2   | 22:LN:90:ARG:HG2   | 1.89                     | 0.55              |
| 51:S1:228:G:OP2    | 64:SK:160:ARG:NE   | 2.35                     | 0.55              |
| 51:S1:878:C:H2'    | 51:S1:879:A:C8     | 2.42                     | 0.55              |
| 52:S4:31:U:H4'     | 68:SO:59:ARG:HH22  | 1.71                     | 0.55              |
| 54:SA:44:ALA:HB2   | 68:SO:40:MET:HE2   | 1.88                     | 0.55              |
| 86:Sg:89:ILE:HB    | 86:Sg:103:PHE:HB2  | 1.88                     | 0.55              |
| 1:L1:170:U:O2      | 35:La:107:LYS:NZ   | 2.38                     | 0.55              |
| 1:L1:398:G:N2      | 1:L1:401:A:OP2     | 2.37                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:L2:746:A:H2'     | 2:L2:747:A:C8      | 2.42                     | 0.55              |
| 2:L2:1281:U:O4     | 2:L2:1336:G:N2     | 2.40                     | 0.55              |
| 51:S1:1684:U:H3    | 51:S1:1820:G:H22   | 1.55                     | 0.55              |
| 55:SB:77:VAL:HG22  | 55:SB:124:VAL:HB   | 1.87                     | 0.55              |
| 78:SY:42:ALA:HA    | 78:SY:54:THR:HG22  | 1.88                     | 0.55              |
| 1:L1:1017:PSU:OP1  | 20:LL:44:ASN:ND2   | 2.38                     | 0.55              |
| 2:L2:849:C:H42     | 2:L2:949:U:H3      | 1.55                     | 0.55              |
| 20:LL:134:ILE:HG21 | 20:LL:141:VAL:HG23 | 1.88                     | 0.55              |
| 29:LU:42:ASP:O     | 29:LU:46:ASN:ND2   | 2.39                     | 0.55              |
| 39:Le:96:LEU:HD11  | 39:Le:108:ALA:HB2  | 1.88                     | 0.55              |
| 51:S1:1360:U:H4'   | 51:S1:1361:U:O5'   | 2.06                     | 0.55              |
| 1:L1:1683:C:H2'    | 1:L1:1684:G:C8     | 2.43                     | 0.54              |
| 51:S1:594:A:H61    | 51:S1:643:A:H5''   | 1.72                     | 0.54              |
| 64:SK:26:LYS:HG2   | 64:SK:29:LEU:HD23  | 1.89                     | 0.54              |
| 1:L1:510:U:O2'     | 1:L1:511:A:OP1     | 2.24                     | 0.54              |
| 3:L3:62:U:O4       | 29:LU:96:LYS:NZ    | 2.40                     | 0.54              |
| 12:LD:89:LYS:HE3   | 12:LD:106:PHE:HB2  | 1.88                     | 0.54              |
| 51:S1:1273:A:N7    | 51:S1:2175:C:O2'   | 2.38                     | 0.54              |
| 51:S1:1961:G:H5'   | 77:SX:99:GLY:HA2   | 1.87                     | 0.54              |
| 2:L2:382:A2M:O5'   | 2:L2:382:A2M:H8    | 2.07                     | 0.54              |
| 4:L4:149:U:H1'     | 4:L4:150:A:H5''    | 1.89                     | 0.54              |
| 8:L8:16:C:OP2      | 8:L8:71:C:O2'      | 2.25                     | 0.54              |
| 22:LN:44:ASP:OD1   | 22:LN:185:ARG:NH1  | 2.39                     | 0.54              |
| 44:Lj:27:TYR:HA    | 44:Lj:34:CYS:HA    | 1.90                     | 0.54              |
| 51:S1:68:A:OP1     | 60:SG:175:LYS:NZ   | 2.39                     | 0.54              |
| 52:S4:46:U:O2'     | 52:S4:47:U:O5'     | 2.24                     | 0.54              |
| 61:SH:47:PHE:HD1   | 61:SH:130:MET:HE2  | 1.71                     | 0.54              |
| 66:SM:23:SER:HB3   | 66:SM:29:VAL:HB    | 1.88                     | 0.54              |
| 1:L1:1688:G:H22    | 1:L1:1712:G:H22    | 1.55                     | 0.54              |
| 45:Lk:57:GLU:HA    | 45:Lk:60:ILE:HD12  | 1.88                     | 0.54              |
| 60:SG:162:ARG:HG2  | 60:SG:176:ALA:HB2  | 1.89                     | 0.54              |
| 74:SU:30:ASN:HB3   | 74:SU:33:MET:HG2   | 1.88                     | 0.54              |
| 62:SI:55:PRO:O     | 62:SI:170:ARG:NH2  | 2.41                     | 0.54              |
| 85:Sf:120:CYS:HA   | 85:Sf:131:MET:HE2  | 1.88                     | 0.54              |
| 1:L1:1348:A:H2'    | 1:L1:1349:A:H4'    | 1.88                     | 0.54              |
| 10:LB:209:ARG:HH22 | 10:LB:292:ARG:HD2  | 1.72                     | 0.54              |
| 62:SI:40:GLU:OE1   | 62:SI:43:ARG:NH2   | 2.41                     | 0.54              |
| 63:SJ:18:GLU:HG3   | 63:SJ:69:LEU:HD23  | 1.88                     | 0.54              |
| 1:L1:1213:C:OP2    | 37:Lc:104:LYS:NZ   | 2.41                     | 0.54              |
| 2:L2:1450:G:O2'    | 6:L6:14:A:N6       | 2.30                     | 0.54              |
| 11:LC:162:LYS:HB2  | 11:LC:165:GLU:HG3  | 1.89                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:S2:37:MIA:H2'   | 52:S2:38:A:O4'     | 2.08                     | 0.54              |
| 2:L2:1360:OMG:HN21 | 52:S2:75:C:H42     | 1.55                     | 0.54              |
| 51:S1:701:G:H1     | 51:S1:745:G:H22    | 1.56                     | 0.54              |
| 54:SA:5:LYS:NZ     | 68:SO:58:ASP:OD2   | 2.39                     | 0.54              |
| 2:L2:954:A:C8      | 42:Lh:114:MET:HE1  | 2.43                     | 0.54              |
| 3:L3:173:U:H2'     | 3:L3:174:C:C6      | 2.43                     | 0.54              |
| 63:SJ:80:ASP:HA    | 63:SJ:124:LYS:HA   | 1.89                     | 0.54              |
| 89:L1:1815:SPD:H22 | 21:LM:83:LYS:HG3   | 1.90                     | 0.54              |
| 2:L2:14:OMC:HM22   | 2:L2:15:C:O4'      | 2.08                     | 0.54              |
| 2:L2:646:G:N7      | 2:L2:647:A:N6      | 2.55                     | 0.54              |
| 50:Lp:74:CYS:SG    | 50:Lp:77:CYS:HB2   | 2.47                     | 0.54              |
| 51:S1:1551:G:H5''  | 72:SS:30:ALA:HB2   | 1.90                     | 0.54              |
| 1:L1:1363:A:H4'    | 1:L1:1364:A:H5''   | 1.89                     | 0.53              |
| 1:L1:1773:C:O2'    | 7:L7:139:A:N3      | 2.37                     | 0.53              |
| 7:L7:71:A:H4'      | 7:L7:72:A:O5'      | 2.08                     | 0.53              |
| 1:L1:1243:G:OP2    | 26:LR:2:VAL:N      | 2.42                     | 0.53              |
| 6:L6:24[B]:C:OP1   | 13:LE:23:ARG:NH1   | 2.33                     | 0.53              |
| 19:LK:16:LEU:HD21  | 19:LK:57:GLU:HB2   | 1.90                     | 0.53              |
| 44:Lj:55:LYS:HA    | 44:Lj:58:ARG:HD2   | 1.90                     | 0.53              |
| 51:S1:461:G:O2'    | 60:SG:60:ASP:OD2   | 2.25                     | 0.53              |
| 51:S1:810:G:OP1    | 87:Sh:125:THR:OG1  | 2.26                     | 0.53              |
| 51:S1:955:A:O2'    | 51:S1:956:A:O5'    | 2.25                     | 0.53              |
| 51:S1:1358:A:N6    | 78:SY:79:ASP:OD1   | 2.39                     | 0.53              |
| 51:S1:1869:U:O2'   | 51:S1:1961:G:OP1   | 2.26                     | 0.53              |
| 1:L1:73:U:H5''     | 17:LI:63:VAL:HB    | 1.90                     | 0.53              |
| 51:S1:266:U:H5''   | 87:Sh:164:ARG:NH2  | 2.24                     | 0.53              |
| 54:SA:154:ARG:HG2  | 54:SA:154:ARG:NH1  | 2.24                     | 0.53              |
| 56:SC:134:GLU:OE1  | 56:SC:186:LYS:NZ   | 2.41                     | 0.53              |
| 3:L3:19:A:H2       | 3:L3:215:G:H21     | 1.55                     | 0.53              |
| 14:LF:168:ASP:OD1  | 14:LF:169:ALA:N    | 2.42                     | 0.53              |
| 51:S1:167:C:OP1    | 60:SG:84:GLY:N     | 2.32                     | 0.53              |
| 60:SG:214:ARG:HH11 | 60:SG:214:ARG:HG3  | 1.73                     | 0.53              |
| 62:SI:132:MET:HE2  | 62:SI:175:VAL:HG12 | 1.91                     | 0.53              |
| 1:L1:959:OMG:N1    | 2:L2:660:G:OP1     | 2.33                     | 0.53              |
| 2:L2:19:C:O2'      | 2:L2:25:A:N1       | 2.34                     | 0.53              |
| 25:LQ:69:ALA:HA    | 25:LQ:72:MET:HE2   | 1.90                     | 0.53              |
| 39:Le:6:MET:HG2    | 39:Le:16:LYS:HE3   | 1.89                     | 0.53              |
| 51:S1:754:G:OP2    | 51:S1:754:G:N2     | 2.36                     | 0.53              |
| 51:S1:1908:A:H5'   | 51:S1:1909:C:H5    | 1.72                     | 0.53              |
| 87:Sh:195:PHE:HB3  | 87:Sh:200:LEU:HD13 | 1.91                     | 0.53              |
| 1:L1:1052:A:N1     | 8:L8:106:C:O2'     | 2.41                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L1:1105:A:H5''   | 2:L2:1064:A:N6     | 2.24                     | 0.53              |
| 2:L2:603:A:H5'     | 28:LT:137:THR:HG23 | 1.91                     | 0.53              |
| 2:L2:1276:A:H4'    | 22:LN:74:LYS:HG2   | 1.89                     | 0.53              |
| 23:LO:142:ASP:N    | 23:LO:142:ASP:OD1  | 2.38                     | 0.53              |
| 50:Lp:2:VAL:N      | 50:Lp:90:HIS:O     | 2.42                     | 0.53              |
| 71:SR:85:LEU:HD12  | 71:SR:96:THR:HG22  | 1.89                     | 0.53              |
| 77:SX:19:LEU:HD11  | 77:SX:75:ARG:HG3   | 1.90                     | 0.53              |
| 4:L4:21:C:O2'      | 5:L5:135:U:O4      | 2.26                     | 0.53              |
| 51:S1:90:C:O2'     | 89:S1:2302:SPD:N1  | 2.41                     | 0.53              |
| 51:S1:934:U:O2'    | 51:S1:936:U:OP2    | 2.26                     | 0.53              |
| 51:S1:1836:G:O6    | 67:SN:71:TYR:OH    | 2.21                     | 0.53              |
| 1:L1:1627:U:OP1    | 30:LV:126:TYR:OH   | 2.24                     | 0.53              |
| 51:S1:277:U:H3     | 51:S1:945:G:HO2'   | 1.57                     | 0.53              |
| 51:S1:792:G:H3'    | 51:S1:793:G:H21    | 1.74                     | 0.53              |
| 51:S1:1019:U:H4'   | 62:SI:80:ALA:HA    | 1.91                     | 0.53              |
| 51:S1:1889:G:H3'   | 51:S1:1932:A:N6    | 2.24                     | 0.53              |
| 79:SZ:64:LEU:HB3   | 79:SZ:67:PHE:HE2   | 1.73                     | 0.53              |
| 85:Sf:102:LYS:N    | 85:Sf:114:GLU:O    | 2.41                     | 0.53              |
| 1:L1:1626:OMG:N2   | 2:L2:18:A:N3       | 2.57                     | 0.53              |
| 51:S1:1603:U:O2    | 85:Sf:139:TYR:OH   | 2.22                     | 0.53              |
| 57:SD:87:GLU:CD    | 57:SD:87:GLU:H     | 2.16                     | 0.53              |
| 66:SM:53:LEU:HD23  | 66:SM:83:LYS:HG2   | 1.91                     | 0.53              |
| 68:SO:75:VAL:HG22  | 68:SO:117:MET:HG3  | 1.89                     | 0.53              |
| 1:L1:1003:A:OP1    | 36:Lb:18:ARG:NH1   | 2.30                     | 0.53              |
| 1:L1:1574:C:H2'    | 1:L1:1575:G:C8     | 2.44                     | 0.53              |
| 2:L2:954:A:H5'     | 2:L2:955:C:H5'     | 1.91                     | 0.53              |
| 23:LO:162:GLY:HA2  | 23:LO:187:PRO:HD3  | 1.91                     | 0.53              |
| 51:S1:323:U:O2'    | 51:S1:325:G:N2     | 2.42                     | 0.53              |
| 1:L1:24:A:N3       | 1:L1:366:C:O2'     | 2.41                     | 0.52              |
| 1:L1:31:G:H21      | 1:L1:49:C:H5       | 1.55                     | 0.52              |
| 2:L2:644:A:OP1     | 96:L2:1801:HOH:O   | 2.18                     | 0.52              |
| 2:L2:1101:A:H5''   | 12:LD:107:GLY:HA3  | 1.91                     | 0.52              |
| 2:L2:1510:A:H2     | 10:LB:209:ARG:HE   | 1.56                     | 0.52              |
| 51:S1:969:A2M:H61  | 62:SI:101:GLN:N    | 2.07                     | 0.52              |
| 55:SB:204:LEU:HD21 | 75:SV:85:ALA:HB2   | 1.91                     | 0.52              |
| 64:SK:161:GLU:OE1  | 64:SK:164:ARG:NH1  | 2.42                     | 0.52              |
| 11:LC:148:GLU:HG3  | 34:LZ:73:LYS:HD3   | 1.91                     | 0.52              |
| 14:LF:55:LYS:HD2   | 14:LF:98:THR:HG23  | 1.91                     | 0.52              |
| 80:Sa:65:ILE:HG13  | 80:Sa:80:LEU:HD21  | 1.91                     | 0.52              |
| 1:L1:1650:U:H5''   | 21:LM:67:ARG:HD2   | 1.91                     | 0.52              |
| 2:L2:1383:G:O2'    | 2:L2:1386:C:OP2    | 2.20                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L3:118:G:OP1     | 25:LQ:118:HIS:ND1  | 2.43                     | 0.52              |
| 51:S1:146:U:H4'    | 60:SG:183:ILE:HD13 | 1.90                     | 0.52              |
| 51:S1:1209:C:O2'   | 51:S1:1210:C:OP1   | 2.26                     | 0.52              |
| 51:S1:1619:G:O2'   | 51:S1:1849:G:O2'   | 2.26                     | 0.52              |
| 1:L1:51:G:H4'      | 1:L1:863:G:H4'     | 1.90                     | 0.52              |
| 2:L2:97:A:O2'      | 2:L2:366:C:O2      | 2.22                     | 0.52              |
| 3:L3:7:U:OP1       | 33:LY:47:LYS:NZ    | 2.35                     | 0.52              |
| 5:L5:117:A:H1'     | 10:LB:400:ARG:HH12 | 1.75                     | 0.52              |
| 12:LD:7:ALA:HA     | 12:LD:12:ARG:HD3   | 1.92                     | 0.52              |
| 33:LY:23:ALA:HA    | 33:LY:45:GLY:HA2   | 1.92                     | 0.52              |
| 68:SO:86:LEU:HG    | 68:SO:117:MET:HE2  | 1.91                     | 0.52              |
| 86:Sg:102:LYS:HD2  | 86:Sg:104:LEU:HD11 | 1.92                     | 0.52              |
| 1:L1:1715:U:H2'    | 1:L1:1716:G:C8     | 2.42                     | 0.52              |
| 51:S1:1530:G:H5'   | 51:S1:1542:C:H42   | 1.74                     | 0.52              |
| 83:Sd:21:ALA:HA    | 83:Sd:76:MET:HA    | 1.91                     | 0.52              |
| 2:L2:1127:G:H5''   | 27:LS:17:LYS:HG2   | 1.90                     | 0.52              |
| 17:L1:172:GLU:HG2  | 20:LL:98:VAL:HG21  | 1.91                     | 0.52              |
| 51:S1:979:U:H3     | 51:S1:1094:G:H1    | 1.58                     | 0.52              |
| 83:Sd:30:LEU:HD12  | 83:Sd:41:GLN:HG2   | 1.92                     | 0.52              |
| 1:L1:1524:OMG:N2   | 96:L1:2015:HOH:O   | 2.30                     | 0.52              |
| 51:S1:1160:A:OP1   | 54:SA:10:SER:OG    | 2.28                     | 0.52              |
| 51:S1:1397:A:O2'   | 51:S1:1399:G:OP2   | 2.21                     | 0.52              |
| 51:S1:1539:PSU:HN3 | 51:S1:1550:OMG:HN1 | 1.57                     | 0.52              |
| 1:L1:38:A:H5''     | 20:LL:35:ALA:HB1   | 1.91                     | 0.52              |
| 6:L6:48:C:C2       | 14:LF:185:LYS:HD3  | 2.45                     | 0.52              |
| 22:LN:48:VAL:HG22  | 22:LN:178:ARG:HH12 | 1.75                     | 0.52              |
| 51:S1:889:A:OP2    | 58:SE:105:ARG:NH2  | 2.42                     | 0.52              |
| 1:L1:839:U:H2'     | 1:L1:840:G:C8      | 2.45                     | 0.51              |
| 1:L1:1764:A:H3'    | 1:L1:1766:G:OP2    | 2.09                     | 0.51              |
| 2:L2:590:U:H2'     | 2:L2:591:A2M:H8    | 1.91                     | 0.51              |
| 14:LF:30:ARG:NH2   | 41:Lg:144:ILE:OXT  | 2.37                     | 0.51              |
| 22:LN:206:ILE:HD13 | 23:LO:296:VAL:HG23 | 1.92                     | 0.51              |
| 51:S1:294:G:O2'    | 51:S1:295:A:OP1    | 2.27                     | 0.51              |
| 51:S1:558:U:H2'    | 51:S1:559:G:C8     | 2.45                     | 0.51              |
| 71:SR:103:MET:HE3  | 71:SR:103:MET:HA   | 1.91                     | 0.51              |
| 6:L6:64:U:OP2      | 14:LF:78:ARG:NE    | 2.36                     | 0.51              |
| 9:LA:32:LEU:HD13   | 9:LA:163:ARG:HD3   | 1.91                     | 0.51              |
| 13:LE:173:LYS:HB2  | 47:Lm:127:LEU:HD11 | 1.92                     | 0.51              |
| 86:Sg:240:GLN:HG2  | 86:Sg:285:ILE:HG12 | 1.92                     | 0.51              |
| 86:Sg:256:ARG:HG2  | 86:Sg:256:ARG:HH11 | 1.75                     | 0.51              |
| 1:L1:1741:A:O2'    | 3:L3:204:A:N1      | 2.40                     | 0.51              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:LB:57:VAL:HB     | 10:LB:365:PHE:HB3  | 1.92                     | 0.51              |
| 19:LK:27:ILE:O      | 19:LK:29:ASP:N     | 2.39                     | 0.51              |
| 1:L1:1489:U:H2'     | 1:L1:1490:G:C8     | 2.45                     | 0.51              |
| 2:L2:1233:U:OP2     | 50:Lp:63:LYS:HG2   | 2.09                     | 0.51              |
| 6:L6:23:A:H4'       | 6:L6:24[B]:C:H5''  | 1.92                     | 0.51              |
| 10:LB:92:TYR:HB2    | 10:LB:159:VAL:HB   | 1.92                     | 0.51              |
| 22:LN:48:VAL:HG11   | 22:LN:145:VAL:HG22 | 1.93                     | 0.51              |
| 60:SG:80:ARG:HG2    | 60:SG:87:THR:HA    | 1.90                     | 0.51              |
| 66:SM:48:HIS:HB2    | 66:SM:87:ASP:HB2   | 1.92                     | 0.51              |
| 1:L1:687:C:H2'      | 1:L1:688:A:C8      | 2.45                     | 0.51              |
| 41:Lg:75:VAL:HG11   | 41:Lg:119:VAL:HG11 | 1.93                     | 0.51              |
| 55:SB:114:GLN:HG2   | 55:SB:115:ILE:HG23 | 1.93                     | 0.51              |
| 1:L1:1185:U:H2'     | 1:L1:1186:A:O4'    | 2.10                     | 0.51              |
| 1:L1:1293:A:O2'     | 1:L1:1294:C:H5'    | 2.10                     | 0.51              |
| 11:LC:292:GLN:HG2   | 11:LC:297:ARG:NH2  | 2.26                     | 0.51              |
| 14:LF:80:ASP:HB3    | 14:LF:83:TYR:HD2   | 1.74                     | 0.51              |
| 50:Lp:55:LYS:NZ     | 52:S4:67:C:O2      | 2.44                     | 0.51              |
| 51:S1:342:C:H1'     | 58:SE:30:PRO:HG3   | 1.92                     | 0.51              |
| 59:SF:250:ASP:OD2   | 59:SF:252:THR:OG1  | 2.27                     | 0.51              |
| 51:S1:1858:G:N2     | 51:S1:1978:A:OP2   | 2.43                     | 0.51              |
| 1:L1:162:U:H3       | 1:L1:293:C:H42     | 1.59                     | 0.51              |
| 1:L1:759:A:H2       | 1:L1:761:A:H61     | 1.58                     | 0.51              |
| 2:L2:25:A:H5''      | 46:L1:45:ARG:HH21  | 1.76                     | 0.51              |
| 2:L2:1156:G:H5''    | 27:LS:83:ARG:NH2   | 2.25                     | 0.51              |
| 4:L4:77:U:H4'       | 10:LB:371:LYS:HE3  | 1.93                     | 0.51              |
| 20:LL:116:GLN:HB3   | 24:LP:100:ALA:HB2  | 1.92                     | 0.51              |
| 51:S1:373:G:H5'     | 64:SK:98:LYS:HB3   | 1.92                     | 0.51              |
| 51:S1:617:G:OP2     | 69:SP:68:LYS:NZ    | 2.44                     | 0.51              |
| 1:L1:83:A:H61       | 1:L1:98:A:H3'      | 1.76                     | 0.51              |
| 10:LB:356:GLN:CD    | 10:LB:356:GLN:H    | 2.18                     | 0.51              |
| 11:LC:299:VAL:HG21  | 24:LP:138:PRO:HB2  | 1.92                     | 0.51              |
| 51:S1:972:A:H61     | 51:S1:1100:U:H2'   | 1.76                     | 0.51              |
| 51:S1:1718:A:O2'    | 51:S1:1949:A:N6    | 2.43                     | 0.51              |
| 54:SA:41:ARG:NH2    | 54:SA:234:HIS:O    | 2.41                     | 0.51              |
| 67:SN:5:VAL:HG11    | 67:SN:52:LEU:HD21  | 1.93                     | 0.51              |
| 2:L2:696:A:H4'      | 2:L2:697:G:OP1     | 2.11                     | 0.51              |
| 2:L2:782:G:O2'      | 2:L2:786:A:O5'     | 2.28                     | 0.51              |
| 25:LQ:105:LEU:HD22  | 25:LQ:135:LYS:HG3  | 1.93                     | 0.51              |
| 51:S1:17:C:O2'      | 51:S1:1489:A:N1    | 2.40                     | 0.51              |
| 51:S1:251:A:H1'     | 51:S1:784:C:H1'    | 1.92                     | 0.51              |
| 51:S1:2008:OMG:HM21 | 61:SH:71:ARG:CZ    | 2.41                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:SF:66:ILE:HA    | 59:SF:71:MET:HE3   | 1.93                     | 0.51              |
| 1:L1:1160:G:OP1    | 37:Lc:119:ARG:NH2  | 2.43                     | 0.50              |
| 18:LJ:8:VAL:HB     | 18:LJ:127:LEU:HD22 | 1.93                     | 0.50              |
| 23:LO:152:LEU:HD22 | 23:LO:169:LEU:HD22 | 1.93                     | 0.50              |
| 29:LU:108:ARG:NH1  | 29:LU:110:LEU:HD21 | 2.26                     | 0.50              |
| 33:LY:14:THR:HB    | 42:Lh:89:ARG:HG3   | 1.93                     | 0.50              |
| 57:SD:27:MET:HG3   | 84:Se:44:PHE:HE2   | 1.75                     | 0.50              |
| 1:L1:779:A:N1      | 24:LP:74:LYS:NZ    | 2.59                     | 0.50              |
| 16:LH:217:LYS:HG2  | 16:LH:222:ALA:HB3  | 1.94                     | 0.50              |
| 35:La:72:MET:O     | 35:La:72:MET:HE3   | 2.11                     | 0.50              |
| 2:L2:1398:C:H2'    | 2:L2:1399:G:C8     | 2.46                     | 0.50              |
| 6:L6:63:A:C6       | 14:LF:108:ARG:HD3  | 2.46                     | 0.50              |
| 31:LW:35:GLU:H     | 31:LW:35:GLU:CD    | 2.19                     | 0.50              |
| 59:SF:177:VAL:HG11 | 59:SF:222:LEU:HA   | 1.93                     | 0.50              |
| 1:L1:1342:C:H2'    | 1:L1:1343:A:C8     | 2.46                     | 0.50              |
| 2:L2:341:A:OP2     | 25:LQ:114:LYS:NZ   | 2.42                     | 0.50              |
| 40:Lf:42:PRO:HB2   | 40:Lf:50:GLN:HG3   | 1.93                     | 0.50              |
| 51:S1:1369:U:H3    | 51:S1:1401:G:H1    | 1.59                     | 0.50              |
| 66:SM:63:ARG:HH21  | 66:SM:65:THR:HG21  | 1.77                     | 0.50              |
| 1:L1:377:G:OP2     | 11:LC:197:ASN:ND2  | 2.25                     | 0.50              |
| 1:L1:409:U:H5      | 46:Ll:34:ARG:HB3   | 1.77                     | 0.50              |
| 1:L1:1525:A:H5'    | 1:L1:1526:U:H5'    | 1.94                     | 0.50              |
| 2:L2:957:C:H2'     | 2:L2:958:A:H8      | 1.77                     | 0.50              |
| 37:Lc:95:VAL:HG21  | 37:Lc:157:MET:HE1  | 1.94                     | 0.50              |
| 39:Le:45:MET:O     | 39:Le:50:ARG:NH2   | 2.44                     | 0.50              |
| 59:SF:83:ILE:HG21  | 59:SF:88:LEU:HD13  | 1.93                     | 0.50              |
| 80:Sa:81:LYS:O     | 80:Sa:85:ARG:HG3   | 2.12                     | 0.50              |
| 1:L1:881:A:O2'     | 2:L2:49:A:OP1      | 2.27                     | 0.50              |
| 1:L1:1085:C:H4'    | 1:L1:1085:C:OP1    | 2.11                     | 0.50              |
| 10:LB:92:TYR:HB3   | 10:LB:99:LEU:HD22  | 1.92                     | 0.50              |
| 10:LB:315:MET:HE1  | 10:LB:377:PHE:HB2  | 1.94                     | 0.50              |
| 51:S1:967:A:OP1    | 62:SI:9:ARG:NH2    | 2.43                     | 0.50              |
| 51:S1:2198:A:H5'   | 81:Sb:83:ILE:HD11  | 1.94                     | 0.50              |
| 20:LL:75:LEU:HG    | 20:LL:111:GLY:HA2  | 1.94                     | 0.50              |
| 37:Lc:230:HIS:CE1  | 37:Lc:238:GLY:HA3  | 2.46                     | 0.50              |
| 51:S1:506:U:OP1    | 79:SZ:115:LYS:NZ   | 2.45                     | 0.50              |
| 51:S1:1923:A:HO2'  | 51:S1:1969:A:HO2'  | 1.60                     | 0.50              |
| 51:S1:1948:U:OP2   | 77:SX:26:ARG:NH2   | 2.41                     | 0.50              |
| 15:LG:187:LEU:HB3  | 15:LG:196:ALA:HB3  | 1.93                     | 0.50              |
| 51:S1:124:A:OP2    | 60:SG:201:LYS:NZ   | 2.34                     | 0.50              |
| 2:L2:1410:G:N7     | 96:L2:1843:HOH:O   | 2.35                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:Lh:10:ARG:HH21 | 42:Lh:35:LYS:HD3   | 1.77                     | 0.50              |
| 51:S1:1860:C:OP2  | 71:SR:137:THR:OG1  | 2.25                     | 0.50              |
| 2:L2:972:C:N4     | 38:Ld:49:ASN:O     | 2.45                     | 0.49              |
| 7:L7:93:C:HO2'    | 7:L7:94:G:P        | 2.33                     | 0.49              |
| 51:S1:566:A:N3    | 79:SZ:40:THR:OG1   | 2.45                     | 0.49              |
| 51:S1:1360:U:H5   | 62:SI:199:THR:H    | 1.59                     | 0.49              |
| 1:L1:1254:C:O2'   | 1:L1:1360:C:OP1    | 2.27                     | 0.49              |
| 55:SB:30:THR:O    | 55:SB:31:ARG:HG2   | 2.11                     | 0.49              |
| 2:L2:389:A:OP2    | 2:L2:570:A2M:H8    | 2.12                     | 0.49              |
| 22:LN:30:LYS:HG2  | 22:LN:63:GLU:HB3   | 1.94                     | 0.49              |
| 51:S1:869:U:C2    | 57:SD:142:ILE:HG12 | 2.46                     | 0.49              |
| 76:SW:117:GLU:CD  | 76:SW:117:GLU:H    | 2.19                     | 0.49              |
| 14:LF:57:LEU:HD12 | 14:LF:62:PRO:HG2   | 1.94                     | 0.49              |
| 14:LF:66:SER:HB2  | 14:LF:76:ILE:HG12  | 1.94                     | 0.49              |
| 14:LF:104:GLU:HA  | 14:LF:107:GLN:HG2  | 1.94                     | 0.49              |
| 25:LQ:171:ASN:OD1 | 25:LQ:174:ARG:NH1  | 2.45                     | 0.49              |
| 51:S1:810:G:HO2'  | 51:S1:811:C:H6     | 1.56                     | 0.49              |
| 51:S1:1605:U:O4   | 85:Sf:90:HIS:NE2   | 2.44                     | 0.49              |
| 54:SA:8:ARG:HD3   | 54:SA:11:LYS:HA    | 1.93                     | 0.49              |
| 59:SF:50:LYS:HD2  | 59:SF:259:LEU:HD13 | 1.93                     | 0.49              |
| 15:LG:117:LYS:NZ  | 15:LG:123:LYS:O    | 2.37                     | 0.49              |
| 43:Li:66:VAL:HG23 | 43:Li:68:LYS:HG3   | 1.94                     | 0.49              |
| 51:S1:327:U:H2'   | 51:S1:328:C:H5''   | 1.95                     | 0.49              |
| 51:S1:498:C:O2'   | 79:SZ:91:ARG:O     | 2.30                     | 0.49              |
| 51:S1:1527:U:H2'  | 51:S1:1528:G:C8    | 2.48                     | 0.49              |
| 51:S1:1967:G:OP2  | 51:S1:1967:G:N2    | 2.36                     | 0.49              |
| 53:S3:9:G:O2'     | 53:S3:10:G:N7      | 2.46                     | 0.49              |
| 57:SD:150:SER:HA  | 57:SD:153:ARG:HH12 | 1.78                     | 0.49              |
| 67:SN:11:ASP:HA   | 67:SN:14:TYR:HB2   | 1.94                     | 0.49              |
| 1:L1:235:A2M:O5'  | 1:L1:235:A2M:H8    | 2.13                     | 0.49              |
| 7:L7:29:C:OP1     | 17:LI:36:GLN:NE2   | 2.42                     | 0.49              |
| 19:LK:147:MET:HE1 | 41:Lg:13:LYS:HG3   | 1.94                     | 0.49              |
| 2:L2:386:U:O2'    | 2:L2:1416:U:H5''   | 2.12                     | 0.49              |
| 2:L2:658:G:OP1    | 96:L2:1803:HOH:O   | 2.20                     | 0.49              |
| 6:L6:43:A:N6      | 16:LH:220:GLY:O    | 2.40                     | 0.49              |
| 16:LH:29:LEU:HD13 | 16:LH:59:LEU:HD11  | 1.95                     | 0.49              |
| 19:LK:13:VAL:HG12 | 19:LK:58:PRO:HA    | 1.94                     | 0.49              |
| 31:LW:3:SER:O     | 31:LW:3:SER:OG     | 2.23                     | 0.49              |
| 51:S1:777:A:H4'   | 51:S1:778:G:O5'    | 2.12                     | 0.49              |
| 51:S1:1649:G:N2   | 51:S1:1652:A:OP2   | 2.45                     | 0.49              |
| 76:SW:97:VAL:HA   | 76:SW:114:ILE:HG22 | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:Sg:98:GLN:O     | 86:Sg:100:GLN:NE2  | 2.42                     | 0.49              |
| 1:L1:984:A:OP2     | 89:L1:1813:SPD:H52 | 2.12                     | 0.49              |
| 2:L2:968:U:O4      | 2:L2:969:A:N6      | 2.45                     | 0.49              |
| 13:LE:93:CYS:HB2   | 13:LE:141:ASP:HB3  | 1.94                     | 0.49              |
| 28:LT:67:ILE:HD11  | 28:LT:80:LYS:HB3   | 1.94                     | 0.49              |
| 41:Lg:34:TYR:CE1   | 41:Lg:136:ARG:HG2  | 2.47                     | 0.49              |
| 44:Lj:39:TYR:CD1   | 44:Lj:40:PRO:HA    | 2.48                     | 0.49              |
| 51:S1:1837:A:HO2'  | 56:SC:175:TYR:HH   | 1.60                     | 0.49              |
| 77:SX:30:THR:HB    | 77:SX:147:LEU:HD21 | 1.94                     | 0.49              |
| 2:L2:1482:C:H3'    | 2:L2:1483:U:H5''   | 1.95                     | 0.49              |
| 3:L3:72:A:H5'      | 42:Lh:26:THR:HA    | 1.95                     | 0.49              |
| 30:LV:144:LEU:HA   | 35:La:38:THR:HG21  | 1.94                     | 0.49              |
| 51:S1:876:G:H1     | 51:S1:885:C:H5     | 1.61                     | 0.49              |
| 51:S1:916:G:H22    | 73:ST:133:LYS:HB2  | 1.77                     | 0.49              |
| 86:Sg:214:LYS:HD2  | 86:Sg:237:PRO:HB3  | 1.95                     | 0.49              |
| 2:L2:1515:A:H5''   | 10:LB:109:HIS:CD2  | 2.48                     | 0.49              |
| 9:LA:42:ARG:HG2    | 9:LA:42:ARG:HH11   | 1.78                     | 0.49              |
| 10:LB:266:MET:HG2  | 16:LH:82:THR:HG22  | 1.95                     | 0.49              |
| 23:LO:284:SER:OG   | 23:LO:287:GLU:OE1  | 2.26                     | 0.49              |
| 51:S1:29:OMU:HM21  | 69:SP:123:VAL:HG11 | 1.95                     | 0.49              |
| 62:SI:61:VAL:HG11  | 62:SI:175:VAL:HG21 | 1.95                     | 0.49              |
| 71:SR:87:ARG:HD2   | 71:SR:99:LEU:HD11  | 1.95                     | 0.49              |
| 77:SX:57:GLU:HG3   | 77:SX:58:ARG:HG3   | 1.95                     | 0.49              |
| 51:S1:2198:A:N6    | 81:Sb:9:GLY:HA3    | 2.28                     | 0.48              |
| 64:SK:210:PHE:O    | 64:SK:214:ARG:HG2  | 2.13                     | 0.48              |
| 1:L1:369:A:O2'     | 44:Lj:58:ARG:NH2   | 2.46                     | 0.48              |
| 1:L1:412:G:N1      | 1:L1:415:A:OP2     | 2.46                     | 0.48              |
| 1:L1:835:G:H2'     | 1:L1:835:G:N3      | 2.27                     | 0.48              |
| 1:L1:1684:G:N2     | 1:L1:1716:G:H1     | 2.08                     | 0.48              |
| 2:L2:782:G:H8      | 2:L2:782:G:OP2     | 1.95                     | 0.48              |
| 9:LA:62:GLU:OE1    | 9:LA:71:ARG:HD2    | 2.12                     | 0.48              |
| 9:LA:178:PRO:HG2   | 49:Lo:26:ALA:HB2   | 1.94                     | 0.48              |
| 15:LG:183:ASP:HB3  | 15:LG:186:ARG:H    | 1.78                     | 0.48              |
| 51:S1:38:OMC:O2'   | 57:SD:5:ASN:ND2    | 2.46                     | 0.48              |
| 51:S1:377:A:H5'    | 64:SK:48:ALA:HB1   | 1.95                     | 0.48              |
| 51:S1:1202:A:OP1   | 73:ST:2:VAL:HG23   | 2.13                     | 0.48              |
| 65:SL:23:ALA:HB2   | 65:SL:75:VAL:HG13  | 1.95                     | 0.48              |
| 68:SO:90:MET:HE1   | 68:SO:105:ALA:HB1  | 1.95                     | 0.48              |
| 73:ST:110:ASP:O    | 73:ST:114:ARG:HG2  | 2.12                     | 0.48              |
| 2:L2:1246:A:H5''   | 2:L2:1248:OMC:O5'  | 2.13                     | 0.48              |
| 23:LO:107:ARG:HH21 | 23:LO:110:LEU:HD12 | 1.77                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:LU:44:LEU:HG    | 29:LU:72:MET:HE2   | 1.95                     | 0.48              |
| 29:LU:91:LYS:HB2   | 29:LU:117:TYR:CE2  | 2.49                     | 0.48              |
| 51:S1:522:A:H5'    | 57:SD:143:PRO:HD2  | 1.95                     | 0.48              |
| 51:S1:784:C:H41    | 51:S1:834:U:H3     | 1.60                     | 0.48              |
| 51:S1:969:A2M:H2   | 62:SI:118:SER:HB2  | 1.95                     | 0.48              |
| 86:Sg:234:VAL:HG21 | 86:Sg:254:THR:HG21 | 1.95                     | 0.48              |
| 1:L1:1147:A:O2'    | 1:L1:1150:A:N1     | 2.45                     | 0.48              |
| 1:L1:1683:C:H2'    | 1:L1:1684:G:H8     | 1.78                     | 0.48              |
| 38:Ld:18:LEU:HD13  | 38:Ld:100:SER:HA   | 1.94                     | 0.48              |
| 52:S2:74:C:H2'     | 52:S2:75:C:O4'     | 2.13                     | 0.48              |
| 57:SD:31:GLY:HA3   | 84:Se:40:TYR:CG    | 2.49                     | 0.48              |
| 86:Sg:67:PHE:HB2   | 86:Sg:85:TRP:CG    | 2.48                     | 0.48              |
| 2:L2:1485:G:N3     | 19:LK:164:MET:HG2  | 2.29                     | 0.48              |
| 2:L2:1510:A:HO2'   | 10:LB:170:LYS:HZ1  | 1.57                     | 0.48              |
| 6:L6:66:A:OP1      | 14:LF:47:ARG:NH2   | 2.45                     | 0.48              |
| 7:L7:47:C:H1'      | 7:L7:61:A:H2'      | 1.95                     | 0.48              |
| 12:LD:25:VAL:HG12  | 12:LD:27:GLU:HG2   | 1.93                     | 0.48              |
| 51:S1:1:G:OP1      | 57:SD:49:SER:OG    | 2.30                     | 0.48              |
| 51:S1:251:A:N1     | 51:S1:835:C:O2'    | 2.43                     | 0.48              |
| 51:S1:1523:A:H2'   | 51:S1:1524:G:C8    | 2.48                     | 0.48              |
| 86:Sg:237:PRO:HD2  | 86:Sg:255:GLU:HG2  | 1.94                     | 0.48              |
| 2:L2:1250:C:H2'    | 2:L2:1251:A:C8     | 2.48                     | 0.48              |
| 11:LC:286:ASP:OD2  | 11:LC:289:ARG:NH1  | 2.46                     | 0.48              |
| 26:LR:70:LYS:O     | 26:LR:74:ARG:NH2   | 2.44                     | 0.48              |
| 51:S1:527:A:H4'    | 57:SD:119:LYS:HG3  | 1.96                     | 0.48              |
| 51:S1:656:G:H5'    | 51:S1:662:G:N2     | 2.28                     | 0.48              |
| 51:S1:1123:G:H1'   | 51:S1:1191:A:O4'   | 2.13                     | 0.48              |
| 85:Sf:103:VAL:HA   | 85:Sf:113:VAL:HA   | 1.95                     | 0.48              |
| 1:L1:1371:OMU:HM23 | 1:L1:1371:OMU:H1'  | 1.72                     | 0.48              |
| 3:L3:174:C:O2'     | 3:L3:175:A:OP1     | 2.29                     | 0.48              |
| 19:LK:25:GLY:HA2   | 19:LK:40:ASN:HB2   | 1.96                     | 0.48              |
| 56:SC:210:ILE:HD11 | 75:SV:40:ILE:HD11  | 1.96                     | 0.48              |
| 84:Se:64:LYS:HB3   | 84:Se:64:LYS:HE3   | 1.68                     | 0.48              |
| 7:L7:142:C:O3'     | 30:LV:94:ASN:ND2   | 2.47                     | 0.48              |
| 23:LO:206:PHE:CE1  | 23:LO:250:LYS:HG2  | 2.49                     | 0.48              |
| 38:Ld:20:MET:HG3   | 38:Ld:83:CYS:O     | 2.13                     | 0.48              |
| 41:Lg:32:ARG:NH1   | 41:Lg:36:LYS:HG3   | 2.29                     | 0.48              |
| 74:SU:14:ASP:OD2   | 74:SU:67:LYS:NZ    | 2.44                     | 0.48              |
| 86:Sg:222:ASP:OD2  | 86:Sg:224:SER:OG   | 2.20                     | 0.48              |
| 1:L1:297:A:H1'     | 1:L1:298:U:C5      | 2.49                     | 0.48              |
| 1:L1:1611:G:N7     | 96:L1:2024:HOH:O   | 2.35                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:L2:638:C:O2'     | 10:LB:271:ARG:NH1  | 2.45                     | 0.48              |
| 7:L7:70:C:OP1      | 31:LW:118:ARG:NH2  | 2.36                     | 0.48              |
| 51:S1:1614:U:H2'   | 51:S1:1615:G:C8    | 2.47                     | 0.48              |
| 1:L1:159:U:O2'     | 1:L1:160:C:H5'     | 2.14                     | 0.48              |
| 9:LA:48:ILE:HG21   | 49:Lo:65:ALA:HB2   | 1.96                     | 0.48              |
| 51:S1:1853:U:OP1   | 72:SS:10:ARG:NH2   | 2.46                     | 0.48              |
| 64:SK:150:ASP:OD1  | 64:SK:150:ASP:N    | 2.41                     | 0.48              |
| 77:SX:110:THR:HA   | 77:SX:113:LEU:HD12 | 1.95                     | 0.48              |
| 1:L1:215:U:OP1     | 34:LZ:129:LYS:NZ   | 2.46                     | 0.47              |
| 6:L6:60:A:OP1      | 14:LF:45:ARG:NH2   | 2.47                     | 0.47              |
| 58:SE:95:ARG:HH21  | 58:SE:112:SER:HA   | 1.79                     | 0.47              |
| 60:SG:34:GLY:HA2   | 60:SG:52:ARG:HE    | 1.79                     | 0.47              |
| 79:SZ:6:LYS:NZ     | 79:SZ:7:LYS:O      | 2.46                     | 0.47              |
| 1:L1:205:A:C6      | 34:LZ:55:PRO:HG3   | 2.49                     | 0.47              |
| 2:L2:1484:U:N3     | 2:L2:1486:G:O4'    | 2.48                     | 0.47              |
| 13:LE:91:VAL:HG22  | 13:LE:143:ILE:HB   | 1.96                     | 0.47              |
| 51:S1:2006:A:OP1   | 65:SL:139:SER:OG   | 2.29                     | 0.47              |
| 94:S1:2446:PAR:H24 | 94:S1:2446:PAR:H33 | 1.68                     | 0.47              |
| 57:SD:50:LYS:O     | 57:SD:54:THR:HG22  | 2.14                     | 0.47              |
| 86:Sg:135:ASN:HD22 | 86:Sg:137:ALA:H    | 1.59                     | 0.47              |
| 2:L2:664:G:H5'     | 2:L2:664:G:N3      | 2.29                     | 0.47              |
| 2:L2:1486:G:H2'    | 2:L2:1487:G:C8     | 2.49                     | 0.47              |
| 8:L8:121:U:OP1     | 23:LO:266:LYS:NZ   | 2.48                     | 0.47              |
| 51:S1:1250:A:O2'   | 51:S1:1252:A:N7    | 2.45                     | 0.47              |
| 51:S1:1974:A:OP2   | 76:SW:54:ARG:NH1   | 2.47                     | 0.47              |
| 58:SE:84:MET:HE3   | 58:SE:97:ARG:HD3   | 1.97                     | 0.47              |
| 60:SG:121:ASP:N    | 60:SG:121:ASP:OD1  | 2.47                     | 0.47              |
| 67:SN:86:TYR:HD1   | 67:SN:87:LEU:HD23  | 1.79                     | 0.47              |
| 69:SP:53:GLU:OE2   | 69:SP:71:ARG:NH1   | 2.43                     | 0.47              |
| 77:SX:55:GLY:HA2   | 77:SX:96:LYS:HD2   | 1.95                     | 0.47              |
| 79:SZ:47:ARG:HG3   | 79:SZ:62:VAL:HB    | 1.96                     | 0.47              |
| 1:L1:746:G:N2      | 1:L1:749:A:OP2     | 2.43                     | 0.47              |
| 2:L2:1239:A:O2'    | 2:L2:1240:A:H2'    | 2.14                     | 0.47              |
| 4:L4:174:A:H5'     | 16:LH:3:PHE:HB2    | 1.96                     | 0.47              |
| 9:LA:59:ALA:HB2    | 9:LA:78:ALA:HB2    | 1.95                     | 0.47              |
| 20:LL:51:GLY:HA2   | 24:LP:182:ARG:N    | 2.30                     | 0.47              |
| 25:LQ:89:MET:HE2   | 25:LQ:94:LEU:HG    | 1.96                     | 0.47              |
| 1:L1:553:A:C8      | 11:LC:337:THR:HG21 | 2.50                     | 0.47              |
| 94:L7:208:PAR:O43  | 94:L7:208:PAR:O62  | 2.25                     | 0.47              |
| 11:LC:290:ILE:HG23 | 24:LP:135:MET:SD   | 2.54                     | 0.47              |
| 13:LE:91:VAL:HA    | 13:LE:180:VAL:HA   | 1.95                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:LQ:2:VAL:HG23   | 25:LQ:33:GLN:HG3  | 1.95                     | 0.47              |
| 51:S1:1433:G:H4'   | 63:SJ:19:ARG:HH21 | 1.79                     | 0.47              |
| 51:S1:1932:A:O2'   | 51:S1:1934:A:OP2  | 2.28                     | 0.47              |
| 1:L1:1238:C:C5'    | 1:L1:1239:U:H5'   | 2.45                     | 0.47              |
| 1:L1:1766:G:H2'    | 1:L1:1767:A:C8    | 2.49                     | 0.47              |
| 6:L6:6:G:H5''      | 6:L6:7:A:OP2      | 2.15                     | 0.47              |
| 10:LB:286:LYS:NZ   | 10:LB:359:GLU:O   | 2.48                     | 0.47              |
| 43:Li:90:ARG:O     | 43:Li:94:GLU:HG3  | 2.14                     | 0.47              |
| 51:S1:3:U:O2       | 57:SD:16:ARG:NH2  | 2.42                     | 0.47              |
| 51:S1:1714:C:H5''  | 77:SX:8:ILE:HD11  | 1.96                     | 0.47              |
| 71:SR:25:ARG:HB2   | 71:SR:30:ALA:HB2  | 1.97                     | 0.47              |
| 80:Sa:41:MET:HE2   | 80:Sa:41:MET:HB3  | 1.85                     | 0.47              |
| 1:L1:633:U:H4'     | 1:L1:634:G:H5''   | 1.97                     | 0.47              |
| 1:L1:1023:G:OP2    | 89:L1:1808:SPD:N6 | 2.32                     | 0.47              |
| 2:L2:638:C:O2'     | 10:LB:271:ARG:NH2 | 2.47                     | 0.47              |
| 3:L3:71:U:O2'      | 3:L3:149:A:N1     | 2.44                     | 0.47              |
| 32:LX:82:VAL:HG11  | 60:SG:9:ARG:HG2   | 1.97                     | 0.47              |
| 51:S1:1566:PSU:OP1 | 51:S1:1598:U:O2'  | 2.26                     | 0.47              |
| 67:SN:80:ILE:HA    | 67:SN:83:MET:HB2  | 1.96                     | 0.47              |
| 1:L1:1686:C:H2'    | 1:L1:1687:G:C8    | 2.50                     | 0.47              |
| 2:L2:772:A:OP1     | 9:LA:37:ARG:NH2   | 2.48                     | 0.47              |
| 4:L4:75:C:H5'      | 10:LB:336:SER:HA  | 1.97                     | 0.47              |
| 45:Lk:5:ILE:HD11   | 45:Lk:43:TYR:HB3  | 1.97                     | 0.47              |
| 65:SL:11:GLN:HG3   | 65:SL:28:THR:HB   | 1.97                     | 0.47              |
| 85:Sf:139:TYR:H    | 85:Sf:139:TYR:HD2 | 1.61                     | 0.47              |
| 86:Sg:82:THR:HG22  | 86:Sg:92:TRP:HE1  | 1.79                     | 0.47              |
| 1:L1:47:C:O2       | 93:L1:1977:PUT:N1 | 2.40                     | 0.47              |
| 1:L1:700:A:H2'     | 1:L1:701:G:C8     | 2.50                     | 0.47              |
| 1:L1:967:G:H5'     | 1:L1:968:A:OP1    | 2.15                     | 0.47              |
| 5:L5:106:G:N3      | 39:Le:94:LYS:HA   | 2.30                     | 0.47              |
| 10:LB:374:HIS:O    | 32:LX:37:ARG:NH2  | 2.47                     | 0.47              |
| 17:LI:60:ARG:HD2   | 17:LI:77:GLY:O    | 2.14                     | 0.47              |
| 51:S1:701:G:H1     | 51:S1:745:G:H1    | 1.62                     | 0.47              |
| 51:S1:1931:G:O6    | 56:SC:2:GLY:N     | 2.48                     | 0.47              |
| 53:S3:51:U:H3      | 53:S3:65:G:H1     | 1.63                     | 0.47              |
| 55:SB:114:GLN:HA   | 55:SB:119:PHE:CG  | 2.49                     | 0.47              |
| 58:SE:178:VAL:HG12 | 58:SE:224:VAL:HA  | 1.96                     | 0.47              |
| 59:SF:190:ILE:HD12 | 59:SF:201:GLU:HG3 | 1.97                     | 0.47              |
| 61:SH:92:GLU:CD    | 61:SH:93:ASN:H    | 2.23                     | 0.47              |
| 75:SV:72:LYS:HE3   | 75:SV:72:LYS:HB3  | 1.66                     | 0.47              |
| 1:L1:262:C:H5'     | 31:LW:31:PRO:HD3  | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L1:574:G:O2'     | 1:L1:576:G:H2'     | 2.15                     | 0.47              |
| 2:L2:1264:PSU:H5'  | 2:L2:1264:PSU:H6   | 1.78                     | 0.47              |
| 7:L7:71:A:OP1      | 31:LW:25:ARG:NH1   | 2.48                     | 0.47              |
| 26:LR:95:GLU:OE1   | 26:LR:138:HIS:ND1  | 2.47                     | 0.47              |
| 40:Lf:3:LYS:HE2    | 40:Lf:4:PRO:HD2    | 1.97                     | 0.47              |
| 51:S1:1227:G:H4'   | 51:S1:2179:A:H4'   | 1.96                     | 0.47              |
| 51:S1:1800:U:H2'   | 51:S1:1801:G:O4'   | 2.15                     | 0.47              |
| 53:S3:7:G:P        | 53:S3:16:C:H42     | 2.38                     | 0.47              |
| 69:SP:88:ASP:OD2   | 84:Se:15:LYS:HB2   | 2.14                     | 0.47              |
| 1:L1:1526:U:H5''   | 1:L1:1527:OMC:H5'  | 1.96                     | 0.46              |
| 1:L1:1597:G:O6     | 46:Ll:2:GLY:N      | 2.48                     | 0.46              |
| 33:LY:35:GLU:H     | 33:LY:35:GLU:CD    | 2.23                     | 0.46              |
| 51:S1:904:G:OP2    | 51:S1:904:G:N2     | 2.40                     | 0.46              |
| 56:SC:210:ILE:O    | 75:SV:20:TYR:OH    | 2.30                     | 0.46              |
| 61:SH:21:GLU:HG3   | 61:SH:103:SER:HB3  | 1.97                     | 0.46              |
| 62:SI:25:LYS:HB3   | 62:SI:25:LYS:NZ    | 2.30                     | 0.46              |
| 76:SW:67:LEU:HD21  | 76:SW:101:VAL:HG22 | 1.95                     | 0.46              |
| 81:Sb:93:VAL:HG22  | 81:Sb:96:ARG:NH2   | 2.30                     | 0.46              |
| 86:Sg:125:ALA:HB1  | 86:Sg:153:VAL:HB   | 1.97                     | 0.46              |
| 2:L2:1512:G:H1'    | 2:L2:1513:G:OP2    | 2.15                     | 0.46              |
| 4:L4:125:C:OP1     | 10:LB:332:LYS:NZ   | 2.45                     | 0.46              |
| 4:L4:126:G:N7      | 96:L4:302:HOH:O    | 2.36                     | 0.46              |
| 22:LN:47:PRO:HB3   | 22:LN:171:TRP:CZ2  | 2.50                     | 0.46              |
| 29:LU:70:LEU:HD23  | 29:LU:79:ILE:HG12  | 1.96                     | 0.46              |
| 51:S1:366:G:N7     | 96:S1:2524:HOH:O   | 2.36                     | 0.46              |
| 51:S1:1692:G:H5'   | 86:Sg:65:THR:HG21  | 1.97                     | 0.46              |
| 51:S1:1788:U:H5'   | 75:SV:48:ASN:CB    | 2.45                     | 0.46              |
| 61:SH:174:TYR:CZ   | 61:SH:178:LYS:HE3  | 2.50                     | 0.46              |
| 86:Sg:134:TRP:N    | 86:Sg:134:TRP:CD1  | 2.83                     | 0.46              |
| 2:L2:949:U:H2'     | 2:L2:950:G:C8      | 2.50                     | 0.46              |
| 7:L7:167:C:OP1     | 15:LG:182:LYS:NZ   | 2.42                     | 0.46              |
| 37:Lc:198:ILE:HD11 | 37:Lc:212:MET:HE1  | 1.98                     | 0.46              |
| 51:S1:52:U:H2'     | 51:S1:53:G:C8      | 2.51                     | 0.46              |
| 51:S1:1793:U:H3'   | 51:S1:1794:U:H5''  | 1.98                     | 0.46              |
| 56:SC:115:ARG:HG2  | 56:SC:151:PHE:CE2  | 2.50                     | 0.46              |
| 75:SV:35:ILE:HA    | 75:SV:38:VAL:HG22  | 1.96                     | 0.46              |
| 75:SV:88:THR:O     | 75:SV:93:LYS:NZ    | 2.48                     | 0.46              |
| 76:SW:66:ARG:HH11  | 76:SW:66:ARG:HB3   | 1.80                     | 0.46              |
| 83:Sd:60:VAL:HG12  | 83:Sd:82:ALA:HB3   | 1.98                     | 0.46              |
| 87:Sh:182:ALA:HA   | 87:Sh:185:LYS:HG2  | 1.98                     | 0.46              |
| 1:L1:1525:A:H5'    | 1:L1:1526:U:H5''   | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L1:1667:G:N2     | 2:L2:769:A:OP1     | 2.34                     | 0.46              |
| 9:LA:83:PHE:HB3    | 49:Lo:64:VAL:HG22  | 1.97                     | 0.46              |
| 29:LU:87:LYS:HE2   | 29:LU:117:TYR:CZ   | 2.50                     | 0.46              |
| 34:LZ:49:LYS:HE2   | 34:LZ:99:VAL:HG13  | 1.97                     | 0.46              |
| 51:S1:442:A:OP1    | 64:SK:49:ARG:NH2   | 2.49                     | 0.46              |
| 51:S1:1862:C:H2'   | 51:S1:1863:G:H8    | 1.80                     | 0.46              |
| 65:SL:99:PHE:HB3   | 65:SL:108:LYS:HB2  | 1.98                     | 0.46              |
| 75:SV:35:ILE:HD13  | 75:SV:50:ILE:HG22  | 1.97                     | 0.46              |
| 87:Sh:161:LYS:HE3  | 87:Sh:178:ASP:CG   | 2.41                     | 0.46              |
| 1:L1:171:U:H2'     | 1:L1:172:G:C8      | 2.50                     | 0.46              |
| 3:L3:169:A:H5'     | 3:L3:170:C:H5'     | 1.98                     | 0.46              |
| 15:LG:101:GLU:HG3  | 15:LG:106:ARG:HB2  | 1.98                     | 0.46              |
| 51:S1:1145:A:H5''  | 68:SO:53:MET:HE3   | 1.98                     | 0.46              |
| 51:S1:1581:G:H3'   | 85:Sf:92:LEU:HD11  | 1.96                     | 0.46              |
| 78:SY:75:HIS:ND1   | 82:Sc:5:ASP:OD2    | 2.37                     | 0.46              |
| 82:Sc:35:ASP:CG    | 82:Sc:83:LYS:HZ3   | 2.24                     | 0.46              |
| 1:L1:412:G:H4'     | 1:L1:437:A:N1      | 2.30                     | 0.46              |
| 1:L1:547:U:H4'     | 26:LR:65:VAL:HG21  | 1.98                     | 0.46              |
| 1:L1:1390:G:H4'    | 1:L1:1391:U:O5'    | 2.16                     | 0.46              |
| 1:L1:1564:C:H5''   | 5:L5:127:A:N6      | 2.30                     | 0.46              |
| 2:L2:414:G:OP2     | 2:L2:414:G:N2      | 2.38                     | 0.46              |
| 4:L4:4:G:H1        | 4:L4:20:U:H3       | 1.64                     | 0.46              |
| 10:LB:47:MET:HB2   | 10:LB:84:MET:HE3   | 1.98                     | 0.46              |
| 29:LU:50:PHE:O     | 29:LU:54:ASN:HB2   | 2.16                     | 0.46              |
| 51:S1:917:C:O2'    | 51:S1:918:A:H4'    | 2.15                     | 0.46              |
| 51:S1:1699:A:H2    | 51:S1:1778:C:H42   | 1.64                     | 0.46              |
| 54:SA:246:ARG:NH2  | 68:SO:11:GLY:O     | 2.39                     | 0.46              |
| 61:SH:52:MET:HG2   | 61:SH:53:PRO:HD2   | 1.98                     | 0.46              |
| 64:SK:177:ASP:O    | 64:SK:181:GLU:HG2  | 2.15                     | 0.46              |
| 76:SW:90:VAL:HB    | 76:SW:123:LEU:HD12 | 1.97                     | 0.46              |
| 1:L1:1650:U:OP1    | 21:LM:67:ARG:NH1   | 2.41                     | 0.46              |
| 1:L1:1652:A:OP1    | 21:LM:71:ARG:NH1   | 2.49                     | 0.46              |
| 10:LB:93:ARG:HD3   | 10:LB:102:ILE:HG12 | 1.98                     | 0.46              |
| 16:LH:131:VAL:HG12 | 16:LH:132:ARG:HG3  | 1.98                     | 0.46              |
| 51:S1:2200:A:C6    | 81:Sb:88:VAL:HG22  | 2.51                     | 0.46              |
| 65:SL:104:ASN:ND2  | 65:SL:106:VAL:HG23 | 2.30                     | 0.46              |
| 67:SN:37:LEU:HD13  | 67:SN:42:PHE:CE1   | 2.51                     | 0.46              |
| 86:Sg:81:LEU:HD11  | 86:Sg:122:ILE:HG12 | 1.97                     | 0.46              |
| 2:L2:590:U:H2'     | 2:L2:591:A2M:C8    | 2.45                     | 0.46              |
| 41:Lg:20:LYS:HB2   | 41:Lg:20:LYS:HE3   | 1.59                     | 0.46              |
| 42:Lh:115:LYS:HB2  | 42:Lh:115:LYS:HZ3  | 1.81                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:S1:98:A2M:HM'3  | 51:S1:98:A2M:H1'   | 1.84                     | 0.46              |
| 51:S1:784:C:N4     | 51:S1:834:U:H3     | 2.14                     | 0.46              |
| 51:S1:1511:C:N4    | 51:S1:1637:A:O5'   | 2.47                     | 0.46              |
| 51:S1:1527:U:H2'   | 51:S1:1528:G:H8    | 1.81                     | 0.46              |
| 65:SL:28:THR:HG23  | 65:SL:70:ARG:HB3   | 1.98                     | 0.46              |
| 69:SP:17:ARG:NH1   | 69:SP:17:ARG:HA    | 2.30                     | 0.46              |
| 82:Sc:3:PHE:HD1    | 82:Sc:4:PHE:H      | 1.62                     | 0.46              |
| 86:Sg:191:LYS:HB3  | 86:Sg:191:LYS:HE3  | 1.76                     | 0.46              |
| 1:L1:719:U:O2'     | 1:L1:720:A:H5''    | 2.16                     | 0.46              |
| 2:L2:957:C:H2'     | 2:L2:958:A:C8      | 2.50                     | 0.46              |
| 51:S1:17:C:H2'     | 51:S1:18:OMC:C6    | 2.51                     | 0.46              |
| 51:S1:756:C:H42    | 51:S1:772:A:H62    | 1.64                     | 0.46              |
| 54:SA:26:ARG:O     | 54:SA:50:LYS:HG3   | 2.16                     | 0.46              |
| 64:SK:119:ILE:HD11 | 64:SK:166:ARG:HD3  | 1.96                     | 0.46              |
| 2:L2:501:A:N1      | 51:S1:2064:C:O2'   | 2.46                     | 0.46              |
| 2:L2:507:G:H21     | 2:L2:508:A:N6      | 2.14                     | 0.46              |
| 2:L2:1336:G:H5''   | 2:L2:1337:C:H5'    | 1.98                     | 0.46              |
| 2:L2:1510:A:H61    | 10:LB:327:ASP:H    | 1.63                     | 0.46              |
| 3:L3:20:C:H5       | 42:Lh:71:HIS:NE2   | 2.14                     | 0.46              |
| 10:LB:390:LEU:O    | 10:LB:394:ARG:HG3  | 2.15                     | 0.46              |
| 14:LF:101:ILE:HG12 | 14:LF:153:LEU:HD11 | 1.98                     | 0.46              |
| 51:S1:45:U:O2'     | 51:S1:46:U:H2'     | 2.16                     | 0.46              |
| 51:S1:546:U:C2     | 51:S1:547:U:H1'    | 2.51                     | 0.46              |
| 51:S1:878:C:H5     | 51:S1:883:G:H1     | 1.64                     | 0.46              |
| 63:SJ:67:GLY:HA3   | 78:SY:26:THR:HB    | 1.98                     | 0.46              |
| 80:Sa:60:ILE:HG23  | 80:Sa:65:ILE:HD11  | 1.98                     | 0.46              |
| 87:Sh:185:LYS:HG3  | 87:Sh:186:PHE:N    | 2.31                     | 0.46              |
| 1:L1:84:G:O6       | 89:LM:301:SPD:H91  | 2.16                     | 0.45              |
| 1:L1:358:G:N7      | 89:L1:1811:SPD:N6  | 2.63                     | 0.45              |
| 18:LJ:106:ASN:OD1  | 18:LJ:110:GLU:N    | 2.50                     | 0.45              |
| 51:S1:328:C:O2'    | 51:S1:329:C:OP1    | 2.32                     | 0.45              |
| 69:SP:95:GLU:O     | 69:SP:98:ASP:HB2   | 2.15                     | 0.45              |
| 1:L1:163:U:H2'     | 1:L1:164:G:C8      | 2.51                     | 0.45              |
| 1:L1:678:A2M:HM'3  | 1:L1:678:A2M:H1'   | 1.86                     | 0.45              |
| 1:L1:1039:OMU:HM23 | 1:L1:1039:OMU:H1'  | 1.64                     | 0.45              |
| 2:L2:83:G:O2'      | 2:L2:580:U:O4      | 2.28                     | 0.45              |
| 2:L2:488:A:H5''    | 9:LA:244:GLY:HA3   | 1.97                     | 0.45              |
| 12:LD:111:HIS:CD2  | 12:LD:124:ILE:HA   | 2.51                     | 0.45              |
| 12:LD:165:PHE:HD2  | 12:LD:173:ILE:HD11 | 1.81                     | 0.45              |
| 22:LN:69:ARG:HG3   | 22:LN:70:ILE:N     | 2.32                     | 0.45              |
| 51:S1:811:C:HO2'   | 51:S1:812:A:H8     | 1.63                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:S1:824:C:H5'    | 51:S1:825:C:H5'    | 1.98                     | 0.45              |
| 51:S1:933:G:N2     | 96:S1:2579:HOH:O   | 2.49                     | 0.45              |
| 52:S4:54:C:H2'     | 52:S4:55:G:H8      | 1.82                     | 0.45              |
| 57:SD:91:LYS:HB2   | 57:SD:94:TYR:CE2   | 2.52                     | 0.45              |
| 60:SG:59:LYS:HD3   | 60:SG:110:ALA:HB2  | 1.97                     | 0.45              |
| 1:L1:531:C:H1'     | 26:LR:132:PRO:HG3  | 1.98                     | 0.45              |
| 2:L2:1192:C:O3'    | 50:Lp:39:GLY:HA3   | 2.17                     | 0.45              |
| 12:LD:30:ASP:OD1   | 12:LD:34:ARG:NE    | 2.37                     | 0.45              |
| 13:LE:56:VAL:HG22  | 13:LE:69:LEU:HD23  | 1.98                     | 0.45              |
| 18:LJ:19:LEU:HD13  | 18:LJ:25:VAL:HG11  | 1.98                     | 0.45              |
| 32:LX:84:ARG:H     | 60:SG:134:ARG:NH2  | 2.14                     | 0.45              |
| 51:S1:29:OMU:H2'   | 51:S1:30:G:H8      | 1.81                     | 0.45              |
| 58:SE:138:THR:OG1  | 58:SE:140:ASP:OD1  | 2.30                     | 0.45              |
| 86:Sg:135:ASN:ND2  | 86:Sg:137:ALA:H    | 2.15                     | 0.45              |
| 1:L1:1753:U:O4     | 1:L1:1754:A:N6     | 2.49                     | 0.45              |
| 2:L2:382:A2M:HM'3  | 2:L2:382:A2M:H1'   | 1.85                     | 0.45              |
| 2:L2:1333:G:O2'    | 47:Lm:100:TYR:O    | 2.25                     | 0.45              |
| 2:L2:1368:A:O2'    | 18:LJ:40:SER:OG    | 2.28                     | 0.45              |
| 7:L7:83:A:O2'      | 7:L7:84:U:O5'      | 2.29                     | 0.45              |
| 15:LG:163:LEU:HD23 | 21:LM:7:LEU:HD21   | 1.99                     | 0.45              |
| 20:LL:72:THR:HB    | 20:LL:110:LEU:HG   | 1.98                     | 0.45              |
| 23:LO:83:LEU:HB3   | 23:LO:88:ILE:HB    | 1.98                     | 0.45              |
| 42:Lh:10:ARG:HG2   | 42:Lh:10:ARG:NH1   | 2.29                     | 0.45              |
| 50:Lp:7:LYS:HD3    | 50:Lp:24:LYS:HA    | 1.97                     | 0.45              |
| 54:SA:85:LYS:NZ    | 54:SA:108:THR:HA   | 2.32                     | 0.45              |
| 62:SI:95:MET:HE1   | 62:SI:172:VAL:HA   | 1.98                     | 0.45              |
| 76:SW:63:LEU:HD13  | 76:SW:85:THR:HB    | 1.98                     | 0.45              |
| 94:L2:1729:PAR:H24 | 94:L2:1729:PAR:H33 | 1.80                     | 0.45              |
| 18:LJ:29:ASP:HB3   | 18:LJ:31:THR:HG23  | 1.97                     | 0.45              |
| 19:LK:39:GLU:OE1   | 19:LK:48:ARG:HB2   | 2.17                     | 0.45              |
| 51:S1:309:G:O2'    | 51:S1:311:G:OP2    | 2.21                     | 0.45              |
| 1:L1:195:G:H1'     | 1:L1:196:C:C6      | 2.52                     | 0.45              |
| 1:L1:1286:C:H1'    | 1:L1:1348:A:H61    | 1.82                     | 0.45              |
| 1:L1:1672:U:H2'    | 1:L1:1673:G:O4'    | 2.16                     | 0.45              |
| 1:L1:1766:G:H2'    | 1:L1:1767:A:H8     | 1.80                     | 0.45              |
| 2:L2:806:C:H2'     | 2:L2:807:A:O4'     | 2.17                     | 0.45              |
| 2:L2:1224:U:OP1    | 50:Lp:38:ARG:N     | 2.35                     | 0.45              |
| 8:L8:52:G:OP2      | 23:LO:94:ASN:HB3   | 2.17                     | 0.45              |
| 33:LY:77:HIS:HB3   | 38:Ld:37:ARG:HD3   | 1.99                     | 0.45              |
| 55:SB:183:ARG:HD3  | 55:SB:187:ARG:CZ   | 2.47                     | 0.45              |
| 56:SC:126:MET:HE2  | 56:SC:153:ASP:OD2  | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:SG:33:LEU:HD11  | 60:SG:64:MET:HB2   | 1.97                     | 0.45              |
| 62:SI:41:LEU:N     | 62:SI:42:PRO:HD2   | 2.31                     | 0.45              |
| 77:SX:17:ALA:HB3   | 77:SX:149:PHE:HA   | 1.99                     | 0.45              |
| 85:Sf:85:LYS:HG3   | 85:Sf:86:PRO:HD2   | 1.99                     | 0.45              |
| 1:L1:1037:A:O2'    | 37:Lc:132:PRO:O    | 2.35                     | 0.45              |
| 2:L2:1404:G:C5'    | 9:LA:220:GLY:HA3   | 2.47                     | 0.45              |
| 22:LN:38:ARG:HG3   | 22:LN:83:ASP:HA    | 1.98                     | 0.45              |
| 2:L2:383:U:OP2     | 2:L2:388:A:N6      | 2.39                     | 0.45              |
| 2:L2:1510:A:C6     | 10:LB:83:PRO:HD3   | 2.51                     | 0.45              |
| 15:LG:73:PRO:HG3   | 21:LM:18:VAL:HA    | 1.98                     | 0.45              |
| 51:S1:528:G:H1     | 51:S1:553:U:H3     | 1.65                     | 0.45              |
| 51:S1:1598:U:OP2   | 72:SS:3:HIS:ND1    | 2.38                     | 0.45              |
| 55:SB:194:ARG:HE   | 78:SY:48:GLY:HA3   | 1.82                     | 0.45              |
| 60:SG:59:LYS:HG2   | 60:SG:108:ASP:O    | 2.16                     | 0.45              |
| 79:SZ:12:ILE:HG21  | 79:SZ:50:LEU:HG    | 1.98                     | 0.45              |
| 86:Sg:21:GLN:HA    | 86:Sg:289:ALA:HB2  | 1.98                     | 0.45              |
| 87:Sh:150:LYS:HA   | 87:Sh:167:MET:HE1  | 1.98                     | 0.45              |
| 2:L2:4:C:O2        | 3:L3:18:A:O2'      | 2.28                     | 0.45              |
| 2:L2:748:C:N4      | 2:L2:749:G:O6      | 2.49                     | 0.45              |
| 37:Lc:142:PRO:HA   | 37:Lc:237:TYR:CG   | 2.51                     | 0.45              |
| 37:Lc:230:HIS:ND1  | 37:Lc:232:VAL:HG22 | 2.32                     | 0.45              |
| 80:Sa:71:ILE:HB    | 80:Sa:75:ILE:HD11  | 1.98                     | 0.45              |
| 1:L1:921:A:C5      | 89:L1:1802:SPD:H32 | 2.52                     | 0.45              |
| 2:L2:25:A:H5''     | 46:Ll:45:ARG:NH2   | 2.31                     | 0.45              |
| 3:L3:111:A:O2'     | 3:L3:112:C:H5''    | 2.17                     | 0.45              |
| 3:L3:123:G:N2      | 3:L3:124:U:O4      | 2.49                     | 0.45              |
| 8:L8:109:U:H2'     | 8:L8:110:G:H8      | 1.81                     | 0.45              |
| 18:LJ:106:ASN:ND2  | 18:LJ:110:GLU:HB2  | 2.32                     | 0.45              |
| 19:LK:141:LYS:HA   | 19:LK:141:LYS:HD3  | 1.71                     | 0.45              |
| 24:LP:92:ASP:OD1   | 24:LP:92:ASP:N     | 2.50                     | 0.45              |
| 51:S1:29:OMU:HM23  | 51:S1:29:OMU:H1'   | 1.63                     | 0.45              |
| 51:S1:481:A:O2'    | 51:S1:513:G:N2     | 2.33                     | 0.45              |
| 51:S1:2015:U:H5''  | 51:S1:2016:C:H5    | 1.82                     | 0.45              |
| 58:SE:121:MET:HB3  | 58:SE:138:THR:HB   | 1.99                     | 0.45              |
| 65:SL:66:TYR:HA    | 65:SL:69:LEU:HD12  | 1.99                     | 0.45              |
| 87:Sh:81:VAL:H     | 87:Sh:94:PHE:C     | 2.25                     | 0.45              |
| 1:L1:196:C:O2'     | 1:L1:198:A:OP2     | 2.35                     | 0.44              |
| 1:L1:550:A:OP1     | 37:Lc:150:SER:OG   | 2.25                     | 0.44              |
| 1:L1:752:G:OP1     | 20:LL:128:LYS:HG2  | 2.17                     | 0.44              |
| 1:L1:1479:A:H4'    | 1:L1:1480:C:O5'    | 2.16                     | 0.44              |
| 10:LB:226:THR:HG22 | 10:LB:336:SER:HB3  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:Lb:22:LYS:HA    | 36:Lb:22:LYS:HD3   | 1.79                     | 0.44              |
| 51:S1:664:U:O2'    | 51:S1:670:A:N1     | 2.42                     | 0.44              |
| 51:S1:1449:U:C4    | 59:SF:213:ARG:HD3  | 2.52                     | 0.44              |
| 51:S1:2198:A:N6    | 81:Sb:36:LYS:HE3   | 2.31                     | 0.44              |
| 59:SF:164:HIS:ND1  | 59:SF:207:ASP:OD2  | 2.49                     | 0.44              |
| 66:SM:21:ILE:HG22  | 66:SM:29:VAL:HG23  | 1.98                     | 0.44              |
| 4:L4:24:A:N1       | 4:L4:181:C:O2'     | 2.49                     | 0.44              |
| 18:LJ:86:SER:HA    | 18:LJ:96:TYR:HB3   | 1.99                     | 0.44              |
| 27:LS:48:VAL:HG12  | 27:LS:50:GLU:H     | 1.82                     | 0.44              |
| 61:SH:58:LEU:HD23  | 61:SH:58:LEU:HA    | 1.88                     | 0.44              |
| 75:SV:96:GLN:HA    | 75:SV:119:ARG:HH21 | 1.82                     | 0.44              |
| 1:L1:743:A:H4'     | 1:L1:744:C:H5'     | 2.00                     | 0.44              |
| 2:L2:1187:C:N3     | 50:Lp:63:LYS:HE3   | 2.32                     | 0.44              |
| 10:LB:224:SER:HB3  | 10:LB:343:MET:HG2  | 2.00                     | 0.44              |
| 22:LN:75:TYR:CZ    | 22:LN:79:ARG:HG3   | 2.52                     | 0.44              |
| 25:LQ:105:LEU:HD23 | 25:LQ:138:LEU:HD23 | 1.99                     | 0.44              |
| 51:S1:701:G:H22    | 51:S1:745:G:N2     | 2.15                     | 0.44              |
| 51:S1:1518:C:H2'   | 51:S1:1519:G:O4'   | 2.17                     | 0.44              |
| 76:SW:102:ALA:HB1  | 76:SW:109:PHE:HB3  | 1.99                     | 0.44              |
| 86:Sg:283:ILE:HD11 | 86:Sg:299:LYS:HE3  | 1.99                     | 0.44              |
| 1:L1:409:U:H5'     | 1:L1:410:U:H2'     | 1.99                     | 0.44              |
| 1:L1:597:C:H2'     | 1:L1:598:G:H8      | 1.82                     | 0.44              |
| 1:L1:824:U:O2'     | 1:L1:1128:A:N6     | 2.30                     | 0.44              |
| 2:L2:5:A:H2'       | 2:L2:6:A:C8        | 2.52                     | 0.44              |
| 6:L6:51:A:C6       | 41:Lg:23:ARG:HD2   | 2.52                     | 0.44              |
| 7:L7:106:G:H4'     | 7:L7:149:A:H5'     | 1.98                     | 0.44              |
| 31:LW:108:LEU:HD13 | 31:LW:113:LYS:HD3  | 2.00                     | 0.44              |
| 51:S1:580:A:H8     | 51:S1:584:U:H5''   | 1.82                     | 0.44              |
| 51:S1:1502:G:H22   | 88:S5:4:C:H3'      | 1.82                     | 0.44              |
| 51:S1:1603:U:O2'   | 85:Sf:132:ALA:HB1  | 2.18                     | 0.44              |
| 51:S1:1916:G:H3'   | 51:S1:1917:A:H8    | 1.83                     | 0.44              |
| 51:S1:2015:U:H5'   | 51:S1:2016:C:OP2   | 2.18                     | 0.44              |
| 57:SD:88:GLU:CD    | 57:SD:88:GLU:H     | 2.26                     | 0.44              |
| 59:SF:63:LEU:HD12  | 59:SF:83:ILE:HD11  | 2.00                     | 0.44              |
| 68:SO:24:VAL:HB    | 68:SO:86:LEU:HD13  | 1.99                     | 0.44              |
| 86:Sg:33:SER:OG    | 86:Sg:34:ARG:N     | 2.51                     | 0.44              |
| 87:Sh:170:GLN:HB2  | 87:Sh:172:PHE:CD1  | 2.52                     | 0.44              |
| 1:L1:447:G:N2      | 7:L7:15:G:O2'      | 2.50                     | 0.44              |
| 3:L3:109:U:O2'     | 3:L3:111:A:H8      | 2.01                     | 0.44              |
| 8:L8:87:G:O2'      | 8:L8:89:C:OP1      | 2.33                     | 0.44              |
| 60:SG:165:VAL:HB   | 60:SG:173:ARG:HG3  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:SH:151:ASN:OD1  | 61:SH:152:LEU:N    | 2.51                     | 0.44              |
| 62:SI:21:GLU:O     | 62:SI:25:LYS:HG3   | 2.17                     | 0.44              |
| 62:SI:100:ARG:HH22 | 62:SI:131:ASP:CG   | 2.25                     | 0.44              |
| 66:SM:33:THR:HG23  | 66:SM:86:ILE:HD11  | 2.00                     | 0.44              |
| 79:SZ:44:GLN:O     | 79:SZ:48:LYS:HG2   | 2.18                     | 0.44              |
| 79:SZ:84:ASP:N     | 79:SZ:84:ASP:OD1   | 2.51                     | 0.44              |
| 1:L1:1632:C:H5''   | 42:Lh:10:ARG:HH12  | 1.82                     | 0.44              |
| 2:L2:538:U:O2'     | 51:S1:2076:U:O2'   | 2.34                     | 0.44              |
| 2:L2:1116:A:H2'    | 2:L2:1116:A:N3     | 2.33                     | 0.44              |
| 5:L5:39:G:H4'      | 10:LB:372:ILE:O    | 2.17                     | 0.44              |
| 10:LB:261:HIS:HA   | 10:LB:262:PRO:C    | 2.42                     | 0.44              |
| 28:LT:43:LYS:HE3   | 28:LT:43:LYS:HB3   | 1.63                     | 0.44              |
| 51:S1:2132:C:H2'   | 51:S1:2133:G:O4'   | 2.18                     | 0.44              |
| 56:SC:205:ASP:OD1  | 56:SC:205:ASP:N    | 2.50                     | 0.44              |
| 58:SE:258:GLU:HA   | 58:SE:258:GLU:OE2  | 2.16                     | 0.44              |
| 61:SH:42:TRP:CE2   | 61:SH:52:MET:HG3   | 2.53                     | 0.44              |
| 61:SH:45:ARG:HG3   | 61:SH:45:ARG:HH11  | 1.83                     | 0.44              |
| 65:SL:96:ILE:HG23  | 65:SL:108:LYS:HG2  | 1.99                     | 0.44              |
| 1:L1:165:U:H3      | 1:L1:290:G:H1      | 1.66                     | 0.44              |
| 2:L2:1076:G:N3     | 2:L2:1185:A2M:H2   | 2.33                     | 0.44              |
| 2:L2:1175:A:H5'    | 23:LO:181:HIS:HA   | 1.99                     | 0.44              |
| 15:LG:177:PRO:HA   | 15:LG:224:LEU:HD22 | 1.98                     | 0.44              |
| 34:LZ:120:ARG:HD3  | 40:Lf:117:ASP:HB2  | 2.00                     | 0.44              |
| 51:S1:285:A:N1     | 51:S1:815:U:H5''   | 2.33                     | 0.44              |
| 55:SB:94:SER:OG    | 55:SB:101:PHE:HB3  | 2.17                     | 0.44              |
| 66:SM:47:ILE:HG22  | 66:SM:88:LEU:HB3   | 1.99                     | 0.44              |
| 76:SW:28:GLU:N     | 76:SW:28:GLU:OE1   | 2.51                     | 0.44              |
| 86:Sg:172:TRP:HA   | 86:Sg:196:TYR:HB2  | 2.00                     | 0.44              |
| 1:L1:1216:U:O5'    | 1:L1:1402:U:H4'    | 2.18                     | 0.44              |
| 2:L2:337:A:HO2'    | 2:L2:338:C:P       | 2.41                     | 0.44              |
| 2:L2:1360:OMG:H1'  | 2:L2:1389:G:N3     | 2.33                     | 0.44              |
| 4:L4:141:A:H4'     | 13:LE:70:ASN:HB3   | 2.00                     | 0.44              |
| 9:LA:42:ARG:HG2    | 9:LA:42:ARG:NH1    | 2.31                     | 0.44              |
| 18:LJ:106:ASN:HD21 | 18:LJ:110:GLU:HB2  | 1.83                     | 0.44              |
| 27:LS:57:TYR:HA    | 27:LS:60:ARG:HG3   | 2.00                     | 0.44              |
| 28:LT:16:LYS:HG2   | 28:LT:149:PHE:HB3  | 2.00                     | 0.44              |
| 51:S1:198:C:H4'    | 87:Sh:196:ARG:HH12 | 1.83                     | 0.44              |
| 55:SB:109:GLY:N    | 55:SB:139:GLU:OE2  | 2.40                     | 0.44              |
| 87:Sh:164:ARG:HB3  | 87:Sh:176:TYR:HB2  | 1.99                     | 0.44              |
| 1:L1:751:G:O2'     | 1:L1:815:G:H5''    | 2.17                     | 0.44              |
| 1:L1:752:G:OP1     | 20:LL:128:LYS:NZ   | 2.43                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:L1:845:OMU:HM23  | 1:L1:845:OMU:H1'  | 1.82                     | 0.44              |
| 1:L1:1369:G:OP1    | 16:LH:78:LYS:NZ   | 2.40                     | 0.44              |
| 1:L1:1749:G:OP2    | 42:Lh:30:LYS:NZ   | 2.50                     | 0.44              |
| 2:L2:613:A:OP1     | 10:LB:264:ARG:NH2 | 2.51                     | 0.44              |
| 14:LF:97:ASP:C     | 14:LF:99:ALA:H    | 2.26                     | 0.44              |
| 17:LI:55:PRO:HB3   | 17:LI:154:ASP:HB3 | 2.00                     | 0.44              |
| 19:LK:7:ILE:HD11   | 19:LK:58:PRO:HG3  | 2.00                     | 0.44              |
| 35:La:20:LYS:O     | 35:La:24:GLU:HG3  | 2.16                     | 0.44              |
| 39:Le:164:LYS:HG2  | 39:Le:166:PHE:CE1 | 2.53                     | 0.44              |
| 51:S1:700:G:H2'    | 51:S1:701:G:C8    | 2.53                     | 0.44              |
| 51:S1:969:A2M:N6   | 62:SI:101:GLN:O   | 2.51                     | 0.44              |
| 51:S1:2182:G:OP2   | 51:S1:2182:G:N2   | 2.38                     | 0.44              |
| 56:SC:53:LYS:O     | 56:SC:57:VAL:HG12 | 2.18                     | 0.44              |
| 1:L1:947:A:H5'     | 9:LA:183:GLY:HA2  | 2.00                     | 0.43              |
| 2:L2:1318:PSU:H1'  | 10:LB:255:ALA:HB3 | 1.99                     | 0.43              |
| 2:L2:1490:U:H2'    | 2:L2:1491:G:H8    | 1.83                     | 0.43              |
| 11:LC:252:GLN:O    | 11:LC:256:GLU:HG3 | 2.17                     | 0.43              |
| 14:LF:112:GLU:OE1  | 14:LF:112:GLU:N   | 2.42                     | 0.43              |
| 16:LH:22:PRO:HG2   | 16:LH:24:ILE:HD11 | 1.99                     | 0.43              |
| 17:LI:48:ALA:HB2   | 17:LI:56:LEU:HD22 | 1.99                     | 0.43              |
| 27:LS:83:ARG:NE    | 27:LS:85:LEU:HD21 | 2.33                     | 0.43              |
| 32:LX:1:MET:HG3    | 32:LX:15:PRO:HG3  | 2.00                     | 0.43              |
| 51:S1:2015:U:H5''  | 51:S1:2016:C:C5   | 2.53                     | 0.43              |
| 56:SC:89:ARG:HG3   | 56:SC:89:ARG:HH11 | 1.82                     | 0.43              |
| 86:Sg:185:LYS:HE2  | 86:Sg:185:LYS:HB2 | 1.90                     | 0.43              |
| 1:L1:1010:OMC:HN42 | 2:L2:1239:A:H5''  | 1.84                     | 0.43              |
| 12:LD:51:ARG:HA    | 12:LD:66:LYS:HA   | 2.00                     | 0.43              |
| 25:LQ:198:GLN:HA   | 25:LQ:201:LYS:HD2 | 1.99                     | 0.43              |
| 42:Lh:10:ARG:HH11  | 42:Lh:10:ARG:CG   | 2.31                     | 0.43              |
| 42:Lh:95:ALA:O     | 42:Lh:99:GLU:HG3  | 2.18                     | 0.43              |
| 51:S1:98:A2M:O5'   | 51:S1:98:A2M:H8   | 2.18                     | 0.43              |
| 51:S1:866:G:C6     | 57:SD:148:ARG:HG3 | 2.52                     | 0.43              |
| 51:S1:1439:G:O2'   | 51:S1:1445:A:N1   | 2.49                     | 0.43              |
| 60:SG:184:THR:O    | 60:SG:188:LYS:HG3 | 2.18                     | 0.43              |
| 82:Sc:39:PRO:HA    | 82:Sc:42:ARG:HH11 | 1.83                     | 0.43              |
| 1:L1:320:G:O6      | 1:L1:342:G:H1'    | 2.18                     | 0.43              |
| 1:L1:447:G:H1'     | 7:L7:15:G:N2      | 2.33                     | 0.43              |
| 1:L1:745:U:OP1     | 1:L1:831:C:O2'    | 2.32                     | 0.43              |
| 2:L2:382:A2M:H2    | 2:L2:389:A:N7     | 2.33                     | 0.43              |
| 2:L2:1308:5MC:H6   | 2:L2:1308:5MC:H2' | 1.75                     | 0.43              |
| 4:L4:92:U:H2'      | 4:L4:93:U:C6      | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:LV:91:SER:HA    | 30:LV:123:LYS:HB2  | 2.01                     | 0.43              |
| 42:Lh:43:ILE:HD12  | 42:Lh:57:THR:HB    | 2.01                     | 0.43              |
| 47:Lm:79:GLU:HG3   | 47:Lm:82:LEU:H     | 1.83                     | 0.43              |
| 51:S1:288:A:H5'    | 60:SG:213:LEU:HD22 | 2.00                     | 0.43              |
| 51:S1:1870:A:H4'   | 51:S1:1960:G:H4'   | 2.01                     | 0.43              |
| 54:SA:22:GLU:OE1   | 54:SA:23:THR:N     | 2.52                     | 0.43              |
| 57:SD:125:ARG:HD2  | 84:Se:33:ARG:HD3   | 2.00                     | 0.43              |
| 58:SE:99:MET:HE2   | 58:SE:99:MET:HB3   | 1.72                     | 0.43              |
| 62:SI:9:ARG:HG3    | 62:SI:12:LYS:HG2   | 1.99                     | 0.43              |
| 1:L1:37:A:H5''     | 20:LL:35:ALA:HB2   | 2.00                     | 0.43              |
| 1:L1:307:U:H2'     | 1:L1:308:A:H8      | 1.82                     | 0.43              |
| 1:L1:678:A2M:H5''  | 96:L1:2728:HOH:O   | 2.19                     | 0.43              |
| 2:L2:1038:U:H2'    | 2:L2:1039:U:C6     | 2.53                     | 0.43              |
| 94:L2:1729:PAR:H62 | 94:L2:1729:PAR:H13 | 1.68                     | 0.43              |
| 3:L3:100:U:H2'     | 3:L3:101:G:C8      | 2.54                     | 0.43              |
| 7:L7:32:U:H5''     | 7:L7:33:U:OP2      | 2.18                     | 0.43              |
| 8:L8:30:C:H5''     | 23:LO:56:THR:HG21  | 2.00                     | 0.43              |
| 11:LC:140:GLY:HA2  | 34:LZ:17:ARG:HD2   | 2.00                     | 0.43              |
| 12:LD:113:ASP:OD2  | 71:SR:15:ARG:NH2   | 2.51                     | 0.43              |
| 16:LH:161:CYS:HA   | 16:LH:164:VAL:HG22 | 2.01                     | 0.43              |
| 23:LO:40:ASP:HB2   | 23:LO:43:LYS:HG3   | 2.00                     | 0.43              |
| 29:LU:32:ILE:HB    | 29:LU:33:PRO:HD3   | 2.01                     | 0.43              |
| 29:LU:96:LYS:HB3   | 29:LU:96:LYS:HE3   | 1.80                     | 0.43              |
| 30:LV:60:ILE:HD12  | 35:La:26:LYS:HE3   | 1.99                     | 0.43              |
| 35:La:27:LYS:O     | 35:La:31:GLN:HG3   | 2.17                     | 0.43              |
| 46:Ll:28:ARG:HD3   | 46:Ll:36:LYS:HD2   | 1.99                     | 0.43              |
| 51:S1:699:A:N6     | 51:S1:747:C:H42    | 2.17                     | 0.43              |
| 51:S1:783:A:H61    | 51:S1:835:C:H42    | 1.65                     | 0.43              |
| 51:S1:1637:A:H62   | 51:S1:1822:A:N6    | 2.17                     | 0.43              |
| 51:S1:1982:G:OP1   | 77:SX:96:LYS:NZ    | 2.41                     | 0.43              |
| 53:S3:11:A:H2'     | 53:S3:12:G:C8      | 2.53                     | 0.43              |
| 56:SC:6:LYS:O      | 56:SC:10:ILE:HD12  | 2.17                     | 0.43              |
| 61:SH:164:VAL:HG12 | 61:SH:168:LYS:HE3  | 2.01                     | 0.43              |
| 66:SM:19:LEU:O     | 66:SM:85:ILE:HA    | 2.18                     | 0.43              |
| 84:Se:56:HIS:HB3   | 84:Se:59:LYS:HB2   | 2.00                     | 0.43              |
| 2:L2:601:G:OP2     | 28:LT:25:HIS:NE2   | 2.47                     | 0.43              |
| 6:L6:30:C:H3'      | 13:LE:50:LYS:HD3   | 2.00                     | 0.43              |
| 7:L7:162:A2M:H1'   | 7:L7:162:A2M:HM'3  | 1.77                     | 0.43              |
| 49:Lo:55:TRP:NE1   | 49:Lo:66:GLY:O     | 2.51                     | 0.43              |
| 51:S1:124:A:OP2    | 51:S1:124:A:H8     | 2.01                     | 0.43              |
| 51:S1:826:A:H2'    | 51:S1:827:G:H8     | 1.84                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:SB:140:ALA:HB1  | 55:SB:145:ILE:HB   | 2.00                     | 0.43              |
| 55:SB:152:ASP:OD2  | 55:SB:169:ARG:NH1  | 2.50                     | 0.43              |
| 56:SC:30:GLU:H     | 56:SC:30:GLU:CD    | 2.26                     | 0.43              |
| 59:SF:156:TRP:CE2  | 59:SF:185:PRO:HG3  | 2.53                     | 0.43              |
| 62:SI:146:ARG:HA   | 63:SJ:49:GLU:HG3   | 2.00                     | 0.43              |
| 79:SZ:17:PHE:HZ    | 79:SZ:26:LYS:HD2   | 1.83                     | 0.43              |
| 20:LL:70:LYS:HD2   | 20:LL:125:TYR:CE1  | 2.54                     | 0.43              |
| 22:LN:40:ARG:HG3   | 22:LN:40:ARG:HH11  | 1.84                     | 0.43              |
| 51:S1:1672:C:H4'   | 51:S1:1673:A:OP1   | 2.18                     | 0.43              |
| 51:S1:1921:A:N3    | 51:S1:1982:G:O2'   | 2.43                     | 0.43              |
| 65:SL:108:LYS:NZ   | 86:Sg:62:GLU:OE2   | 2.50                     | 0.43              |
| 1:L1:299:U:HO2'    | 1:L1:300:A:H8      | 1.64                     | 0.43              |
| 1:L1:496:C:H2'     | 1:L1:497:A:C8      | 2.53                     | 0.43              |
| 1:L1:709:A:OP1     | 24:LP:115:SER:OG   | 2.35                     | 0.43              |
| 1:L1:1102:U:H5''   | 27:LS:19:PHE:HB2   | 2.00                     | 0.43              |
| 2:L2:1397:OMC:HM22 | 2:L2:1398:C:O4'    | 2.19                     | 0.43              |
| 4:L4:180:C:H1'     | 5:L5:5:C:H1'       | 2.00                     | 0.43              |
| 12:LD:28:SER:HB2   | 12:LD:66:LYS:O     | 2.19                     | 0.43              |
| 12:LD:119:ASP:HB3  | 12:LD:122:THR:HG23 | 2.01                     | 0.43              |
| 13:LE:94:ALA:HB1   | 47:Lm:78:MET:SD    | 2.58                     | 0.43              |
| 38:Ld:26:VAL:HG12  | 38:Ld:93:SER:HB3   | 2.01                     | 0.43              |
| 51:S1:550:C:H2'    | 51:S1:551:A:C8     | 2.53                     | 0.43              |
| 51:S1:552:U:H2'    | 51:S1:553:U:O4'    | 2.18                     | 0.43              |
| 51:S1:918:A:H3'    | 51:S1:919:G:C8     | 2.54                     | 0.43              |
| 51:S1:1718:A:C8    | 80:Sa:85:ARG:HG2   | 2.53                     | 0.43              |
| 54:SA:130:LYS:NZ   | 54:SA:134:GLY:O    | 2.48                     | 0.43              |
| 61:SH:45:ARG:HG3   | 61:SH:45:ARG:NH1   | 2.33                     | 0.43              |
| 64:SK:72:ILE:HG21  | 64:SK:112:TRP:CZ2  | 2.54                     | 0.43              |
| 86:Sg:7:LEU:HB2    | 86:Sg:303:ILE:HB   | 2.00                     | 0.43              |
| 1:L1:981:C:P       | 89:L1:1813:SPD:H42 | 2.59                     | 0.43              |
| 1:L1:1574:C:O2'    | 1:L1:1575:G:OP1    | 2.30                     | 0.43              |
| 2:L2:521:A:OP1     | 94:L2:1729:PAR:N24 | 2.51                     | 0.43              |
| 3:L3:75:C:O2'      | 45:Lk:3:ARG:NH1    | 2.51                     | 0.43              |
| 12:LD:76:LYS:HB2   | 12:LD:76:LYS:HE3   | 1.73                     | 0.43              |
| 15:LG:184:MET:HE3  | 15:LG:195:THR:HG21 | 2.00                     | 0.43              |
| 15:LG:224:LEU:HD12 | 15:LG:224:LEU:HA   | 1.81                     | 0.43              |
| 50:Lp:74:CYS:HB3   | 50:Lp:77:CYS:HB2   | 2.01                     | 0.43              |
| 51:S1:500:A:OP1    | 79:SZ:105:LYS:NZ   | 2.51                     | 0.43              |
| 51:S1:750:U:H2'    | 51:S1:751:G:C8     | 2.54                     | 0.43              |
| 89:L1:1814:SPD:H41 | 2:L2:1037:G:OP1    | 2.18                     | 0.43              |
| 2:L2:453:A:H1'     | 51:S1:1160:A:C5    | 2.54                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:L2:1087:C:H2'   | 2:L2:1088:G:C8     | 2.54                     | 0.43              |
| 11:LC:120:ARG:HG2 | 11:LC:272:LYS:HE3  | 2.01                     | 0.43              |
| 27:LS:80:VAL:HG12 | 27:LS:81:ARG:HG2   | 1.99                     | 0.43              |
| 29:LU:87:LYS:HG2  | 29:LU:117:TYR:CE2  | 2.54                     | 0.43              |
| 46:LI:36:LYS:HD2  | 46:LI:36:LYS:HA    | 1.75                     | 0.43              |
| 51:S1:1450:A:OP1  | 59:SF:171:THR:OG1  | 2.33                     | 0.43              |
| 55:SB:83:ARG:O    | 55:SB:84:LEU:HB3   | 2.19                     | 0.43              |
| 80:Sa:51:ARG:NH1  | 80:Sa:86:GLU:OE1   | 2.52                     | 0.43              |
| 1:L1:247:A:N3     | 11:LC:217:ARG:HD2  | 2.34                     | 0.43              |
| 1:L1:684:G:O2'    | 89:L1:1806:SPD:H41 | 2.19                     | 0.43              |
| 1:L1:1110:G:H5'   | 27:LS:60:ARG:NH1   | 2.34                     | 0.43              |
| 1:L1:1232:U:H5''  | 16:LH:43:LYS:HD3   | 2.01                     | 0.43              |
| 1:L1:1452:C:H2'   | 1:L1:1453:G:H8     | 1.84                     | 0.43              |
| 1:L1:1686:C:H2'   | 1:L1:1687:G:H8     | 1.84                     | 0.43              |
| 2:L2:528:U:O2     | 2:L2:556:U:H4'     | 2.19                     | 0.43              |
| 8:L8:30:C:H2'     | 8:L8:31:A:O4'      | 2.19                     | 0.43              |
| 10:LB:120:LYS:HA  | 10:LB:120:LYS:HD2  | 1.75                     | 0.43              |
| 22:LN:46:PHE:HE1  | 22:LN:141:LYS:HE2  | 1.83                     | 0.43              |
| 23:LO:41:LYS:HA   | 23:LO:41:LYS:HD2   | 1.68                     | 0.43              |
| 23:LO:166:PHE:HA  | 23:LO:169:LEU:HB3  | 2.00                     | 0.43              |
| 26:LR:19:GLU:CD   | 26:LR:19:GLU:H     | 2.27                     | 0.43              |
| 31:LW:74:LYS:HB2  | 31:LW:76:VAL:HG22  | 2.00                     | 0.43              |
| 36:Lb:15:LYS:HB3  | 36:Lb:15:LYS:HE2   | 1.86                     | 0.43              |
| 51:S1:1271:C:O2'  | 51:S1:2177:G:O3'   | 2.36                     | 0.43              |
| 51:S1:2198:A:O2'  | 51:S1:2200:A:N7    | 2.39                     | 0.43              |
| 67:SN:27:LYS:HG3  | 67:SN:71:TYR:CE2   | 2.54                     | 0.43              |
| 69:SP:77:ASN:ND2  | 69:SP:79:LYS:HD2   | 2.34                     | 0.43              |
| 1:L1:135:A:N7     | 1:L1:171:U:H4'     | 2.34                     | 0.42              |
| 1:L1:255:G:OP1    | 31:LW:57:ARG:NH2   | 2.52                     | 0.42              |
| 1:L1:1537:G:O2'   | 2:L2:601:G:O6      | 2.33                     | 0.42              |
| 2:L2:14:OMC:HM21  | 7:L7:113:G:H5'     | 2.00                     | 0.42              |
| 2:L2:795:U:O2'    | 2:L2:798:G:O6      | 2.27                     | 0.42              |
| 2:L2:1127:G:O2'   | 2:L2:1132:A:N1     | 2.45                     | 0.42              |
| 4:L4:161:C:H2'    | 4:L4:162:A:C8      | 2.54                     | 0.42              |
| 7:L7:161:C:H2'    | 7:L7:162:A2M:H8    | 2.01                     | 0.42              |
| 14:LF:177:TYR:OH  | 19:LK:107:ASP:OD2  | 2.26                     | 0.42              |
| 51:S1:29:OMU:H2'  | 51:S1:30:G:C8      | 2.54                     | 0.42              |
| 51:S1:2129:C:H2'  | 51:S1:2130:A:C8    | 2.53                     | 0.42              |
| 62:SI:183:ARG:HG2 | 62:SI:183:ARG:NH1  | 2.30                     | 0.42              |
| 67:SN:76:ASN:O    | 67:SN:80:ILE:HG22  | 2.19                     | 0.42              |
| 71:SR:27:VAL:O    | 71:SR:31:LEU:HG    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 73:ST:2:VAL:HG22   | 73:ST:3:ARG:HG2    | 2.01                     | 0.42              |
| 1:L1:1405:U:H2'    | 1:L1:1406:C:C6     | 2.55                     | 0.42              |
| 1:L1:1569:U:C2     | 28:LT:46:GLN:HG3   | 2.55                     | 0.42              |
| 2:L2:56:OMU:HM23   | 2:L2:56:OMU:H1'    | 1.84                     | 0.42              |
| 2:L2:1183:C:H2'    | 2:L2:1184:C:O4'    | 2.18                     | 0.42              |
| 26:LR:48:ARG:HG3   | 26:LR:54:LYS:HD2   | 2.01                     | 0.42              |
| 39:Le:13:LYS:HA    | 39:Le:13:LYS:HD2   | 1.69                     | 0.42              |
| 51:S1:66:U:H1'     | 60:SG:163:ARG:HH21 | 1.83                     | 0.42              |
| 51:S1:701:G:N2     | 51:S1:745:G:H22    | 2.17                     | 0.42              |
| 51:S1:2098:G:C6    | 51:S1:2099:G:C6    | 3.07                     | 0.42              |
| 57:SD:16:ARG:HB2   | 57:SD:19:GLU:OE2   | 2.18                     | 0.42              |
| 66:SM:26:ALA:HB2   | 66:SM:82:TYR:CZ    | 2.54                     | 0.42              |
| 66:SM:27:LYS:HB2   | 66:SM:27:LYS:NZ    | 2.33                     | 0.42              |
| 69:SP:17:ARG:HA    | 69:SP:17:ARG:HH11  | 1.84                     | 0.42              |
| 74:SU:20:GLU:C     | 74:SU:22:ALA:H     | 2.28                     | 0.42              |
| 1:L1:108:G:N1      | 35:La:120:LYS:HB3  | 2.34                     | 0.42              |
| 1:L1:357:A:N7      | 89:L1:1811:SPD:H71 | 2.35                     | 0.42              |
| 1:L1:624:U:O2'     | 1:L1:625:C:H4'     | 2.19                     | 0.42              |
| 1:L1:823:G:N3      | 1:L1:823:G:H2'     | 2.35                     | 0.42              |
| 2:L2:1354:U:H1'    | 18:LJ:46:GLY:HA3   | 2.00                     | 0.42              |
| 2:L2:1453:U:H4'    | 2:L2:1454:A:H5''   | 2.01                     | 0.42              |
| 5:L5:62:C:H3'      | 5:L5:63:G:N2       | 2.28                     | 0.42              |
| 9:LA:106:GLN:HE21  | 9:LA:106:GLN:HA    | 1.83                     | 0.42              |
| 10:LB:356:GLN:CD   | 10:LB:356:GLN:N    | 2.77                     | 0.42              |
| 22:LN:153:ARG:HD2  | 22:LN:153:ARG:C    | 2.44                     | 0.42              |
| 23:LO:231:GLN:HG3  | 23:LO:232:PHE:CD2  | 2.54                     | 0.42              |
| 31:LW:109:THR:H    | 31:LW:112:ARG:HB3  | 1.85                     | 0.42              |
| 38:Ld:10:ASP:OD1   | 38:Ld:11:THR:N     | 2.51                     | 0.42              |
| 40:Lf:96:VAL:HG22  | 40:Lf:121:ALA:HB3  | 2.00                     | 0.42              |
| 51:S1:471:A:H2'    | 51:S1:472:G:O4'    | 2.18                     | 0.42              |
| 53:S3:44:A:H2'     | 53:S3:45:A:C8      | 2.55                     | 0.42              |
| 57:SD:28:LYS:HE2   | 57:SD:28:LYS:HB2   | 1.89                     | 0.42              |
| 65:SL:55:MET:HB3   | 65:SL:55:MET:HE3   | 1.80                     | 0.42              |
| 75:SV:100:SER:HB3  | 75:SV:123:ALA:HB2  | 2.01                     | 0.42              |
| 1:L1:80:C:H2'      | 1:L1:81:U:O4'      | 2.20                     | 0.42              |
| 1:L1:1775:U:O2'    | 7:L7:127:C:OP1     | 2.34                     | 0.42              |
| 94:L1:1978:PAR:N24 | 94:L1:1978:PAR:O44 | 2.52                     | 0.42              |
| 2:L2:1309:G:H5''   | 2:L2:1310:A:H5''   | 2.01                     | 0.42              |
| 7:L7:43:A2M:HM'3   | 7:L7:43:A2M:H1'    | 1.92                     | 0.42              |
| 13:LE:77:GLN:O     | 13:LE:81:THR:HG22  | 2.20                     | 0.42              |
| 21:LM:146:PRO:HG3  | 35:La:106:ARG:HB3  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:LX:54:PRO:HA    | 32:LX:59:TYR:CG   | 2.54                     | 0.42              |
| 51:S1:1560:A:H5''  | 51:S1:1561:C:OP2  | 2.20                     | 0.42              |
| 51:S1:1686:C:H4'   | 72:SS:56:LEU:HD13 | 2.00                     | 0.42              |
| 51:S1:1905:C:HO2'  | 51:S1:1906:G:P    | 2.39                     | 0.42              |
| 52:S4:33:C:H4'     | 61:SH:184:ARG:HE  | 1.84                     | 0.42              |
| 54:SA:145:THR:HG21 | 54:SA:158:ALA:HB2 | 2.00                     | 0.42              |
| 56:SC:39:HIS:ND1   | 56:SC:39:HIS:C    | 2.77                     | 0.42              |
| 58:SE:84:MET:HE2   | 58:SE:120:LEU:HB2 | 2.00                     | 0.42              |
| 61:SH:37:HIS:CD2   | 61:SH:72:LYS:HG2  | 2.53                     | 0.42              |
| 62:SI:117:ARG:HA   | 62:SI:117:ARG:HD2 | 1.84                     | 0.42              |
| 1:L1:610:A:C2      | 37:Lc:77:ARG:HB3  | 2.54                     | 0.42              |
| 1:L1:739:U:H2'     | 1:L1:740:C:C6     | 2.54                     | 0.42              |
| 2:L2:1101:A:H8     | 12:LD:128:ASP:OD2 | 2.02                     | 0.42              |
| 2:L2:1319:C:H2'    | 2:L2:1320:U:C6    | 2.55                     | 0.42              |
| 9:LA:206:PRO:HD3   | 9:LA:213:GLY:CA   | 2.50                     | 0.42              |
| 21:LM:54:LYS:HD3   | 21:LM:54:LYS:HA   | 1.90                     | 0.42              |
| 34:LZ:41:ARG:HH11  | 34:LZ:102:ASP:HB2 | 1.85                     | 0.42              |
| 41:Lg:61:VAL:HG13  | 41:Lg:66:ASP:HB3  | 2.00                     | 0.42              |
| 55:SB:117:LYS:HD2  | 55:SB:117:LYS:O   | 2.20                     | 0.42              |
| 1:L1:328:U:OP1     | 21:LM:68:ARG:HD2  | 2.19                     | 0.42              |
| 1:L1:1170:G:H4'    | 1:L1:1459:G:H5'   | 2.02                     | 0.42              |
| 2:L2:1000:U:H5'    | 2:L2:1001:C:OP2   | 2.19                     | 0.42              |
| 2:L2:1513:G:N7     | 39:Le:37:ARG:NH2  | 2.66                     | 0.42              |
| 3:L3:174:C:H2'     | 3:L3:175:A:H8     | 1.83                     | 0.42              |
| 5:L5:5:C:H2'       | 5:L5:6:G:O4'      | 2.20                     | 0.42              |
| 5:L5:36:G:OP1      | 10:LB:392:LYS:HE3 | 2.19                     | 0.42              |
| 6:L6:44:G:H2'      | 6:L6:45:G:C8      | 2.54                     | 0.42              |
| 7:L7:169:A:OP2     | 7:L7:169:A:H8     | 2.03                     | 0.42              |
| 11:LC:94:MET:HE3   | 11:LC:94:MET:HB3  | 1.95                     | 0.42              |
| 21:LM:75:VAL:HG23  | 21:LM:78:GLY:HA2  | 2.01                     | 0.42              |
| 24:LP:36:LEU:O     | 24:LP:40:THR:OG1  | 2.31                     | 0.42              |
| 25:LQ:77:GLY:O     | 25:LQ:81:ARG:HG3  | 2.18                     | 0.42              |
| 51:S1:376:U:H5''   | 64:SK:31:ARG:HH11 | 1.85                     | 0.42              |
| 51:S1:462:G:H5'    | 60:SG:73:ARG:HH21 | 1.84                     | 0.42              |
| 51:S1:1978:A:H5''  | 71:SR:134:GLY:HA3 | 2.01                     | 0.42              |
| 87:Sh:67:VAL:HG12  | 87:Sh:70:ALA:N    | 2.31                     | 0.42              |
| 1:L1:114:G:H4'     | 21:LM:49:ARG:HG2  | 2.01                     | 0.42              |
| 1:L1:984:A:OP1     | 17:LI:22:SER:HB3  | 2.20                     | 0.42              |
| 2:L2:1369:C:N3     | 2:L2:1373:C:H5    | 2.18                     | 0.42              |
| 2:L2:1385:G:H4'    | 2:L2:1385:G:OP2   | 2.20                     | 0.42              |
| 2:L2:1485:G:OP2    | 19:LK:171:ARG:NH2 | 2.47                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:LC:356:LYS:HE3 | 11:LC:356:LYS:HB3  | 1.86                     | 0.42              |
| 14:LF:51:ALA:HA   | 14:LF:67:GLY:HA3   | 2.01                     | 0.42              |
| 20:LL:36:GLY:O    | 20:LL:41:HIS:HB2   | 2.19                     | 0.42              |
| 23:LO:262:LYS:HB2 | 23:LO:262:LYS:HE2  | 1.81                     | 0.42              |
| 37:Lc:176:ASN:HA  | 37:Lc:179:ILE:HD12 | 2.02                     | 0.42              |
| 48:Ln:3:THR:HG23  | 51:S1:2174:G:H1'   | 2.02                     | 0.42              |
| 49:Lo:49:ARG:HG3  | 49:Lo:55:TRP:CE2   | 2.55                     | 0.42              |
| 51:S1:58:C:OP1    | 51:S1:504:G:O2'    | 2.38                     | 0.42              |
| 51:S1:230:G:O2'   | 87:Sh:198:HIS:NE2  | 2.47                     | 0.42              |
| 51:S1:1409:U:H2'  | 51:S1:1410:C:C6    | 2.55                     | 0.42              |
| 52:S4:45:G:H2'    | 52:S4:46:U:H5'     | 2.02                     | 0.42              |
| 60:SG:14:LYS:HD3  | 60:SG:14:LYS:HA    | 1.95                     | 0.42              |
| 62:SI:191:ASN:HB3 | 62:SI:196:GLN:HB2  | 2.02                     | 0.42              |
| 1:L1:510:U:O2'    | 26:LR:67:LYS:HE2   | 2.19                     | 0.42              |
| 1:L1:517:U:H2'    | 1:L1:518:C:C6      | 2.55                     | 0.42              |
| 2:L2:72:G:OP1     | 10:LB:251:LEU:N    | 2.52                     | 0.42              |
| 6:L6:68:A:H5'     | 14:LF:47:ARG:NH2   | 2.34                     | 0.42              |
| 6:L6:68:A:H2'     | 6:L6:70:G:C5       | 2.54                     | 0.42              |
| 16:LH:65:GLU:HG3  | 16:LH:155:THR:HG23 | 2.01                     | 0.42              |
| 16:LH:72:TYR:OH   | 16:LH:91:HIS:O     | 2.36                     | 0.42              |
| 21:LM:103:GLU:OE2 | 21:LM:118:SER:OG   | 2.34                     | 0.42              |
| 41:Lg:69:TRP:HZ2  | 41:Lg:144:ILE:HD11 | 1.85                     | 0.42              |
| 49:Lo:67:GLY:HA3  | 49:Lo:70:THR:O     | 2.20                     | 0.42              |
| 50:Lp:11:HIS:HA   | 50:Lp:20:HIS:HA    | 2.01                     | 0.42              |
| 51:S1:1:G:OP2     | 57:SD:52:ARG:NH2   | 2.53                     | 0.42              |
| 51:S1:148:G:H2'   | 51:S1:149:G:C8     | 2.54                     | 0.42              |
| 51:S1:315:A:H5''  | 51:S1:333:G:H22    | 1.84                     | 0.42              |
| 51:S1:969:A2M:H8  | 51:S1:969:A2M:H2'  | 1.80                     | 0.42              |
| 54:SA:11:LYS:O    | 54:SA:11:LYS:HG2   | 2.20                     | 0.42              |
| 73:ST:47:PRO:HG3  | 73:ST:75:LEU:HD12  | 2.01                     | 0.42              |
| 1:L1:246:A:H4'    | 1:L1:248:A:N7      | 2.35                     | 0.42              |
| 1:L1:687:C:H2'    | 1:L1:688:A:H8      | 1.83                     | 0.42              |
| 1:L1:958:G:H5'    | 1:L1:960:A:H1'     | 2.02                     | 0.42              |
| 1:L1:1659:OMU:H6  | 1:L1:1659:OMU:O5'  | 2.20                     | 0.42              |
| 2:L2:459:A:H2'    | 2:L2:460:A:C8      | 2.54                     | 0.42              |
| 2:L2:1507:U:H2'   | 2:L2:1508:A:C8     | 2.54                     | 0.42              |
| 6:L6:11:G:C8      | 14:LF:186:PRO:HG2  | 2.55                     | 0.42              |
| 12:LD:135:ARG:NH2 | 12:LD:155:HIS:O    | 2.48                     | 0.42              |
| 15:LG:88:ARG:HD2  | 15:LG:92:LEU:HD22  | 2.01                     | 0.42              |
| 20:LL:51:GLY:C    | 24:LP:179:GLU:HA   | 2.44                     | 0.42              |
| 22:LN:115:MET:HA  | 22:LN:118:ALA:HB2  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:LQ:89:MET:HE1   | 25:LQ:93:GLU:HB3   | 2.01                     | 0.42              |
| 26:LR:68:ASP:OD1   | 26:LR:100:SER:HB2  | 2.20                     | 0.42              |
| 38:Ld:9:VAL:HG23   | 38:Ld:73:SER:HB2   | 2.01                     | 0.42              |
| 44:Lj:38:ALA:HB2   | 44:Lj:45:ARG:HG3   | 2.02                     | 0.42              |
| 51:S1:259:C:H2'    | 51:S1:260:A:H8     | 1.85                     | 0.42              |
| 51:S1:826:A:H2'    | 51:S1:827:G:C8     | 2.55                     | 0.42              |
| 55:SB:15:GLU:OE2   | 75:SV:118:ARG:HB2  | 2.20                     | 0.42              |
| 59:SF:200:LEU:HD13 | 59:SF:208:VAL:HG11 | 2.02                     | 0.42              |
| 64:SK:171:VAL:O    | 74:SU:7:TYR:HA     | 2.19                     | 0.42              |
| 1:L1:1574:C:HO2'   | 1:L1:1575:G:P      | 2.41                     | 0.42              |
| 1:L1:1685:G:H1     | 1:L1:1715:U:H3     | 1.68                     | 0.42              |
| 2:L2:490:A:H5''    | 9:LA:243:THR:HB    | 2.01                     | 0.42              |
| 2:L2:771:G:H4'     | 15:LG:50:PHE:CE1   | 2.55                     | 0.42              |
| 2:L2:1175:A:OP1    | 23:LO:182:ARG:HD3  | 2.20                     | 0.42              |
| 6:L6:70:G:O2'      | 6:L6:71:A:H8       | 2.02                     | 0.42              |
| 9:LA:36:GLU:OE2    | 9:LA:90:CYS:HB3    | 2.20                     | 0.42              |
| 13:LE:149:ASP:HB3  | 13:LE:152:GLN:HB2  | 2.01                     | 0.42              |
| 34:LZ:53:VAL:HB    | 34:LZ:110:ARG:HG2  | 2.02                     | 0.42              |
| 34:LZ:56:ALA:HB3   | 34:LZ:60:ALA:HB3   | 2.01                     | 0.42              |
| 41:Lg:85:LYS:HG3   | 41:Lg:101:ARG:NH2  | 2.34                     | 0.42              |
| 42:Lh:47:TRP:HA    | 42:Lh:51:HIS:HB2   | 2.02                     | 0.42              |
| 44:Lj:51:VAL:HG12  | 44:Lj:55:LYS:HD2   | 2.02                     | 0.42              |
| 51:S1:27:U:H2'     | 51:S1:28:A2M:H8    | 2.02                     | 0.42              |
| 51:S1:259:C:H2'    | 51:S1:260:A:C8     | 2.55                     | 0.42              |
| 51:S1:1972:G:N1    | 51:S1:1975:A:OP2   | 2.52                     | 0.42              |
| 55:SB:116:GLN:C    | 55:SB:118:LYS:H    | 2.28                     | 0.42              |
| 59:SF:250:ASP:CG   | 59:SF:252:THR:HG1  | 2.26                     | 0.42              |
| 65:SL:107:GLU:O    | 65:SL:108:LYS:HB3  | 2.20                     | 0.42              |
| 66:SM:18:ARG:HD3   | 66:SM:87:ASP:OD2   | 2.19                     | 0.42              |
| 66:SM:96:LYS:HE3   | 66:SM:96:LYS:HB2   | 1.87                     | 0.42              |
| 67:SN:79:GLY:O     | 67:SN:83:MET:HB2   | 2.20                     | 0.42              |
| 73:ST:19:ARG:HB2   | 82:Sc:86:HIS:NE2   | 2.35                     | 0.42              |
| 77:SX:118:LYS:HG2  | 77:SX:122:LYS:HE2  | 2.01                     | 0.42              |
| 1:L1:307:U:H2'     | 1:L1:308:A:C8      | 2.55                     | 0.41              |
| 1:L1:836:G:N1      | 24:LP:96:ASP:HA    | 2.35                     | 0.41              |
| 1:L1:921:A:N3      | 89:L1:1802:SPD:H51 | 2.35                     | 0.41              |
| 1:L1:1031:A:N1     | 1:L1:1161:A:O2'    | 2.52                     | 0.41              |
| 1:L1:1106:A:H5''   | 8:L8:102:G:O2'     | 2.20                     | 0.41              |
| 4:L4:170:G:H4'     | 4:L4:171:A:H3'     | 2.02                     | 0.41              |
| 8:L8:109:U:H2'     | 8:L8:110:G:C8      | 2.55                     | 0.41              |
| 11:LC:295:GLU:HG3  | 11:LC:298:ARG:NH2  | 2.35                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:LF:32:SER:OG    | 41:Lg:144:ILE:O    | 2.33                     | 0.41              |
| 26:LR:29:PHE:CE2   | 26:LR:31:VAL:HB    | 2.55                     | 0.41              |
| 51:S1:402:A:H4'    | 69:SP:33:PHE:HZ    | 1.84                     | 0.41              |
| 51:S1:1535:A:C2    | 76:SW:107:HIS:HB3  | 2.55                     | 0.41              |
| 51:S1:1637:A:H1'   | 51:S1:1638:U:C6    | 2.55                     | 0.41              |
| 51:S1:1915:U:H2'   | 51:S1:1916:G:O4'   | 2.20                     | 0.41              |
| 57:SD:70:LEU:HD12  | 58:SE:247:ILE:HG12 | 2.02                     | 0.41              |
| 66:SM:64:LYS:HE2   | 66:SM:75:ASP:OD1   | 2.20                     | 0.41              |
| 86:Sg:243:PHE:CE1  | 86:Sg:263:LEU:HD11 | 2.55                     | 0.41              |
| 1:L1:159:U:H1'     | 1:L1:160:C:H5'     | 2.02                     | 0.41              |
| 1:L1:169:G:H4'     | 1:L1:170:U:H3'     | 2.02                     | 0.41              |
| 1:L1:454:U:H2'     | 1:L1:455:G:C8      | 2.55                     | 0.41              |
| 1:L1:1044:G:N3     | 2:L2:1064:A:H2'    | 2.35                     | 0.41              |
| 1:L1:1578:G:H4'    | 25:LQ:26:PRO:HD3   | 2.02                     | 0.41              |
| 2:L2:653:C:H2'     | 2:L2:654:U:C6      | 2.56                     | 0.41              |
| 2:L2:822:G:O2'     | 2:L2:823:A:H5'     | 2.20                     | 0.41              |
| 2:L2:970:A:HO2'    | 2:L2:971:A:H8      | 1.66                     | 0.41              |
| 2:L2:1232:G:O2'    | 2:L2:1233:U:OP2    | 2.27                     | 0.41              |
| 2:L2:1385:G:C2     | 10:LB:255:ALA:HB1  | 2.55                     | 0.41              |
| 18:LJ:47:ARG:HD2   | 18:LJ:48:LEU:H     | 1.85                     | 0.41              |
| 31:LW:32:LEU:HB2   | 31:LW:37:ARG:HG3   | 2.02                     | 0.41              |
| 39:Le:24:LYS:HE2   | 39:Le:24:LYS:HB3   | 1.78                     | 0.41              |
| 51:S1:792:G:H5'    | 51:S1:792:G:N3     | 2.35                     | 0.41              |
| 51:S1:1114:G:OP1   | 73:ST:121:ARG:NE   | 2.52                     | 0.41              |
| 51:S1:2119:C:H1'   | 51:S1:2120:C:O5'   | 2.20                     | 0.41              |
| 55:SB:194:ARG:NE   | 78:SY:48:GLY:HA3   | 2.35                     | 0.41              |
| 58:SE:118:ILE:HG23 | 58:SE:158:VAL:HG23 | 2.02                     | 0.41              |
| 87:Sh:165:LEU:HD23 | 87:Sh:165:LEU:HA   | 1.86                     | 0.41              |
| 2:L2:21:C:H5''     | 2:L2:22:A:H5'      | 2.01                     | 0.41              |
| 20:LL:110:LEU:O    | 20:LL:130:ALA:HB2  | 2.21                     | 0.41              |
| 47:Lm:79:GLU:OE1   | 47:Lm:80:PRO:HD2   | 2.21                     | 0.41              |
| 51:S1:668:A2M:H8   | 51:S1:668:A2M:H2'  | 1.90                     | 0.41              |
| 51:S1:1281:C:O2'   | 63:SJ:2:THR:N      | 2.45                     | 0.41              |
| 51:S1:1859:A:H2'   | 51:S1:1859:A:N3    | 2.35                     | 0.41              |
| 52:S4:17:A:H2'     | 52:S4:18:G:C8      | 2.56                     | 0.41              |
| 55:SB:54:VAL:HG22  | 75:SV:108:MET:SD   | 2.60                     | 0.41              |
| 60:SG:4:ASN:ND2    | 60:SG:111:LEU:HD11 | 2.35                     | 0.41              |
| 63:SJ:3:MET:HE3    | 63:SJ:3:MET:HB2    | 1.77                     | 0.41              |
| 71:SR:113:GLU:HA   | 71:SR:116:LYS:HG2  | 2.02                     | 0.41              |
| 85:Sf:92:LEU:HD12  | 85:Sf:92:LEU:HA    | 1.89                     | 0.41              |
| 86:Sg:4:GLU:O      | 86:Sg:47:ARG:NH2   | 2.53                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 87:Sh:75:SER:HA   | 87:Sh:78:GLY:O      | 2.20                     | 0.41              |
| 1:L1:156:A:H8     | 1:L1:156:A:OP2      | 2.03                     | 0.41              |
| 1:L1:712:G:H2'    | 1:L1:713:A:O4'      | 2.21                     | 0.41              |
| 2:L2:742:U:H2'    | 2:L2:743:C:C6       | 2.56                     | 0.41              |
| 2:L2:784:U:H1'    | 2:L2:785:U:OP2      | 2.20                     | 0.41              |
| 10:LB:116:ARG:HG2 | 10:LB:122:TRP:CG    | 2.55                     | 0.41              |
| 11:LC:216:THR:O   | 11:LC:220:ARG:HG3   | 2.20                     | 0.41              |
| 22:LN:46:PHE:HB2  | 22:LN:139:ARG:HG2   | 2.02                     | 0.41              |
| 23:LO:187:PRO:HG2 | 23:LO:201:HIS:CD2   | 2.56                     | 0.41              |
| 39:Le:103:LYS:C   | 39:Le:106:PRO:HD2   | 2.45                     | 0.41              |
| 42:Lh:105:LYS:HE2 | 42:Lh:105:LYS:HB3   | 1.76                     | 0.41              |
| 51:S1:43:A:O2'    | 51:S1:97:C:OP1      | 2.35                     | 0.41              |
| 51:S1:1166:C:H2'  | 51:S1:1167:A:C8     | 2.55                     | 0.41              |
| 51:S1:1715:C:O2'  | 77:SX:154:ARG:NH1   | 2.52                     | 0.41              |
| 51:S1:1873:A:H5'  | 51:S1:1875:G:O4'    | 2.20                     | 0.41              |
| 51:S1:2058:G:H2'  | 51:S1:2059:OMC:O4'  | 2.21                     | 0.41              |
| 53:S3:7:G:OP1     | 53:S3:16:C:N4       | 2.38                     | 0.41              |
| 76:SW:81:LYS:HB3  | 76:SW:81:LYS:HE2    | 1.81                     | 0.41              |
| 79:SZ:119:ASN:HA  | 79:SZ:122:LYS:HE3   | 2.02                     | 0.41              |
| 1:L1:12:U:H2'     | 1:L1:13:G:H8        | 1.85                     | 0.41              |
| 1:L1:540:A:N6     | 26:LR:68:ASP:O      | 2.47                     | 0.41              |
| 1:L1:895:G:N7     | 94:L1:1978:PAR:H221 | 2.36                     | 0.41              |
| 1:L1:954:U:H2'    | 1:L1:955:A2M:H8     | 2.02                     | 0.41              |
| 1:L1:1549:U:H2'   | 1:L1:1550:A:C8      | 2.55                     | 0.41              |
| 1:L1:1554:G:N1    | 1:L1:1557:A:OP1     | 2.53                     | 0.41              |
| 2:L2:958:A:H2'    | 2:L2:959:A:C8       | 2.55                     | 0.41              |
| 5:L5:19:C:O2'     | 28:LT:69:ARG:O      | 2.32                     | 0.41              |
| 7:L7:70:C:H5''    | 31:LW:25:ARG:CZ     | 2.51                     | 0.41              |
| 11:LC:369:LYS:HE2 | 11:LC:369:LYS:HB3   | 1.86                     | 0.41              |
| 12:LD:84:LYS:HZ3  | 12:LD:84:LYS:HG3    | 1.80                     | 0.41              |
| 16:LH:30:LYS:HG2  | 16:LH:31:ASP:OD2    | 2.21                     | 0.41              |
| 17:LI:13:GLN:HE21 | 17:LI:13:GLN:HB2    | 1.67                     | 0.41              |
| 20:LL:51:GLY:N    | 24:LP:182:ARG:O     | 2.48                     | 0.41              |
| 22:LN:12:CYS:SG   | 22:LN:59:GLN:HG3    | 2.61                     | 0.41              |
| 34:LZ:30:ASP:HB3  | 34:LZ:33:ASN:HB2    | 2.03                     | 0.41              |
| 51:S1:889:A:C2    | 58:SE:16:MET:HG2    | 2.56                     | 0.41              |
| 57:SD:87:GLU:CD   | 57:SD:87:GLU:N      | 2.78                     | 0.41              |
| 64:SK:172:GLU:HG3 | 64:SK:175:ILE:HD13  | 2.02                     | 0.41              |
| 75:SV:88:THR:HG23 | 75:SV:93:LYS:NZ     | 2.36                     | 0.41              |
| 87:Sh:81:VAL:HG12 | 87:Sh:82:LYS:HG3    | 2.03                     | 0.41              |
| 3:L3:71:U:H5      | 3:L3:150:A:N7       | 2.18                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:L3:151:A:H5'     | 45:Lk:26:LYS:HE2    | 2.02                     | 0.41              |
| 7:L7:68:A:H2'      | 7:L7:69:PSU:O4'     | 2.20                     | 0.41              |
| 15:LG:166:TRP:CD1  | 15:LG:166:TRP:H     | 2.38                     | 0.41              |
| 17:LI:94:TYR:O     | 17:LI:97:THR:OG1    | 2.37                     | 0.41              |
| 19:LK:148:LEU:HD12 | 19:LK:148:LEU:HA    | 1.85                     | 0.41              |
| 29:LU:88:LYS:HE2   | 29:LU:88:LYS:HB3    | 1.91                     | 0.41              |
| 38:Ld:102:ILE:HD12 | 38:Ld:102:ILE:HA    | 1.84                     | 0.41              |
| 51:S1:275:A:O2'    | 51:S1:276:G:H8      | 2.03                     | 0.41              |
| 51:S1:818:U:O2     | 87:Sh:67:VAL:HG22   | 2.20                     | 0.41              |
| 52:S4:24:G:H2'     | 52:S4:25:A:H8       | 1.86                     | 0.41              |
| 56:SC:44:ARG:HG3   | 56:SC:46:GLU:HG3    | 2.02                     | 0.41              |
| 62:SI:61:VAL:HG22  | 62:SI:93:LEU:HB2    | 2.02                     | 0.41              |
| 65:SL:107:GLU:C    | 65:SL:109:ALA:H     | 2.29                     | 0.41              |
| 68:SO:27:PHE:HB3   | 68:SO:34:PHE:HB2    | 2.02                     | 0.41              |
| 79:SZ:10:VAL:HG13  | 79:SZ:32:VAL:HG13   | 2.02                     | 0.41              |
| 82:Sc:39:PRO:HG3   | 82:Sc:78:CYS:N      | 2.36                     | 0.41              |
| 83:Sd:72:MET:HE3   | 83:Sd:72:MET:HB2    | 1.95                     | 0.41              |
| 1:L1:601:G:N1      | 1:L1:605:G:O6       | 2.53                     | 0.41              |
| 1:L1:1687:G:H2'    | 1:L1:1688:G:C8      | 2.55                     | 0.41              |
| 29:LU:29:ASP:HA    | 29:LU:76:VAL:HG12   | 2.02                     | 0.41              |
| 33:LY:123:GLY:HA2  | 33:LY:126:MET:HE3   | 2.02                     | 0.41              |
| 35:La:49:ARG:HB3   | 35:La:50:PRO:HD3    | 2.02                     | 0.41              |
| 51:S1:1605:U:O4'   | 85:Sf:141:GLY:HA3   | 2.21                     | 0.41              |
| 51:S1:1662:OMU:H1' | 51:S1:1662:OMU:HM23 | 1.63                     | 0.41              |
| 55:SB:58:TRP:O     | 55:SB:62:ILE:HG12   | 2.20                     | 0.41              |
| 56:SC:65:ILE:HD12  | 56:SC:65:ILE:HA     | 1.83                     | 0.41              |
| 61:SH:153:LYS:HG2  | 61:SH:158:CYS:SG    | 2.61                     | 0.41              |
| 65:SL:99:PHE:O     | 65:SL:103:HIS:HB2   | 2.20                     | 0.41              |
| 68:SO:75:VAL:HG21  | 68:SO:115:ALA:HB3   | 2.02                     | 0.41              |
| 85:Sf:74:LYS:HE2   | 85:Sf:74:LYS:HB3    | 1.89                     | 0.41              |
| 87:Sh:149:THR:O    | 87:Sh:153:VAL:HG23  | 2.21                     | 0.41              |
| 1:L1:719:U:OP2     | 17:LI:41:ARG:NH1    | 2.49                     | 0.41              |
| 1:L1:791:C:OP2     | 37:Lc:38:LYS:HD3    | 2.21                     | 0.41              |
| 1:L1:1240:U:OP1    | 26:LR:159:LYS:NZ    | 2.38                     | 0.41              |
| 1:L1:1252:C:O3'    | 1:L1:1253:OMU:H6    | 2.21                     | 0.41              |
| 2:L2:95:A2M:O5'    | 2:L2:95:A2M:H8      | 2.21                     | 0.41              |
| 2:L2:443:OMC:N4    | 2:L2:488:A:O5'      | 2.48                     | 0.41              |
| 2:L2:1254:G:O4'    | 2:L2:1308:5MC:HM52  | 2.20                     | 0.41              |
| 2:L2:1340:A:OP1    | 13:LE:169:LYS:NZ    | 2.50                     | 0.41              |
| 16:LH:31:ASP:HA    | 16:LH:60:ASN:OD1    | 2.21                     | 0.41              |
| 21:LM:47:LYS:HA    | 21:LM:47:LYS:HD2    | 1.94                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 22:LN:166:VAL:HG21  | 27:LS:159:TYR:CD1  | 2.56                     | 0.41              |
| 23:LO:41:LYS:NZ     | 27:LS:30:ILE:O     | 2.54                     | 0.41              |
| 34:LZ:46:LEU:HD12   | 34:LZ:46:LEU:HA    | 1.87                     | 0.41              |
| 51:S1:1597:G:N1     | 51:S1:1601:U:O4    | 2.53                     | 0.41              |
| 51:S1:2008:OMG:HM23 | 51:S1:2008:OMG:H1' | 1.81                     | 0.41              |
| 60:SG:214:ARG:HG3   | 60:SG:214:ARG:NH1  | 2.35                     | 0.41              |
| 62:SI:196:GLN:HG3   | 82:Sc:13:VAL:HG22  | 2.03                     | 0.41              |
| 71:SR:120:ALA:O     | 71:SR:124:VAL:HG23 | 2.20                     | 0.41              |
| 86:Sg:196:TYR:CZ    | 86:Sg:214:LYS:HB2  | 2.56                     | 0.41              |
| 86:Sg:261:TYR:CE2   | 86:Sg:268:VAL:HG22 | 2.55                     | 0.41              |
| 1:L1:23:U:H4'       | 1:L1:24:A:N7       | 2.36                     | 0.41              |
| 1:L1:205:A:N6       | 34:LZ:55:PRO:HG3   | 2.36                     | 0.41              |
| 1:L1:346:U:H1'      | 2:L2:468:A:N3      | 2.35                     | 0.41              |
| 1:L1:669:OMC:HM23   | 1:L1:678:A2M:H4'   | 2.03                     | 0.41              |
| 1:L1:828:U:O5'      | 2:L2:1148:G:H4'    | 2.21                     | 0.41              |
| 1:L1:1161:A:N6      | 24:LP:13:ARG:HD2   | 2.35                     | 0.41              |
| 1:L1:1190:OMG:HM22  | 1:L1:1191:G:H5'    | 2.03                     | 0.41              |
| 1:L1:1524:OMG:H8    | 1:L1:1524:OMG:H2'  | 1.41                     | 0.41              |
| 2:L2:339:A:H1'      | 2:L2:341:A:H2'     | 2.03                     | 0.41              |
| 2:L2:340:A:H4'      | 2:L2:341:A:H5'     | 2.02                     | 0.41              |
| 2:L2:591:A2M:H8     | 2:L2:591:A2M:O5'   | 2.20                     | 0.41              |
| 2:L2:598:A:H5''     | 28:LT:83:TRP:O     | 2.20                     | 0.41              |
| 2:L2:775:C:H1'      | 2:L2:811:U:C4      | 2.56                     | 0.41              |
| 2:L2:1248:OMC:H1'   | 2:L2:1248:OMC:HM23 | 1.77                     | 0.41              |
| 5:L5:112:U:H6       | 5:L5:112:U:H2'     | 1.66                     | 0.41              |
| 9:LA:40:TYR:HA      | 9:LA:91:GLY:HA3    | 2.03                     | 0.41              |
| 10:LB:124:GLN:O     | 39:Le:3:ARG:HD3    | 2.21                     | 0.41              |
| 13:LE:109:ILE:HD11  | 13:LE:131:VAL:HG21 | 2.03                     | 0.41              |
| 13:LE:111:VAL:HB    | 13:LE:121:ARG:HB2  | 2.02                     | 0.41              |
| 17:LI:137:LYS:HB3   | 17:LI:137:LYS:HE2  | 1.57                     | 0.41              |
| 22:LN:54:SER:HB2    | 22:LN:135:LEU:HD11 | 2.02                     | 0.41              |
| 23:LO:107:ARG:NH2   | 23:LO:119:PHE:O    | 2.54                     | 0.41              |
| 29:LU:23:LYS:HB3    | 29:LU:23:LYS:HE2   | 1.82                     | 0.41              |
| 29:LU:120:LYS:HE3   | 29:LU:120:LYS:HB3  | 1.68                     | 0.41              |
| 31:LW:77:ILE:HG23   | 31:LW:98:PRO:HG3   | 2.02                     | 0.41              |
| 38:Ld:53:ILE:HD12   | 38:Ld:53:ILE:HA    | 1.93                     | 0.41              |
| 50:Lp:22:SER:O      | 50:Lp:75:SER:OG    | 2.39                     | 0.41              |
| 51:S1:447:G:H4'     | 60:SG:91:TYR:HE2   | 1.86                     | 0.41              |
| 51:S1:498:C:H4'     | 58:SE:60:MET:HE2   | 2.02                     | 0.41              |
| 51:S1:695:G:H22     | 51:S1:750:U:H3     | 1.68                     | 0.41              |
| 51:S1:784:C:H3'     | 51:S1:787:G:H1     | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:S1:1014:C:H2'   | 51:S1:1015:G:C8    | 2.56                     | 0.41              |
| 51:S1:1588:A:H2'   | 51:S1:1589:G:C8    | 2.56                     | 0.41              |
| 51:S1:1615:G:H2'   | 51:S1:1616:A:O4'   | 2.21                     | 0.41              |
| 51:S1:1983:U:H2'   | 51:S1:1984:C:C6    | 2.56                     | 0.41              |
| 51:S1:2008:OMG:O6  | 89:S1:2447:SPD:H21 | 2.21                     | 0.41              |
| 52:S4:17:A:H2'     | 52:S4:18:G:H8      | 1.85                     | 0.41              |
| 56:SC:41:THR:HG23  | 56:SC:44:ARG:H     | 1.85                     | 0.41              |
| 56:SC:79:LYS:HB2   | 56:SC:82:LYS:HG3   | 2.03                     | 0.41              |
| 62:SI:86:GLU:HG3   | 62:SI:94:VAL:HG23  | 2.02                     | 0.41              |
| 75:SV:76:GLU:O     | 75:SV:80:ARG:HG3   | 2.21                     | 0.41              |
| 75:SV:76:GLU:HA    | 75:SV:79:GLU:HG3   | 2.02                     | 0.41              |
| 80:Sa:26:LYS:HA    | 80:Sa:26:LYS:HD3   | 1.84                     | 0.41              |
| 86:Sg:22:GLN:H     | 86:Sg:22:GLN:HG2   | 1.66                     | 0.41              |
| 1:L1:19:G:OP2      | 1:L1:19:G:N2       | 2.48                     | 0.41              |
| 1:L1:522:G:H8      | 1:L1:522:G:OP2     | 2.04                     | 0.41              |
| 2:L2:976:A:OP2     | 2:L2:976:A:H8      | 2.04                     | 0.41              |
| 2:L2:1287:C:O2'    | 2:L2:1288:G:O5'    | 2.39                     | 0.41              |
| 11:LC:182:VAL:HG11 | 11:LC:224:GLY:HA2  | 2.02                     | 0.41              |
| 51:S1:328:C:H2'    | 51:S1:329:C:C6     | 2.56                     | 0.41              |
| 51:S1:743:A:O2'    | 51:S1:744:G:OP1    | 2.32                     | 0.41              |
| 51:S1:2135:U:H2'   | 51:S1:2136:A:C8    | 2.55                     | 0.41              |
| 52:S4:13:C:H4'     | 52:S4:14:A:OP1     | 2.21                     | 0.41              |
| 67:SN:63:LYS:HB3   | 67:SN:63:LYS:HE3   | 1.75                     | 0.41              |
| 74:SU:73:CYS:O     | 74:SU:77:SER:OG    | 2.31                     | 0.41              |
| 1:L1:415:A:O2'     | 1:L1:417:G:H5'     | 2.20                     | 0.40              |
| 1:L1:1090:U:H2'    | 1:L1:1091:A:C8     | 2.57                     | 0.40              |
| 1:L1:1198:C:H2'    | 1:L1:1199:G:O4'    | 2.22                     | 0.40              |
| 1:L1:1374:C:H2'    | 1:L1:1375:G:O4'    | 2.22                     | 0.40              |
| 1:L1:1390:G:O2'    | 19:LK:50:VAL:N     | 2.45                     | 0.40              |
| 1:L1:1574:C:H2'    | 1:L1:1575:G:H8     | 1.86                     | 0.40              |
| 2:L2:1250:C:H2'    | 2:L2:1251:A:H8     | 1.86                     | 0.40              |
| 2:L2:1275:A:N7     | 89:L2:1602:SPD:H81 | 2.35                     | 0.40              |
| 2:L2:1505:A:H2'    | 2:L2:1506:G:C8     | 2.56                     | 0.40              |
| 23:LO:248:MET:HE3  | 23:LO:248:MET:HB3  | 1.72                     | 0.40              |
| 24:LP:67:ILE:O     | 24:LP:71:MET:HG2   | 2.21                     | 0.40              |
| 51:S1:163:A:H2'    | 51:S1:165:G:O4'    | 2.21                     | 0.40              |
| 51:S1:447:G:H5''   | 89:S1:2302:SPD:HN6 | 1.86                     | 0.40              |
| 51:S1:1796:U:H2'   | 51:S1:1797:A:O4'   | 2.21                     | 0.40              |
| 52:S4:33:C:O2'     | 61:SH:184:ARG:NH2  | 2.54                     | 0.40              |
| 54:SA:139:LEU:HG   | 54:SA:174:ILE:HG21 | 2.03                     | 0.40              |
| 57:SD:112:VAL:HG13 | 57:SD:117:LEU:HB2  | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:Sg:158:PHE:CE1  | 86:Sg:181:VAL:HG11 | 2.57                     | 0.40              |
| 87:Sh:110:GLU:H    | 87:Sh:119:LEU:HD13 | 1.86                     | 0.40              |
| 1:L1:305:A2M:H5''  | 21:LM:47:LYS:NZ    | 2.37                     | 0.40              |
| 1:L1:357:A:N7      | 89:L1:1811:SPD:N10 | 2.62                     | 0.40              |
| 1:L1:681:A2M:HM'2  | 1:L1:682:C:O4'     | 2.22                     | 0.40              |
| 1:L1:830:G:OP1     | 24:LP:192:ARG:NH2  | 2.55                     | 0.40              |
| 1:L1:1442:G:H3'    | 1:L1:1464:G:N2     | 2.35                     | 0.40              |
| 1:L1:1452:C:H2'    | 1:L1:1453:G:C8     | 2.57                     | 0.40              |
| 1:L1:1749:G:H2'    | 1:L1:1751:A:N7     | 2.35                     | 0.40              |
| 2:L2:1416:U:O2'    | 2:L2:1417:U:H5'    | 2.21                     | 0.40              |
| 3:L3:129:A:C6      | 49:Lo:42:CYS:HA    | 2.57                     | 0.40              |
| 5:L5:86:G:H8       | 5:L5:86:G:OP2      | 2.04                     | 0.40              |
| 11:LC:59:MET:HE3   | 11:LC:59:MET:HB3   | 1.97                     | 0.40              |
| 17:LI:123:THR:O    | 17:LI:127:LYS:HG2  | 2.20                     | 0.40              |
| 23:LO:106:ALA:O    | 23:LO:110:LEU:HG   | 2.21                     | 0.40              |
| 25:LQ:66:MET:SD    | 25:LQ:70:LYS:HE3   | 2.62                     | 0.40              |
| 25:LQ:84:SER:O     | 25:LQ:88:ARG:HG3   | 2.21                     | 0.40              |
| 50:Lp:46:LYS:HE3   | 50:Lp:54:THR:HB    | 2.02                     | 0.40              |
| 62:SI:143:TRP:HZ3  | 63:SJ:54:ASP:HB2   | 1.85                     | 0.40              |
| 71:SR:6:ILE:HA     | 80:Sa:41:MET:HE2   | 2.03                     | 0.40              |
| 1:L1:447:G:OP1     | 1:L1:1505:U:O2'    | 2.39                     | 0.40              |
| 1:L1:1245:G:N3     | 26:LR:114:SER:HB2  | 2.35                     | 0.40              |
| 1:L1:1493:G:O6     | 40:Lf:17:ARG:NH1   | 2.54                     | 0.40              |
| 1:L1:1552:OMC:HM23 | 1:L1:1552:OMC:H1'  | 1.64                     | 0.40              |
| 2:L2:616:G:OP2     | 2:L2:616:G:H8      | 2.04                     | 0.40              |
| 4:L4:8:U:H4'       | 28:LT:7:LYS:HG2    | 2.03                     | 0.40              |
| 10:LB:36:ASP:O     | 10:LB:190:GLY:HA2  | 2.21                     | 0.40              |
| 15:LG:65:VAL:O     | 15:LG:69:ARG:HG2   | 2.22                     | 0.40              |
| 34:LZ:28:SER:N     | 34:LZ:36:GLY:O     | 2.55                     | 0.40              |
| 34:LZ:93:SER:HB2   | 34:LZ:108:PHE:HB2  | 2.04                     | 0.40              |
| 37:Lc:241:ASP:OD2  | 37:Lc:242:THR:HG23 | 2.21                     | 0.40              |
| 50:Lp:74:CYS:CB    | 50:Lp:77:CYS:HB2   | 2.51                     | 0.40              |
| 51:S1:70:U:OP1     | 60:SG:167:LYS:NZ   | 2.34                     | 0.40              |
| 56:SC:26:ARG:HD2   | 67:SN:67:ALA:HB2   | 2.03                     | 0.40              |
| 56:SC:172:ARG:HD3  | 56:SC:172:ARG:HA   | 1.95                     | 0.40              |
| 57:SD:12:LYS:HE3   | 57:SD:12:LYS:HB3   | 1.86                     | 0.40              |
| 64:SK:157:LYS:HE2  | 64:SK:157:LYS:HB3  | 1.87                     | 0.40              |
| 1:L1:36:U:H4'      | 20:LL:32:ARG:HD2   | 2.04                     | 0.40              |
| 1:L1:170:U:H1'     | 1:L1:171:U:OP2     | 2.21                     | 0.40              |
| 1:L1:836:G:H1      | 24:LP:96:ASP:HA    | 1.86                     | 0.40              |
| 1:L1:1214:G:H2'    | 1:L1:1215:C:O4'    | 2.22                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:L1:1232:U:H1'    | 16:LH:105:MET:HG2   | 2.04                     | 0.40              |
| 3:L3:45:U:OP1      | 42:Lh:25:ARG:NH2    | 2.47                     | 0.40              |
| 17:LI:210:LYS:O    | 17:LI:214:LYS:HG2   | 2.22                     | 0.40              |
| 18:LJ:12:ARG:HG2   | 18:LJ:13:PHE:O      | 2.21                     | 0.40              |
| 20:LL:64:LYS:HB2   | 20:LL:64:LYS:HE3    | 1.91                     | 0.40              |
| 27:LS:123:LYS:HE2  | 27:LS:123:LYS:HB2   | 1.88                     | 0.40              |
| 37:Lc:124:THR:HB   | 37:Lc:215:PHE:HB2   | 2.02                     | 0.40              |
| 39:Le:46:ASP:O     | 39:Le:50:ARG:HB2    | 2.22                     | 0.40              |
| 51:S1:154:C:OP1    | 79:SZ:127:LYS:HB2   | 2.22                     | 0.40              |
| 51:S1:275:A:O2'    | 51:S1:276:G:H5'     | 2.20                     | 0.40              |
| 51:S1:556:A:H5''   | 57:SD:172:LYS:HE3   | 2.03                     | 0.40              |
| 51:S1:823:G:N7     | 87:Sh:86:ARG:NH2    | 2.69                     | 0.40              |
| 51:S1:877:U:H3     | 51:S1:884:A:H62     | 1.70                     | 0.40              |
| 51:S1:1272:A:H2'   | 51:S1:1274:A:H5''   | 2.03                     | 0.40              |
| 57:SD:96:LEU:HB3   | 59:SF:186:ARG:O     | 2.21                     | 0.40              |
| 68:SO:129:PRO:HB2  | 68:SO:131:ASP:O     | 2.20                     | 0.40              |
| 77:SX:127:GLU:HG2  | 77:SX:137:THR:HG22  | 2.03                     | 0.40              |
| 80:Sa:58:LYS:HG3   | 80:Sa:103:ARG:NH2   | 2.37                     | 0.40              |
| 1:L1:438:A:H4'     | 1:L1:439:U:H3'      | 2.03                     | 0.40              |
| 13:LE:162:GLN:O    | 13:LE:165:LEU:HG    | 2.21                     | 0.40              |
| 24:LP:74:LYS:O     | 24:LP:78:THR:OG1    | 2.33                     | 0.40              |
| 24:LP:145:LEU:HD12 | 24:LP:145:LEU:HA    | 1.94                     | 0.40              |
| 24:LP:178:LYS:HG3  | 24:LP:179:GLU:N     | 2.36                     | 0.40              |
| 33:LY:54:VAL:H     | 33:LY:57:MET:HE2    | 1.87                     | 0.40              |
| 48:Ln:28:ARG:HG3   | 48:Ln:28:ARG:HH11   | 1.87                     | 0.40              |
| 51:S1:2026:U:C4    | 89:S1:2447:SPD:H71  | 2.56                     | 0.40              |
| 51:S1:2140:OMC:H1' | 51:S1:2140:OMC:HM23 | 1.86                     | 0.40              |
| 55:SB:92:LYS:HB3   | 55:SB:92:LYS:HE2    | 1.96                     | 0.40              |
| 69:SP:51:VAL:HG13  | 69:SP:70:VAL:HB     | 2.03                     | 0.40              |
| 77:SX:89:SER:HB2   | 77:SX:108:SER:O     | 2.21                     | 0.40              |
| 86:Sg:118:ASP:OD1  | 86:Sg:118:ASP:N     | 2.43                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 9   | LA    | 257/260 (99%) | 248 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 10  | LB    | 402/419 (96%) | 398 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 11  | LC    | 364/373 (98%) | 355 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 12  | LD    | 173/188 (92%) | 171 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 13  | LE    | 184/190 (97%) | 178 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 14  | LF    | 147/195 (75%) | 141 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 15  | LG    | 240/264 (91%) | 237 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 16  | LH    | 219/222 (99%) | 217 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 17  | LI    | 212/220 (96%) | 207 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 18  | LJ    | 133/139 (96%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 19  | LK    | 167/175 (95%) | 161 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 20  | LL    | 142/145 (98%) | 137 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 21  | LM    | 201/204 (98%) | 198 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 22  | LN    | 196/213 (92%) | 189 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 23  | LO    | 295/305 (97%) | 292 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 24  | LP    | 195/198 (98%) | 190 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 25  | LQ    | 200/254 (79%) | 200 (100%) | 0       | 0        | 100         | 100 |
| 26  | LR    | 176/179 (98%) | 174 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 27  | LS    | 156/159 (98%) | 152 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 28  | LT    | 150/166 (90%) | 149 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 29  | LU    | 120/129 (93%) | 119 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 30  | LV    | 117/145 (81%) | 116 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 31  | LW    | 119/143 (83%) | 116 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 32  | LX    | 81/124 (65%)  | 78 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 33  | LY    | 131/134 (98%) | 130 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 34  | LZ    | 143/147 (97%) | 142 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 35  | La    | 123/127 (97%) | 120 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 36  | Lb    | 66/70 (94%)   | 66 (100%)  | 0       | 0        | 100         | 100 |
| 37  | Lc    | 227/252 (90%) | 222 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 38  | Ld    | 94/104 (90%)  | 94 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 39  | Le    | 184/188 (98%) | 183 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 40  | Lf    | 126/133 (95%) | 123 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 41  | Lg    | 142/144 (99%) | 140 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 42  | Lh    | 125/168 (74%) | 124 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 43  | Li    | 99/105 (94%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 44  | Lj    | 79/83 (95%)   | 78 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 45  | Lk    | 76/83 (92%)   | 76 (100%)  | 0       | 0        | 100         | 100 |
| 46  | Ll    | 48/51 (94%)   | 47 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 47  | Lm    | 50/128 (39%)  | 50 (100%)  | 0       | 0        | 100         | 100 |
| 48  | Ln    | 31/34 (91%)   | 31 (100%)  | 0       | 0        | 100         | 100 |
| 49  | Lo    | 87/92 (95%)   | 82 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 50  | Lp    | 95/106 (90%)  | 94 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 54  | SA    | 234/264 (89%) | 229 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 55  | SB    | 209/246 (85%) | 205 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 56  | SC    | 211/219 (96%) | 208 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 57  | SD    | 181/190 (95%) | 180 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 58  | SE    | 258/273 (94%) | 255 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 59  | SF    | 220/265 (83%) | 218 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 60  | SG    | 232/249 (93%) | 229 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 61  | SH    | 179/190 (94%) | 176 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 62  | SI    | 198/200 (99%) | 192 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 63  | SJ    | 127/130 (98%) | 123 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 64  | SK    | 193/220 (88%) | 191 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 65  | SL    | 142/149 (95%) | 139 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 66  | SM    | 101/116 (87%) | 99 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 67  | SN    | 105/168 (62%) | 103 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 68  | SO    | 135/144 (94%) | 131 (97%)  | 3 (2%)  | 1 (1%)   | 18          | 17  |
| 69  | SP    | 139/143 (97%) | 138 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 70  | SQ    | 91/141 (64%)  | 89 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 71  | SR    | 140/153 (92%) | 137 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 72  | SS    | 54/57 (95%)   | 54 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 73  | ST    | 141/151 (93%)     | 137 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 74  | SU    | 151/173 (87%)     | 146 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 75  | SV    | 120/143 (84%)     | 119 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 76  | SW    | 113/152 (74%)     | 111 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 77  | SX    | 150/161 (93%)     | 146 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 78  | SY    | 87/164 (53%)      | 83 (95%)    | 4 (5%)   | 0        | 100         | 100 |
| 79  | SZ    | 128/137 (93%)     | 125 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 80  | Sa    | 81/120 (68%)      | 81 (100%)   | 0        | 0        | 100         | 100 |
| 81  | Sb    | 102/112 (91%)     | 99 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 82  | Sc    | 83/86 (96%)       | 83 (100%)   | 0        | 0        | 100         | 100 |
| 83  | Sd    | 64/87 (74%)       | 62 (97%)    | 2 (3%)   | 0        | 100         | 100 |
| 84  | Se    | 57/66 (86%)       | 56 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 85  | Sf    | 71/152 (47%)      | 68 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 86  | Sg    | 297/312 (95%)     | 284 (96%)   | 13 (4%)  | 0        | 100         | 100 |
| 87  | Sh    | 167/235 (71%)     | 158 (95%)   | 9 (5%)   | 0        | 100         | 100 |
| All | All   | 11533/12926 (89%) | 11308 (98%) | 224 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | SO    | 131 | ASP  |

### 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 |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 9   | LA    | 201/204 (98%) | 200 (100%) | 1 (0%)   | 81          | 87 |
| 10  | LB    | 337/351 (96%) | 335 (99%)  | 2 (1%)   | 78          | 84 |
| 11  | LC    | 293/301 (97%) | 287 (98%)  | 6 (2%)   | 48          | 59 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 12  | LD    | 148/162 (91%)  | 142 (96%)  | 6 (4%)   | 27          | 33  |
| 13  | LE    | 166/172 (96%)  | 159 (96%)  | 7 (4%)   | 26          | 31  |
| 14  | LF    | 124/153 (81%)  | 122 (98%)  | 2 (2%)   | 55          | 66  |
| 15  | LG    | 193/221 (87%)  | 191 (99%)  | 2 (1%)   | 68          | 77  |
| 16  | LH    | 182/188 (97%)  | 181 (100%) | 1 (0%)   | 81          | 87  |
| 17  | LI    | 178/183 (97%)  | 177 (99%)  | 1 (1%)   | 78          | 84  |
| 18  | LJ    | 106/111 (96%)  | 104 (98%)  | 2 (2%)   | 50          | 61  |
| 19  | LK    | 136/145 (94%)  | 131 (96%)  | 5 (4%)   | 30          | 37  |
| 20  | LL    | 113/114 (99%)  | 112 (99%)  | 1 (1%)   | 70          | 79  |
| 21  | LM    | 178/180 (99%)  | 177 (99%)  | 1 (1%)   | 78          | 84  |
| 22  | LN    | 170/179 (95%)  | 168 (99%)  | 2 (1%)   | 63          | 74  |
| 23  | LO    | 233/242 (96%)  | 227 (97%)  | 6 (3%)   | 40          | 50  |
| 24  | LP    | 163/164 (99%)  | 162 (99%)  | 1 (1%)   | 78          | 84  |
| 25  | LQ    | 171/198 (86%)  | 170 (99%)  | 1 (1%)   | 78          | 84  |
| 26  | LR    | 157/159 (99%)  | 154 (98%)  | 3 (2%)   | 50          | 61  |
| 27  | LS    | 132/134 (98%)  | 132 (100%) | 0        | 100         | 100 |
| 28  | LT    | 129/143 (90%)  | 128 (99%)  | 1 (1%)   | 73          | 80  |
| 29  | LU    | 93/114 (82%)   | 92 (99%)   | 1 (1%)   | 65          | 75  |
| 30  | LV    | 102/124 (82%)  | 101 (99%)  | 1 (1%)   | 68          | 77  |
| 31  | LW    | 104/122 (85%)  | 103 (99%)  | 1 (1%)   | 68          | 77  |
| 32  | LX    | 74/104 (71%)   | 73 (99%)   | 1 (1%)   | 59          | 70  |
| 33  | LY    | 110/116 (95%)  | 108 (98%)  | 2 (2%)   | 51          | 63  |
| 34  | LZ    | 114/118 (97%)  | 112 (98%)  | 2 (2%)   | 51          | 63  |
| 35  | La    | 114/118 (97%)  | 111 (97%)  | 3 (3%)   | 40          | 50  |
| 36  | Lb    | 56/58 (97%)    | 53 (95%)   | 3 (5%)   | 20          | 21  |
| 37  | Lc    | 191/209 (91%)  | 191 (100%) | 0        | 100         | 100 |
| 38  | Ld    | 82/89 (92%)    | 78 (95%)   | 4 (5%)   | 22          | 24  |
| 39  | Le    | 154/158 (98%)  | 151 (98%)  | 3 (2%)   | 50          | 61  |
| 40  | Lf    | 111/115 (96%)  | 111 (100%) | 0        | 100         | 100 |
| 41  | Lg    | 121/121 (100%) | 118 (98%)  | 3 (2%)   | 42          | 52  |
| 42  | Lh    | 107/146 (73%)  | 104 (97%)  | 3 (3%)   | 38          | 48  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 43  | Li    | 82/88 (93%)   | 81 (99%)   | 1 (1%)   | 63          | 74  |
| 44  | Lj    | 67/70 (96%)   | 67 (100%)  | 0        | 100         | 100 |
| 45  | Lk    | 65/74 (88%)   | 65 (100%)  | 0        | 100         | 100 |
| 46  | Ll    | 46/47 (98%)   | 45 (98%)   | 1 (2%)   | 45          | 56  |
| 47  | Lm    | 42/113 (37%)  | 41 (98%)   | 1 (2%)   | 43          | 54  |
| 48  | Ln    | 30/32 (94%)   | 29 (97%)   | 1 (3%)   | 33          | 42  |
| 49  | Lo    | 69/74 (93%)   | 68 (99%)   | 1 (1%)   | 59          | 70  |
| 50  | Lp    | 83/92 (90%)   | 81 (98%)   | 2 (2%)   | 43          | 54  |
| 54  | SA    | 205/222 (92%) | 202 (98%)  | 3 (2%)   | 57          | 68  |
| 55  | SB    | 179/202 (89%) | 177 (99%)  | 2 (1%)   | 65          | 75  |
| 56  | SC    | 176/184 (96%) | 170 (97%)  | 6 (3%)   | 32          | 40  |
| 57  | SD    | 159/164 (97%) | 156 (98%)  | 3 (2%)   | 50          | 61  |
| 58  | SE    | 216/225 (96%) | 214 (99%)  | 2 (1%)   | 70          | 79  |
| 59  | SF    | 182/208 (88%) | 179 (98%)  | 3 (2%)   | 55          | 66  |
| 60  | SG    | 194/208 (93%) | 191 (98%)  | 3 (2%)   | 57          | 68  |
| 61  | SH    | 152/159 (96%) | 152 (100%) | 0        | 100         | 100 |
| 62  | SI    | 181/186 (97%) | 180 (99%)  | 1 (1%)   | 78          | 84  |
| 63  | SJ    | 110/111 (99%) | 109 (99%)  | 1 (1%)   | 70          | 79  |
| 64  | SK    | 159/176 (90%) | 159 (100%) | 0        | 100         | 100 |
| 65  | SL    | 116/120 (97%) | 112 (97%)  | 4 (3%)   | 32          | 40  |
| 66  | SM    | 93/104 (89%)  | 92 (99%)   | 1 (1%)   | 65          | 75  |
| 67  | SN    | 95/128 (74%)  | 92 (97%)   | 3 (3%)   | 34          | 43  |
| 68  | SO    | 104/113 (92%) | 103 (99%)  | 1 (1%)   | 68          | 77  |
| 69  | SP    | 114/117 (97%) | 111 (97%)  | 3 (3%)   | 40          | 50  |
| 71  | SR    | 120/130 (92%) | 114 (95%)  | 6 (5%)   | 22          | 24  |
| 72  | SS    | 47/49 (96%)   | 45 (96%)   | 2 (4%)   | 26          | 31  |
| 73  | ST    | 126/132 (96%) | 125 (99%)  | 1 (1%)   | 73          | 80  |
| 74  | SU    | 136/152 (90%) | 134 (98%)  | 2 (2%)   | 57          | 68  |
| 75  | SV    | 109/126 (86%) | 107 (98%)  | 2 (2%)   | 51          | 63  |
| 76  | SW    | 98/130 (75%)  | 97 (99%)   | 1 (1%)   | 68          | 77  |
| 77  | SX    | 122/131 (93%) | 120 (98%)  | 2 (2%)   | 55          | 66  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 78  | SY    | 73/116 (63%)     | 69 (94%)   | 4 (6%)   | 19          | 20  |
| 79  | SZ    | 111/118 (94%)    | 107 (96%)  | 4 (4%)   | 31          | 39  |
| 80  | Sa    | 71/95 (75%)      | 70 (99%)   | 1 (1%)   | 59          | 70  |
| 81  | Sb    | 85/93 (91%)      | 82 (96%)   | 3 (4%)   | 32          | 39  |
| 82  | Sc    | 70/76 (92%)      | 69 (99%)   | 1 (1%)   | 59          | 70  |
| 83  | Sd    | 52/75 (69%)      | 52 (100%)  | 0        | 100         | 100 |
| 84  | Se    | 44/54 (82%)      | 43 (98%)   | 1 (2%)   | 44          | 55  |
| 85  | Sf    | 26/126 (21%)     | 25 (96%)   | 1 (4%)   | 29          | 36  |
| 86  | Sg    | 255/265 (96%)    | 248 (97%)  | 7 (3%)   | 39          | 49  |
| 87  | Sh    | 104/177 (59%)    | 100 (96%)  | 4 (4%)   | 29          | 36  |
| All | All   | 9611/10678 (90%) | 9448 (98%) | 163 (2%) | 52          | 65  |

All (163) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | LA    | 208 | GLU  |
| 10  | LB    | 120 | LYS  |
| 10  | LB    | 290 | ILE  |
| 11  | LC    | 13  | SER  |
| 11  | LC    | 15  | ASP  |
| 11  | LC    | 109 | ARG  |
| 11  | LC    | 124 | VAL  |
| 11  | LC    | 273 | LYS  |
| 11  | LC    | 285 | THR  |
| 12  | LD    | 44  | GLU  |
| 12  | LD    | 71  | CYS  |
| 12  | LD    | 81  | LEU  |
| 12  | LD    | 108 | ILE  |
| 12  | LD    | 122 | THR  |
| 12  | LD    | 168 | VAL  |
| 13  | LE    | 16  | VAL  |
| 13  | LE    | 28  | THR  |
| 13  | LE    | 81  | THR  |
| 13  | LE    | 130 | LYS  |
| 13  | LE    | 134 | THR  |
| 13  | LE    | 180 | VAL  |
| 13  | LE    | 182 | THR  |
| 14  | LF    | 84  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | LF    | 167 | LYS  |
| 15  | LG    | 148 | GLN  |
| 15  | LG    | 211 | THR  |
| 16  | LH    | 85  | THR  |
| 17  | LI    | 68  | VAL  |
| 18  | LJ    | 124 | SER  |
| 18  | LJ    | 133 | THR  |
| 19  | LK    | 4   | SER  |
| 19  | LK    | 66  | SER  |
| 19  | LK    | 72  | LYS  |
| 19  | LK    | 148 | LEU  |
| 19  | LK    | 156 | SER  |
| 20  | LL    | 132 | LYS  |
| 21  | LM    | 117 | ASN  |
| 22  | LN    | 189 | LYS  |
| 22  | LN    | 198 | LYS  |
| 23  | LO    | 66  | GLN  |
| 23  | LO    | 132 | VAL  |
| 23  | LO    | 233 | SER  |
| 23  | LO    | 244 | SER  |
| 23  | LO    | 273 | VAL  |
| 23  | LO    | 289 | ARG  |
| 24  | LP    | 57  | SER  |
| 25  | LQ    | 183 | LYS  |
| 26  | LR    | 2   | VAL  |
| 26  | LR    | 161 | THR  |
| 26  | LR    | 173 | THR  |
| 28  | LT    | 11  | SER  |
| 29  | LU    | 31  | SER  |
| 30  | LV    | 34  | GLN  |
| 31  | LW    | 101 | VAL  |
| 32  | LX    | 28  | SER  |
| 33  | LY    | 89  | MET  |
| 33  | LY    | 99  | VAL  |
| 34  | LZ    | 17  | ARG  |
| 34  | LZ    | 70  | SER  |
| 35  | La    | 43  | THR  |
| 35  | La    | 92  | THR  |
| 35  | La    | 109 | SER  |
| 36  | Lb    | 4   | SER  |
| 36  | Lb    | 13  | SER  |
| 36  | Lb    | 27  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | Ld    | 9   | VAL  |
| 38  | Ld    | 26  | VAL  |
| 38  | Ld    | 90  | CYS  |
| 38  | Ld    | 101 | ASP  |
| 39  | Le    | 14  | GLU  |
| 39  | Le    | 77  | THR  |
| 39  | Le    | 157 | THR  |
| 41  | Lg    | 38  | THR  |
| 41  | Lg    | 50  | THR  |
| 41  | Lg    | 75  | VAL  |
| 42  | Lh    | 3   | CYS  |
| 42  | Lh    | 10  | ARG  |
| 42  | Lh    | 116 | LEU  |
| 43  | Li    | 5   | THR  |
| 46  | Ll    | 31  | THR  |
| 47  | Lm    | 105 | VAL  |
| 48  | Ln    | 6   | ARG  |
| 49  | Lo    | 41  | PHE  |
| 50  | Lp    | 20  | HIS  |
| 50  | Lp    | 72  | LEU  |
| 54  | SA    | 40  | LYS  |
| 54  | SA    | 117 | ARG  |
| 54  | SA    | 133 | ASP  |
| 55  | SB    | 195 | SER  |
| 55  | SB    | 203 | ASP  |
| 56  | SC    | 39  | HIS  |
| 56  | SC    | 42  | THR  |
| 56  | SC    | 54  | THR  |
| 56  | SC    | 110 | SER  |
| 56  | SC    | 144 | GLN  |
| 56  | SC    | 148 | SER  |
| 57  | SD    | 54  | THR  |
| 57  | SD    | 60  | THR  |
| 57  | SD    | 150 | SER  |
| 58  | SE    | 158 | VAL  |
| 58  | SE    | 249 | GLU  |
| 59  | SF    | 210 | THR  |
| 59  | SF    | 244 | ASP  |
| 59  | SF    | 248 | SER  |
| 60  | SG    | 121 | ASP  |
| 60  | SG    | 129 | ASP  |
| 60  | SG    | 232 | HIS  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 62  | SI    | 167   | SER  |
| 63  | SJ    | 16    | SER  |
| 65  | SL    | 28    | THR  |
| 65  | SL    | 56    | GLU  |
| 65  | SL    | 75    | VAL  |
| 65  | SL    | 106   | VAL  |
| 66  | SM    | 88    | LEU  |
| 67  | SN    | 22    | VAL  |
| 67  | SN    | 36    | THR  |
| 67  | SN    | 44    | VAL  |
| 68  | SO    | 45    | THR  |
| 69  | SP    | 115   | ILE  |
| 69  | SP    | 119   | ARG  |
| 69  | SP    | 137   | LYS  |
| 71  | SR    | 6     | ILE  |
| 71  | SR    | 9     | HIS  |
| 71  | SR    | 32    | ARG  |
| 71  | SR    | 61    | THR  |
| 71  | SR    | 93    | THR  |
| 71  | SR    | 100   | SER  |
| 72  | SS    | 4     | LEU  |
| 72  | SS    | 9     | SER  |
| 73  | ST    | 87    | ASP  |
| 74  | SU    | 67    | LYS  |
| 74  | SU    | 71    | ARG  |
| 75  | SV    | 8     | THR  |
| 75  | SV    | 89    | SER  |
| 76  | SW    | 112   | VAL  |
| 77  | SX    | 49    | ILE  |
| 77  | SX    | 153   | ILE  |
| 78  | SY    | 32[A] | HIS  |
| 78  | SY    | 32[B] | HIS  |
| 78  | SY    | 55    | THR  |
| 78  | SY    | 56    | THR  |
| 79  | SZ    | 53    | LEU  |
| 79  | SZ    | 56    | VAL  |
| 79  | SZ    | 124   | LEU  |
| 79  | SZ    | 127   | LYS  |
| 80  | Sa    | 33    | ARG  |
| 81  | Sb    | 32    | THR  |
| 81  | Sb    | 88    | VAL  |
| 81  | Sb    | 97    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82  | Sc    | 3   | PHE  |
| 84  | Se    | 39  | LYS  |
| 85  | Sf    | 143 | CYS  |
| 86  | Sg    | 134 | TRP  |
| 86  | Sg    | 142 | HIS  |
| 86  | Sg    | 167 | VAL  |
| 86  | Sg    | 179 | TRP  |
| 86  | Sg    | 199 | THR  |
| 86  | Sg    | 225 | THR  |
| 86  | Sg    | 285 | ILE  |
| 87  | Sh    | 80  | VAL  |
| 87  | Sh    | 165 | LEU  |
| 87  | Sh    | 187 | VAL  |
| 87  | Sh    | 212 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | LA    | 38  | HIS  |
| 9   | LA    | 106 | GLN  |
| 9   | LA    | 205 | ASN  |
| 10  | LB    | 11  | HIS  |
| 10  | LB    | 109 | HIS  |
| 10  | LB    | 248 | HIS  |
| 11  | LC    | 40  | HIS  |
| 11  | LC    | 64  | HIS  |
| 11  | LC    | 145 | ASN  |
| 11  | LC    | 158 | GLN  |
| 11  | LC    | 212 | ASN  |
| 13  | LE    | 51  | ASN  |
| 13  | LE    | 108 | ASN  |
| 13  | LE    | 181 | GLN  |
| 14  | LF    | 154 | GLN  |
| 15  | LG    | 78  | GLN  |
| 15  | LG    | 169 | ASN  |
| 16  | LH    | 74  | GLN  |
| 16  | LH    | 187 | HIS  |
| 17  | LI    | 93  | GLN  |
| 18  | LJ    | 26  | ASN  |
| 18  | LJ    | 134 | HIS  |
| 19  | LK    | 68  | ASN  |
| 20  | LL    | 112 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | LN    | 73  | ASN  |
| 23  | LO    | 35  | GLN  |
| 23  | LO    | 90  | HIS  |
| 25  | LQ    | 34  | ASN  |
| 25  | LQ    | 143 | HIS  |
| 25  | LQ    | 176 | GLN  |
| 26  | LR    | 116 | HIS  |
| 26  | LR    | 121 | HIS  |
| 28  | LT    | 111 | GLN  |
| 30  | LV    | 51  | ASN  |
| 30  | LV    | 133 | HIS  |
| 31  | LW    | 83  | ASN  |
| 33  | LY    | 67  | GLN  |
| 34  | LZ    | 15  | ASN  |
| 34  | LZ    | 83  | HIS  |
| 35  | La    | 114 | GLN  |
| 36  | Lb    | 9   | ASN  |
| 37  | Lc    | 82  | HIS  |
| 37  | Lc    | 84  | ASN  |
| 37  | Lc    | 184 | ASN  |
| 39  | Le    | 44  | ASN  |
| 40  | Lf    | 21  | HIS  |
| 40  | Lf    | 89  | GLN  |
| 42  | Lh    | 123 | ASN  |
| 43  | Li    | 18  | HIS  |
| 43  | Li    | 26  | GLN  |
| 43  | Li    | 30  | ASN  |
| 48  | Ln    | 15  | HIS  |
| 49  | Lo    | 75  | ASN  |
| 50  | Lp    | 90  | HIS  |
| 54  | SA    | 103 | HIS  |
| 54  | SA    | 228 | GLN  |
| 56  | SC    | 73  | GLN  |
| 57  | SD    | 45  | ASN  |
| 58  | SE    | 240 | GLN  |
| 59  | SF    | 147 | ASN  |
| 60  | SG    | 86  | ASN  |
| 61  | SH    | 74  | GLN  |
| 62  | SI    | 99  | GLN  |
| 62  | SI    | 178 | GLN  |
| 62  | SI    | 196 | GLN  |
| 63  | SJ    | 9   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | SJ    | 56  | HIS  |
| 63  | SJ    | 120 | ASN  |
| 65  | SL    | 11  | GLN  |
| 65  | SL    | 76  | HIS  |
| 65  | SL    | 138 | HIS  |
| 67  | SN    | 70  | HIS  |
| 67  | SN    | 98  | GLN  |
| 72  | SS    | 38  | ASN  |
| 73  | ST    | 49  | GLN  |
| 74  | SU    | 24  | GLN  |
| 74  | SU    | 32  | ASN  |
| 74  | SU    | 40  | HIS  |
| 74  | SU    | 91  | HIS  |
| 74  | SU    | 104 | ASN  |
| 74  | SU    | 113 | GLN  |
| 75  | SV    | 110 | GLN  |
| 77  | SX    | 34  | HIS  |
| 77  | SX    | 114 | HIS  |
| 77  | SX    | 141 | HIS  |
| 79  | SZ    | 36  | HIS  |
| 81  | Sb    | 27  | ASN  |
| 82  | Sc    | 43  | GLN  |
| 86  | Sg    | 135 | ASN  |
| 87  | Sh    | 163 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | L1    | 1678/1782 (94%) | 320 (19%)         | 14 (0%)         |
| 2   | L2    | 1153/1526 (75%) | 207 (17%)         | 6 (0%)          |
| 3   | L3    | 178/216 (82%)   | 34 (19%)          | 2 (1%)          |
| 4   | L4    | 183/184 (99%)   | 31 (16%)          | 1 (0%)          |
| 5   | L5    | 118/135 (87%)   | 24 (20%)          | 0               |
| 51  | S1    | 1831/2204 (83%) | 354 (19%)         | 18 (0%)         |
| 52  | S2    | 13/76 (17%)     | 3 (23%)           | 1 (7%)          |
| 52  | S4    | 65/76 (85%)     | 24 (36%)          | 3 (4%)          |
| 53  | S3    | 73/77 (94%)     | 10 (13%)          | 0               |
| 6   | L6    | 69/73 (94%)     | 22 (31%)          | 0               |
| 7   | L7    | 164/171 (95%)   | 22 (13%)          | 3 (1%)          |
| 8   | L8    | 119/124 (95%)   | 11 (9%)           | 0               |
| 88  | S5    | 11/13 (84%)     | 3 (27%)           | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| All | All   | 5655/6657 (84%) | 1065 (18%)        | 48 (0%)         |

All (1065) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L1    | 16  | G    |
| 1   | L1    | 24  | A    |
| 1   | L1    | 32  | A    |
| 1   | L1    | 38  | A    |
| 1   | L1    | 41  | A    |
| 1   | L1    | 47  | C    |
| 1   | L1    | 58  | A    |
| 1   | L1    | 63  | A    |
| 1   | L1    | 64  | A    |
| 1   | L1    | 84  | G    |
| 1   | L1    | 86  | G    |
| 1   | L1    | 87  | A    |
| 1   | L1    | 91  | G    |
| 1   | L1    | 110 | A    |
| 1   | L1    | 134 | A    |
| 1   | L1    | 135 | A    |
| 1   | L1    | 136 | G    |
| 1   | L1    | 141 | U    |
| 1   | L1    | 142 | G    |
| 1   | L1    | 147 | G    |
| 1   | L1    | 156 | A    |
| 1   | L1    | 158 | A    |
| 1   | L1    | 160 | C    |
| 1   | L1    | 161 | A    |
| 1   | L1    | 162 | U    |
| 1   | L1    | 166 | G    |
| 1   | L1    | 170 | U    |
| 1   | L1    | 171 | U    |
| 1   | L1    | 176 | C    |
| 1   | L1    | 188 | A    |
| 1   | L1    | 191 | U    |
| 1   | L1    | 192 | C    |
| 1   | L1    | 195 | G    |
| 1   | L1    | 199 | A    |
| 1   | L1    | 201 | A    |
| 1   | L1    | 202 | G    |
| 1   | L1    | 205 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L1    | 206 | A    |
| 1   | L1    | 209 | C    |
| 1   | L1    | 210 | G    |
| 1   | L1    | 218 | A    |
| 1   | L1    | 223 | A    |
| 1   | L1    | 233 | U    |
| 1   | L1    | 234 | G    |
| 1   | L1    | 236 | G    |
| 1   | L1    | 237 | U    |
| 1   | L1    | 243 | G    |
| 1   | L1    | 251 | A    |
| 1   | L1    | 256 | U    |
| 1   | L1    | 273 | A    |
| 1   | L1    | 280 | A    |
| 1   | L1    | 281 | G    |
| 1   | L1    | 293 | C    |
| 1   | L1    | 294 | U    |
| 1   | L1    | 297 | A    |
| 1   | L1    | 299 | U    |
| 1   | L1    | 300 | A    |
| 1   | L1    | 301 | A    |
| 1   | L1    | 306 | G    |
| 1   | L1    | 322 | A    |
| 1   | L1    | 323 | U    |
| 1   | L1    | 332 | A    |
| 1   | L1    | 337 | G    |
| 1   | L1    | 342 | G    |
| 1   | L1    | 343 | U    |
| 1   | L1    | 344 | A    |
| 1   | L1    | 357 | A    |
| 1   | L1    | 367 | A    |
| 1   | L1    | 369 | A    |
| 1   | L1    | 374 | G    |
| 1   | L1    | 376 | A    |
| 1   | L1    | 383 | U    |
| 1   | L1    | 409 | U    |
| 1   | L1    | 410 | U    |
| 1   | L1    | 414 | A    |
| 1   | L1    | 415 | A    |
| 1   | L1    | 417 | G    |
| 1   | L1    | 439 | U    |
| 1   | L1    | 440 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L1    | 443 | A    |
| 1   | L1    | 444 | C    |
| 1   | L1    | 461 | G    |
| 1   | L1    | 463 | C    |
| 1   | L1    | 464 | A    |
| 1   | L1    | 471 | G    |
| 1   | L1    | 477 | C    |
| 1   | L1    | 488 | G    |
| 1   | L1    | 489 | C    |
| 1   | L1    | 494 | A    |
| 1   | L1    | 495 | C    |
| 1   | L1    | 500 | C    |
| 1   | L1    | 502 | U    |
| 1   | L1    | 503 | A    |
| 1   | L1    | 511 | A    |
| 1   | L1    | 522 | G    |
| 1   | L1    | 523 | A    |
| 1   | L1    | 525 | C    |
| 1   | L1    | 527 | A    |
| 1   | L1    | 539 | C    |
| 1   | L1    | 542 | C    |
| 1   | L1    | 544 | A    |
| 1   | L1    | 546 | G    |
| 1   | L1    | 547 | U    |
| 1   | L1    | 551 | A    |
| 1   | L1    | 553 | A    |
| 1   | L1    | 554 | A    |
| 1   | L1    | 555 | U    |
| 1   | L1    | 557 | U    |
| 1   | L1    | 563 | C    |
| 1   | L1    | 569 | G    |
| 1   | L1    | 571 | A    |
| 1   | L1    | 572 | A    |
| 1   | L1    | 573 | U    |
| 1   | L1    | 575 | A    |
| 1   | L1    | 585 | U    |
| 1   | L1    | 599 | G    |
| 1   | L1    | 605 | G    |
| 1   | L1    | 606 | C    |
| 1   | L1    | 611 | C    |
| 1   | L1    | 616 | U    |
| 1   | L1    | 620 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L1    | 621 | U    |
| 1   | L1    | 625 | C    |
| 1   | L1    | 631 | G    |
| 1   | L1    | 632 | A    |
| 1   | L1    | 635 | C    |
| 1   | L1    | 641 | G    |
| 1   | L1    | 648 | A    |
| 1   | L1    | 651 | G    |
| 1   | L1    | 652 | A    |
| 1   | L1    | 663 | C    |
| 1   | L1    | 668 | C    |
| 1   | L1    | 681 | A2M  |
| 1   | L1    | 692 | A    |
| 1   | L1    | 709 | A    |
| 1   | L1    | 710 | G    |
| 1   | L1    | 723 | G    |
| 1   | L1    | 729 | A    |
| 1   | L1    | 736 | C    |
| 1   | L1    | 737 | U    |
| 1   | L1    | 743 | A    |
| 1   | L1    | 750 | G    |
| 1   | L1    | 753 | A    |
| 1   | L1    | 762 | A    |
| 1   | L1    | 763 | U    |
| 1   | L1    | 769 | U    |
| 1   | L1    | 771 | U    |
| 1   | L1    | 778 | C    |
| 1   | L1    | 783 | G    |
| 1   | L1    | 790 | C    |
| 1   | L1    | 794 | U    |
| 1   | L1    | 795 | U    |
| 1   | L1    | 803 | C    |
| 1   | L1    | 810 | C    |
| 1   | L1    | 818 | C    |
| 1   | L1    | 822 | C    |
| 1   | L1    | 823 | G    |
| 1   | L1    | 828 | U    |
| 1   | L1    | 832 | G    |
| 1   | L1    | 836 | G    |
| 1   | L1    | 838 | G    |
| 1   | L1    | 850 | G    |
| 1   | L1    | 867 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L1    | 868  | A    |
| 1   | L1    | 895  | G    |
| 1   | L1    | 900  | C    |
| 1   | L1    | 912  | C    |
| 1   | L1    | 925  | U    |
| 1   | L1    | 930  | U    |
| 1   | L1    | 947  | A    |
| 1   | L1    | 959  | OMG  |
| 1   | L1    | 965  | A    |
| 1   | L1    | 967  | G    |
| 1   | L1    | 968  | A    |
| 1   | L1    | 972  | A    |
| 1   | L1    | 974  | C    |
| 1   | L1    | 975  | G    |
| 1   | L1    | 976  | A    |
| 1   | L1    | 988  | G    |
| 1   | L1    | 995  | C    |
| 1   | L1    | 1010 | OMC  |
| 1   | L1    | 1011 | PSU  |
| 1   | L1    | 1013 | A    |
| 1   | L1    | 1025 | G    |
| 1   | L1    | 1031 | A    |
| 1   | L1    | 1036 | U    |
| 1   | L1    | 1045 | G    |
| 1   | L1    | 1052 | A    |
| 1   | L1    | 1053 | A    |
| 1   | L1    | 1085 | C    |
| 1   | L1    | 1094 | C    |
| 1   | L1    | 1098 | A    |
| 1   | L1    | 1100 | C    |
| 1   | L1    | 1101 | U    |
| 1   | L1    | 1114 | A    |
| 1   | L1    | 1116 | A    |
| 1   | L1    | 1122 | U    |
| 1   | L1    | 1123 | G    |
| 1   | L1    | 1129 | G    |
| 1   | L1    | 1148 | A    |
| 1   | L1    | 1150 | A    |
| 1   | L1    | 1156 | A    |
| 1   | L1    | 1159 | A    |
| 1   | L1    | 1161 | A    |
| 1   | L1    | 1162 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L1    | 1165 | A    |
| 1   | L1    | 1169 | A    |
| 1   | L1    | 1170 | G    |
| 1   | L1    | 1171 | PSU  |
| 1   | L1    | 1172 | G    |
| 1   | L1    | 1174 | G    |
| 1   | L1    | 1179 | C    |
| 1   | L1    | 1188 | G    |
| 1   | L1    | 1196 | G    |
| 1   | L1    | 1201 | U    |
| 1   | L1    | 1202 | G    |
| 1   | L1    | 1207 | A    |
| 1   | L1    | 1210 | A    |
| 1   | L1    | 1217 | U    |
| 1   | L1    | 1225 | U    |
| 1   | L1    | 1239 | U    |
| 1   | L1    | 1240 | U    |
| 1   | L1    | 1242 | U    |
| 1   | L1    | 1243 | G    |
| 1   | L1    | 1248 | C    |
| 1   | L1    | 1251 | U    |
| 1   | L1    | 1254 | C    |
| 1   | L1    | 1258 | A    |
| 1   | L1    | 1261 | U    |
| 1   | L1    | 1263 | A    |
| 1   | L1    | 1270 | U    |
| 1   | L1    | 1271 | G    |
| 1   | L1    | 1274 | G    |
| 1   | L1    | 1286 | C    |
| 1   | L1    | 1287 | A    |
| 1   | L1    | 1294 | C    |
| 1   | L1    | 1342 | C    |
| 1   | L1    | 1346 | C    |
| 1   | L1    | 1348 | A    |
| 1   | L1    | 1349 | A    |
| 1   | L1    | 1350 | U    |
| 1   | L1    | 1364 | A    |
| 1   | L1    | 1367 | U    |
| 1   | L1    | 1369 | G    |
| 1   | L1    | 1371 | OMU  |
| 1   | L1    | 1378 | U    |
| 1   | L1    | 1379 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L1    | 1388 | U    |
| 1   | L1    | 1389 | A    |
| 1   | L1    | 1390 | G    |
| 1   | L1    | 1391 | U    |
| 1   | L1    | 1395 | U    |
| 1   | L1    | 1399 | C    |
| 1   | L1    | 1401 | U    |
| 1   | L1    | 1413 | U    |
| 1   | L1    | 1420 | G    |
| 1   | L1    | 1421 | G    |
| 1   | L1    | 1422 | A    |
| 1   | L1    | 1426 | A    |
| 1   | L1    | 1438 | A    |
| 1   | L1    | 1440 | G    |
| 1   | L1    | 1444 | A    |
| 1   | L1    | 1445 | G    |
| 1   | L1    | 1455 | U    |
| 1   | L1    | 1464 | G    |
| 1   | L1    | 1480 | C    |
| 1   | L1    | 1481 | G    |
| 1   | L1    | 1489 | U    |
| 1   | L1    | 1490 | G    |
| 1   | L1    | 1504 | A    |
| 1   | L1    | 1505 | U    |
| 1   | L1    | 1509 | C    |
| 1   | L1    | 1519 | G    |
| 1   | L1    | 1524 | OMG  |
| 1   | L1    | 1525 | A    |
| 1   | L1    | 1526 | U    |
| 1   | L1    | 1527 | OMC  |
| 1   | L1    | 1536 | C    |
| 1   | L1    | 1540 | OMG  |
| 1   | L1    | 1545 | G    |
| 1   | L1    | 1547 | U    |
| 1   | L1    | 1557 | A    |
| 1   | L1    | 1560 | U    |
| 1   | L1    | 1566 | A    |
| 1   | L1    | 1569 | U    |
| 1   | L1    | 1574 | C    |
| 1   | L1    | 1575 | G    |
| 1   | L1    | 1582 | A    |
| 1   | L1    | 1586 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L1    | 1590 | G    |
| 1   | L1    | 1612 | G    |
| 1   | L1    | 1613 | C    |
| 1   | L1    | 1627 | U    |
| 1   | L1    | 1639 | U    |
| 1   | L1    | 1654 | A    |
| 1   | L1    | 1661 | U    |
| 1   | L1    | 1662 | G    |
| 1   | L1    | 1663 | U    |
| 1   | L1    | 1666 | G    |
| 1   | L1    | 1667 | G    |
| 1   | L1    | 1671 | G    |
| 1   | L1    | 1672 | U    |
| 1   | L1    | 1676 | G    |
| 1   | L1    | 1677 | G    |
| 1   | L1    | 1683 | C    |
| 1   | L1    | 1715 | U    |
| 1   | L1    | 1716 | G    |
| 1   | L1    | 1717 | G    |
| 1   | L1    | 1723 | A    |
| 1   | L1    | 1726 | G    |
| 1   | L1    | 1734 | G    |
| 1   | L1    | 1739 | A    |
| 1   | L1    | 1744 | A    |
| 1   | L1    | 1747 | U    |
| 1   | L1    | 1756 | A    |
| 1   | L1    | 1757 | U    |
| 1   | L1    | 1758 | U    |
| 1   | L1    | 1766 | G    |
| 1   | L1    | 1771 | U    |
| 1   | L1    | 1774 | A    |
| 2   | L2    | 5    | A    |
| 2   | L2    | 7    | C    |
| 2   | L2    | 13   | A    |
| 2   | L2    | 22   | A    |
| 2   | L2    | 25   | A    |
| 2   | L2    | 30   | A    |
| 2   | L2    | 49   | A    |
| 2   | L2    | 61   | C    |
| 2   | L2    | 62   | A    |
| 2   | L2    | 63   | U    |
| 2   | L2    | 68   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L2    | 69  | A    |
| 2   | L2    | 75  | C    |
| 2   | L2    | 90  | G    |
| 2   | L2    | 98  | G    |
| 2   | L2    | 137 | A    |
| 2   | L2    | 336 | C    |
| 2   | L2    | 338 | C    |
| 2   | L2    | 339 | A    |
| 2   | L2    | 340 | A    |
| 2   | L2    | 341 | A    |
| 2   | L2    | 342 | U    |
| 2   | L2    | 343 | U    |
| 2   | L2    | 361 | U    |
| 2   | L2    | 364 | G    |
| 2   | L2    | 368 | G    |
| 2   | L2    | 377 | A    |
| 2   | L2    | 386 | U    |
| 2   | L2    | 388 | A    |
| 2   | L2    | 390 | A    |
| 2   | L2    | 395 | A    |
| 2   | L2    | 404 | A    |
| 2   | L2    | 434 | A    |
| 2   | L2    | 451 | U    |
| 2   | L2    | 453 | A    |
| 2   | L2    | 454 | A    |
| 2   | L2    | 490 | A    |
| 2   | L2    | 495 | G    |
| 2   | L2    | 502 | A2M  |
| 2   | L2    | 514 | U    |
| 2   | L2    | 518 | G    |
| 2   | L2    | 519 | G    |
| 2   | L2    | 527 | A2M  |
| 2   | L2    | 528 | U    |
| 2   | L2    | 529 | G    |
| 2   | L2    | 530 | C    |
| 2   | L2    | 534 | OMG  |
| 2   | L2    | 544 | U    |
| 2   | L2    | 552 | C    |
| 2   | L2    | 553 | G    |
| 2   | L2    | 554 | C    |
| 2   | L2    | 556 | U    |
| 2   | L2    | 559 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L2    | 561 | G    |
| 2   | L2    | 571 | G    |
| 2   | L2    | 580 | U    |
| 2   | L2    | 582 | U    |
| 2   | L2    | 616 | G    |
| 2   | L2    | 619 | A    |
| 2   | L2    | 620 | C    |
| 2   | L2    | 621 | G    |
| 2   | L2    | 639 | G    |
| 2   | L2    | 640 | G    |
| 2   | L2    | 643 | A    |
| 2   | L2    | 647 | A    |
| 2   | L2    | 648 | A    |
| 2   | L2    | 649 | G    |
| 2   | L2    | 650 | A    |
| 2   | L2    | 657 | U    |
| 2   | L2    | 658 | G    |
| 2   | L2    | 664 | G    |
| 2   | L2    | 665 | A2M  |
| 2   | L2    | 681 | G    |
| 2   | L2    | 695 | G    |
| 2   | L2    | 696 | A    |
| 2   | L2    | 697 | G    |
| 2   | L2    | 698 | G    |
| 2   | L2    | 745 | G    |
| 2   | L2    | 746 | A    |
| 2   | L2    | 747 | A    |
| 2   | L2    | 749 | G    |
| 2   | L2    | 750 | U    |
| 2   | L2    | 751 | U    |
| 2   | L2    | 752 | G    |
| 2   | L2    | 760 | U    |
| 2   | L2    | 761 | A    |
| 2   | L2    | 769 | A    |
| 2   | L2    | 777 | A    |
| 2   | L2    | 778 | A    |
| 2   | L2    | 780 | G    |
| 2   | L2    | 782 | G    |
| 2   | L2    | 783 | U    |
| 2   | L2    | 785 | U    |
| 2   | L2    | 787 | G    |
| 2   | L2    | 789 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | L2    | 799  | G    |
| 2   | L2    | 808  | C    |
| 2   | L2    | 810  | G    |
| 2   | L2    | 819  | U    |
| 2   | L2    | 823  | A    |
| 2   | L2    | 824  | G    |
| 2   | L2    | 851  | C    |
| 2   | L2    | 954  | A    |
| 2   | L2    | 970  | A    |
| 2   | L2    | 971  | A    |
| 2   | L2    | 972  | C    |
| 2   | L2    | 1001 | C    |
| 2   | L2    | 1010 | U    |
| 2   | L2    | 1011 | G    |
| 2   | L2    | 1012 | U    |
| 2   | L2    | 1019 | A    |
| 2   | L2    | 1021 | A    |
| 2   | L2    | 1022 | U    |
| 2   | L2    | 1025 | G    |
| 2   | L2    | 1033 | G    |
| 2   | L2    | 1034 | G    |
| 2   | L2    | 1041 | G    |
| 2   | L2    | 1046 | OMG  |
| 2   | L2    | 1053 | A    |
| 2   | L2    | 1055 | A    |
| 2   | L2    | 1064 | A    |
| 2   | L2    | 1075 | G    |
| 2   | L2    | 1079 | U    |
| 2   | L2    | 1083 | A    |
| 2   | L2    | 1096 | U    |
| 2   | L2    | 1101 | A    |
| 2   | L2    | 1104 | G    |
| 2   | L2    | 1108 | U    |
| 2   | L2    | 1115 | U    |
| 2   | L2    | 1116 | A    |
| 2   | L2    | 1118 | A    |
| 2   | L2    | 1121 | A    |
| 2   | L2    | 1123 | A    |
| 2   | L2    | 1129 | A    |
| 2   | L2    | 1137 | G    |
| 2   | L2    | 1141 | G    |
| 2   | L2    | 1147 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | L2    | 1148 | G    |
| 2   | L2    | 1156 | G    |
| 2   | L2    | 1157 | U    |
| 2   | L2    | 1162 | A    |
| 2   | L2    | 1176 | A    |
| 2   | L2    | 1177 | G    |
| 2   | L2    | 1179 | A    |
| 2   | L2    | 1180 | A    |
| 2   | L2    | 1181 | G    |
| 2   | L2    | 1183 | C    |
| 2   | L2    | 1189 | A    |
| 2   | L2    | 1199 | A    |
| 2   | L2    | 1204 | U    |
| 2   | L2    | 1206 | G    |
| 2   | L2    | 1207 | G    |
| 2   | L2    | 1209 | A    |
| 2   | L2    | 1215 | A    |
| 2   | L2    | 1216 | A    |
| 2   | L2    | 1229 | OMG  |
| 2   | L2    | 1233 | U    |
| 2   | L2    | 1234 | G    |
| 2   | L2    | 1237 | A    |
| 2   | L2    | 1238 | G    |
| 2   | L2    | 1239 | A    |
| 2   | L2    | 1241 | U    |
| 2   | L2    | 1246 | A    |
| 2   | L2    | 1248 | OMC  |
| 2   | L2    | 1252 | G    |
| 2   | L2    | 1255 | A    |
| 2   | L2    | 1264 | PSU  |
| 2   | L2    | 1283 | A    |
| 2   | L2    | 1288 | G    |
| 2   | L2    | 1289 | A    |
| 2   | L2    | 1299 | U    |
| 2   | L2    | 1309 | G    |
| 2   | L2    | 1325 | A    |
| 2   | L2    | 1337 | C    |
| 2   | L2    | 1361 | PSU  |
| 2   | L2    | 1373 | C    |
| 2   | L2    | 1374 | A    |
| 2   | L2    | 1379 | A    |
| 2   | L2    | 1380 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | L2    | 1385 | G    |
| 2   | L2    | 1409 | A    |
| 2   | L2    | 1416 | U    |
| 2   | L2    | 1421 | C    |
| 2   | L2    | 1428 | U    |
| 2   | L2    | 1433 | G    |
| 2   | L2    | 1437 | A    |
| 2   | L2    | 1441 | C    |
| 2   | L2    | 1443 | A    |
| 2   | L2    | 1444 | G    |
| 2   | L2    | 1445 | A    |
| 2   | L2    | 1448 | A    |
| 2   | L2    | 1450 | G    |
| 2   | L2    | 1453 | U    |
| 2   | L2    | 1454 | A    |
| 2   | L2    | 1462 | A    |
| 2   | L2    | 1463 | A    |
| 2   | L2    | 1465 | G    |
| 2   | L2    | 1483 | U    |
| 2   | L2    | 1485 | G    |
| 2   | L2    | 1486 | G    |
| 2   | L2    | 1496 | G    |
| 2   | L2    | 1498 | G    |
| 2   | L2    | 1506 | G    |
| 2   | L2    | 1510 | A    |
| 2   | L2    | 1511 | U    |
| 2   | L2    | 1512 | G    |
| 2   | L2    | 1513 | G    |
| 3   | L3    | 6    | G    |
| 3   | L3    | 16   | G    |
| 3   | L3    | 19   | A    |
| 3   | L3    | 20   | C    |
| 3   | L3    | 21   | A    |
| 3   | L3    | 22   | C    |
| 3   | L3    | 24   | U    |
| 3   | L3    | 25   | G    |
| 3   | L3    | 34   | C    |
| 3   | L3    | 35   | A    |
| 3   | L3    | 41   | A    |
| 3   | L3    | 49   | A    |
| 3   | L3    | 70   | A    |
| 3   | L3    | 111  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L3    | 112 | C    |
| 3   | L3    | 113 | U    |
| 3   | L3    | 114 | U    |
| 3   | L3    | 124 | U    |
| 3   | L3    | 125 | U    |
| 3   | L3    | 132 | G    |
| 3   | L3    | 142 | G    |
| 3   | L3    | 146 | G    |
| 3   | L3    | 149 | A    |
| 3   | L3    | 150 | A    |
| 3   | L3    | 151 | A    |
| 3   | L3    | 169 | A    |
| 3   | L3    | 174 | C    |
| 3   | L3    | 175 | A    |
| 3   | L3    | 182 | U    |
| 3   | L3    | 187 | U    |
| 3   | L3    | 192 | G    |
| 3   | L3    | 196 | U    |
| 3   | L3    | 199 | A    |
| 3   | L3    | 202 | A    |
| 4   | L4    | 8   | U    |
| 4   | L4    | 9   | G    |
| 4   | L4    | 10  | U    |
| 4   | L4    | 20  | U    |
| 4   | L4    | 24  | A    |
| 4   | L4    | 40  | G    |
| 4   | L4    | 50  | G    |
| 4   | L4    | 60  | A    |
| 4   | L4    | 61  | A    |
| 4   | L4    | 83  | U    |
| 4   | L4    | 85  | C    |
| 4   | L4    | 86  | U    |
| 4   | L4    | 87  | G    |
| 4   | L4    | 89  | G    |
| 4   | L4    | 102 | G    |
| 4   | L4    | 106 | G    |
| 4   | L4    | 114 | A    |
| 4   | L4    | 120 | U    |
| 4   | L4    | 121 | C    |
| 4   | L4    | 128 | U    |
| 4   | L4    | 133 | C    |
| 4   | L4    | 144 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L4    | 148 | C    |
| 4   | L4    | 150 | A    |
| 4   | L4    | 153 | C    |
| 4   | L4    | 158 | A    |
| 4   | L4    | 159 | G    |
| 4   | L4    | 168 | A    |
| 4   | L4    | 171 | A    |
| 4   | L4    | 173 | C    |
| 4   | L4    | 180 | C    |
| 5   | L5    | 3   | U    |
| 5   | L5    | 4   | A    |
| 5   | L5    | 15  | C    |
| 5   | L5    | 24  | G    |
| 5   | L5    | 29  | U    |
| 5   | L5    | 50  | C    |
| 5   | L5    | 51  | A    |
| 5   | L5    | 52  | U    |
| 5   | L5    | 62  | C    |
| 5   | L5    | 65  | U    |
| 5   | L5    | 68  | G    |
| 5   | L5    | 86  | G    |
| 5   | L5    | 87  | U    |
| 5   | L5    | 88  | C    |
| 5   | L5    | 92  | A    |
| 5   | L5    | 99  | G    |
| 5   | L5    | 105 | U    |
| 5   | L5    | 106 | G    |
| 5   | L5    | 109 | G    |
| 5   | L5    | 113 | G    |
| 5   | L5    | 117 | A    |
| 5   | L5    | 118 | U    |
| 5   | L5    | 120 | C    |
| 5   | L5    | 135 | U    |
| 6   | L6    | 7   | A    |
| 6   | L6    | 14  | A    |
| 6   | L6    | 15  | C    |
| 6   | L6    | 22  | G    |
| 6   | L6    | 25  | U    |
| 6   | L6    | 26  | G    |
| 6   | L6    | 31  | U    |
| 6   | L6    | 33  | G    |
| 6   | L6    | 41  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | L6    | 42  | A    |
| 6   | L6    | 43  | A    |
| 6   | L6    | 52  | G    |
| 6   | L6    | 54  | A    |
| 6   | L6    | 55  | U    |
| 6   | L6    | 56  | A    |
| 6   | L6    | 64  | U    |
| 6   | L6    | 67  | C    |
| 6   | L6    | 68  | A    |
| 6   | L6    | 70  | G    |
| 6   | L6    | 71  | A    |
| 6   | L6    | 72  | C    |
| 6   | L6    | 73  | A    |
| 7   | L7    | 16  | A    |
| 7   | L7    | 33  | U    |
| 7   | L7    | 59  | A    |
| 7   | L7    | 62  | A    |
| 7   | L7    | 63  | G    |
| 7   | L7    | 72  | A    |
| 7   | L7    | 80  | A    |
| 7   | L7    | 81  | U    |
| 7   | L7    | 82  | C    |
| 7   | L7    | 84  | U    |
| 7   | L7    | 94  | G    |
| 7   | L7    | 101 | OMU  |
| 7   | L7    | 102 | G    |
| 7   | L7    | 103 | A    |
| 7   | L7    | 105 | C    |
| 7   | L7    | 110 | A    |
| 7   | L7    | 120 | G    |
| 7   | L7    | 124 | A    |
| 7   | L7    | 125 | A    |
| 7   | L7    | 127 | C    |
| 7   | L7    | 157 | U    |
| 7   | L7    | 158 | U    |
| 8   | L8    | 11  | G    |
| 8   | L8    | 26  | A    |
| 8   | L8    | 37  | U    |
| 8   | L8    | 52  | G    |
| 8   | L8    | 57  | U    |
| 8   | L8    | 58  | A    |
| 8   | L8    | 63  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | L8    | 68  | A    |
| 8   | L8    | 95  | U    |
| 8   | L8    | 104 | A    |
| 8   | L8    | 114 | G    |
| 51  | S1    | 3   | U    |
| 51  | S1    | 26  | A    |
| 51  | S1    | 34  | G    |
| 51  | S1    | 42  | G    |
| 51  | S1    | 45  | U    |
| 51  | S1    | 47  | A    |
| 51  | S1    | 66  | U    |
| 51  | S1    | 68  | A    |
| 51  | S1    | 85  | C    |
| 51  | S1    | 102 | A    |
| 51  | S1    | 109 | C    |
| 51  | S1    | 112 | A    |
| 51  | S1    | 114 | U    |
| 51  | S1    | 117 | G    |
| 51  | S1    | 124 | A    |
| 51  | S1    | 129 | U    |
| 51  | S1    | 145 | A    |
| 51  | S1    | 146 | U    |
| 51  | S1    | 147 | U    |
| 51  | S1    | 149 | G    |
| 51  | S1    | 158 | G    |
| 51  | S1    | 164 | C    |
| 51  | S1    | 165 | G    |
| 51  | S1    | 167 | C    |
| 51  | S1    | 173 | A    |
| 51  | S1    | 174 | A    |
| 51  | S1    | 175 | U    |
| 51  | S1    | 181 | A    |
| 51  | S1    | 194 | U    |
| 51  | S1    | 195 | U    |
| 51  | S1    | 227 | U    |
| 51  | S1    | 228 | G    |
| 51  | S1    | 249 | A    |
| 51  | S1    | 252 | G    |
| 51  | S1    | 253 | U    |
| 51  | S1    | 255 | A    |
| 51  | S1    | 257 | A    |
| 51  | S1    | 264 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | S1    | 265 | C    |
| 51  | S1    | 266 | U    |
| 51  | S1    | 275 | A    |
| 51  | S1    | 276 | G    |
| 51  | S1    | 277 | U    |
| 51  | S1    | 278 | A    |
| 51  | S1    | 281 | A    |
| 51  | S1    | 287 | C    |
| 51  | S1    | 288 | A    |
| 51  | S1    | 295 | A    |
| 51  | S1    | 309 | G    |
| 51  | S1    | 313 | G    |
| 51  | S1    | 316 | A    |
| 51  | S1    | 322 | C    |
| 51  | S1    | 326 | U    |
| 51  | S1    | 329 | C    |
| 51  | S1    | 356 | A    |
| 51  | S1    | 358 | C    |
| 51  | S1    | 360 | G    |
| 51  | S1    | 364 | G    |
| 51  | S1    | 377 | A    |
| 51  | S1    | 381 | G    |
| 51  | S1    | 382 | A    |
| 51  | S1    | 396 | G    |
| 51  | S1    | 404 | C    |
| 51  | S1    | 413 | A    |
| 51  | S1    | 423 | U    |
| 51  | S1    | 433 | G    |
| 51  | S1    | 443 | A    |
| 51  | S1    | 444 | A    |
| 51  | S1    | 445 | U    |
| 51  | S1    | 446 | A    |
| 51  | S1    | 447 | G    |
| 51  | S1    | 455 | PSU  |
| 51  | S1    | 460 | C    |
| 51  | S1    | 464 | G    |
| 51  | S1    | 467 | C    |
| 51  | S1    | 469 | G    |
| 51  | S1    | 477 | G    |
| 51  | S1    | 481 | A    |
| 51  | S1    | 482 | U    |
| 51  | S1    | 487 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | S1    | 488 | A    |
| 51  | S1    | 497 | A    |
| 51  | S1    | 508 | A    |
| 51  | S1    | 523 | A    |
| 51  | S1    | 525 | A    |
| 51  | S1    | 548 | G    |
| 51  | S1    | 551 | A    |
| 51  | S1    | 552 | U    |
| 51  | S1    | 565 | U    |
| 51  | S1    | 575 | C    |
| 51  | S1    | 580 | A    |
| 51  | S1    | 581 | A    |
| 51  | S1    | 584 | U    |
| 51  | S1    | 585 | C    |
| 51  | S1    | 588 | G    |
| 51  | S1    | 589 | U    |
| 51  | S1    | 590 | A    |
| 51  | S1    | 591 | A    |
| 51  | S1    | 592 | C    |
| 51  | S1    | 593 | A    |
| 51  | S1    | 594 | A    |
| 51  | S1    | 600 | OMG  |
| 51  | S1    | 604 | A    |
| 51  | S1    | 606 | G    |
| 51  | S1    | 608 | C    |
| 51  | S1    | 609 | PSU  |
| 51  | S1    | 610 | G    |
| 51  | S1    | 614 | C    |
| 51  | S1    | 617 | G    |
| 51  | S1    | 626 | G    |
| 51  | S1    | 628 | A    |
| 51  | S1    | 631 | U    |
| 51  | S1    | 643 | A    |
| 51  | S1    | 660 | U    |
| 51  | S1    | 668 | A2M  |
| 51  | S1    | 669 | A    |
| 51  | S1    | 670 | A    |
| 51  | S1    | 671 | G    |
| 51  | S1    | 672 | G    |
| 51  | S1    | 673 | G    |
| 51  | S1    | 687 | U    |
| 51  | S1    | 688 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | S1    | 690 | G    |
| 51  | S1    | 698 | C    |
| 51  | S1    | 699 | A    |
| 51  | S1    | 744 | G    |
| 51  | S1    | 749 | U    |
| 51  | S1    | 755 | C    |
| 51  | S1    | 757 | C    |
| 51  | S1    | 758 | G    |
| 51  | S1    | 762 | A    |
| 51  | S1    | 774 | A    |
| 51  | S1    | 775 | C    |
| 51  | S1    | 776 | A    |
| 51  | S1    | 778 | G    |
| 51  | S1    | 779 | A    |
| 51  | S1    | 782 | C    |
| 51  | S1    | 786 | G    |
| 51  | S1    | 788 | A    |
| 51  | S1    | 789 | G    |
| 51  | S1    | 791 | G    |
| 51  | S1    | 792 | G    |
| 51  | S1    | 811 | C    |
| 51  | S1    | 812 | A    |
| 51  | S1    | 814 | G    |
| 51  | S1    | 815 | U    |
| 51  | S1    | 817 | A    |
| 51  | S1    | 818 | U    |
| 51  | S1    | 819 | G    |
| 51  | S1    | 825 | C    |
| 51  | S1    | 826 | A    |
| 51  | S1    | 830 | G    |
| 51  | S1    | 841 | U    |
| 51  | S1    | 844 | U    |
| 51  | S1    | 845 | U    |
| 51  | S1    | 856 | A    |
| 51  | S1    | 866 | G    |
| 51  | S1    | 867 | A    |
| 51  | S1    | 872 | A    |
| 51  | S1    | 880 | U    |
| 51  | S1    | 883 | G    |
| 51  | S1    | 886 | U    |
| 51  | S1    | 887 | U    |
| 51  | S1    | 890 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | S1    | 892  | U    |
| 51  | S1    | 914  | G    |
| 51  | S1    | 919  | G    |
| 51  | S1    | 925  | A    |
| 51  | S1    | 926  | G    |
| 51  | S1    | 930  | A    |
| 51  | S1    | 935  | U    |
| 51  | S1    | 936  | U    |
| 51  | S1    | 937  | C    |
| 51  | S1    | 938  | G    |
| 51  | S1    | 944  | U    |
| 51  | S1    | 945  | G    |
| 51  | S1    | 951  | U    |
| 51  | S1    | 954  | A    |
| 51  | S1    | 956  | A    |
| 51  | S1    | 959  | U    |
| 51  | S1    | 967  | A    |
| 51  | S1    | 970  | U    |
| 51  | S1    | 972  | A    |
| 51  | S1    | 1101 | A    |
| 51  | S1    | 1102 | G    |
| 51  | S1    | 1105 | A    |
| 51  | S1    | 1109 | A    |
| 51  | S1    | 1119 | U    |
| 51  | S1    | 1123 | G    |
| 51  | S1    | 1133 | U    |
| 51  | S1    | 1139 | G    |
| 51  | S1    | 1180 | A    |
| 51  | S1    | 1181 | C    |
| 51  | S1    | 1182 | A    |
| 51  | S1    | 1191 | A    |
| 51  | S1    | 1207 | U    |
| 51  | S1    | 1210 | C    |
| 51  | S1    | 1213 | A    |
| 51  | S1    | 1217 | A    |
| 51  | S1    | 1232 | G    |
| 51  | S1    | 1235 | A    |
| 51  | S1    | 1239 | A    |
| 51  | S1    | 1251 | A    |
| 51  | S1    | 1252 | A    |
| 51  | S1    | 1271 | C    |
| 51  | S1    | 1272 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | S1    | 1273 | A    |
| 51  | S1    | 1275 | C    |
| 51  | S1    | 1359 | C    |
| 51  | S1    | 1360 | U    |
| 51  | S1    | 1361 | U    |
| 51  | S1    | 1365 | U    |
| 51  | S1    | 1366 | A    |
| 51  | S1    | 1371 | U    |
| 51  | S1    | 1398 | C    |
| 51  | S1    | 1399 | G    |
| 51  | S1    | 1443 | U    |
| 51  | S1    | 1444 | G    |
| 51  | S1    | 1448 | U    |
| 51  | S1    | 1449 | U    |
| 51  | S1    | 1452 | A    |
| 51  | S1    | 1466 | G    |
| 51  | S1    | 1490 | A    |
| 51  | S1    | 1502 | G    |
| 51  | S1    | 1510 | C    |
| 51  | S1    | 1516 | G    |
| 51  | S1    | 1537 | U    |
| 51  | S1    | 1543 | B8N  |
| 51  | S1    | 1546 | A    |
| 51  | S1    | 1548 | A    |
| 51  | S1    | 1551 | G    |
| 51  | S1    | 1552 | G    |
| 51  | S1    | 1554 | A    |
| 51  | S1    | 1555 | A    |
| 51  | S1    | 1559 | U    |
| 51  | S1    | 1560 | A    |
| 51  | S1    | 1564 | G    |
| 51  | S1    | 1569 | G    |
| 51  | S1    | 1570 | G    |
| 51  | S1    | 1580 | G    |
| 51  | S1    | 1581 | G    |
| 51  | S1    | 1591 | U    |
| 51  | S1    | 1595 | G    |
| 51  | S1    | 1597 | G    |
| 51  | S1    | 1603 | U    |
| 51  | S1    | 1604 | C    |
| 51  | S1    | 1608 | A    |
| 51  | S1    | 1609 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | S1    | 1611 | C    |
| 51  | S1    | 1612 | C    |
| 51  | S1    | 1613 | C    |
| 51  | S1    | 1614 | U    |
| 51  | S1    | 1622 | G    |
| 51  | S1    | 1637 | A    |
| 51  | S1    | 1638 | U    |
| 51  | S1    | 1653 | U    |
| 51  | S1    | 1658 | U    |
| 51  | S1    | 1659 | U    |
| 51  | S1    | 1666 | U    |
| 51  | S1    | 1667 | U    |
| 51  | S1    | 1673 | A    |
| 51  | S1    | 1677 | G    |
| 51  | S1    | 1699 | A    |
| 51  | S1    | 1706 | A    |
| 51  | S1    | 1712 | G    |
| 51  | S1    | 1713 | C    |
| 51  | S1    | 1715 | C    |
| 51  | S1    | 1720 | G    |
| 51  | S1    | 1723 | A    |
| 51  | S1    | 1725 | C    |
| 51  | S1    | 1762 | A    |
| 51  | S1    | 1766 | G    |
| 51  | S1    | 1768 | U    |
| 51  | S1    | 1769 | C    |
| 51  | S1    | 1770 | G    |
| 51  | S1    | 1773 | U    |
| 51  | S1    | 1784 | G    |
| 51  | S1    | 1788 | U    |
| 51  | S1    | 1789 | U    |
| 51  | S1    | 1790 | C    |
| 51  | S1    | 1794 | U    |
| 51  | S1    | 1795 | G    |
| 51  | S1    | 1799 | U    |
| 51  | S1    | 1800 | U    |
| 51  | S1    | 1806 | A    |
| 51  | S1    | 1814 | U    |
| 51  | S1    | 1816 | U    |
| 51  | S1    | 1823 | A    |
| 51  | S1    | 1826 | G    |
| 51  | S1    | 1828 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | S1    | 1829 | OMG  |
| 51  | S1    | 1833 | OMU  |
| 51  | S1    | 1836 | G    |
| 51  | S1    | 1839 | G    |
| 51  | S1    | 1846 | A    |
| 51  | S1    | 1847 | A    |
| 51  | S1    | 1860 | C    |
| 51  | S1    | 1872 | A    |
| 51  | S1    | 1874 | U    |
| 51  | S1    | 1884 | A    |
| 51  | S1    | 1887 | A    |
| 51  | S1    | 1889 | G    |
| 51  | S1    | 1890 | A    |
| 51  | S1    | 1891 | A    |
| 51  | S1    | 1893 | A    |
| 51  | S1    | 1896 | G    |
| 51  | S1    | 1898 | C    |
| 51  | S1    | 1904 | U    |
| 51  | S1    | 1906 | G    |
| 51  | S1    | 1907 | A    |
| 51  | S1    | 1916 | G    |
| 51  | S1    | 1917 | A    |
| 51  | S1    | 1918 | U    |
| 51  | S1    | 1923 | A    |
| 51  | S1    | 1933 | A    |
| 51  | S1    | 1938 | C    |
| 51  | S1    | 1944 | C    |
| 51  | S1    | 1948 | U    |
| 51  | S1    | 1949 | A    |
| 51  | S1    | 1950 | G    |
| 51  | S1    | 1956 | C    |
| 51  | S1    | 1961 | G    |
| 51  | S1    | 1962 | A    |
| 51  | S1    | 1976 | U    |
| 51  | S1    | 1978 | A    |
| 51  | S1    | 1988 | C    |
| 51  | S1    | 1989 | A    |
| 51  | S1    | 2003 | C    |
| 51  | S1    | 2004 | G    |
| 51  | S1    | 2010 | G    |
| 51  | S1    | 2015 | U    |
| 51  | S1    | 2021 | A2M  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | S1    | 2031 | A    |
| 51  | S1    | 2097 | C    |
| 51  | S1    | 2101 | C    |
| 51  | S1    | 2118 | G    |
| 51  | S1    | 2119 | C    |
| 51  | S1    | 2120 | C    |
| 51  | S1    | 2121 | C    |
| 51  | S1    | 2134 | A    |
| 51  | S1    | 2158 | A    |
| 51  | S1    | 2163 | G    |
| 51  | S1    | 2169 | A    |
| 51  | S1    | 2170 | G    |
| 51  | S1    | 2172 | U    |
| 51  | S1    | 2183 | G    |
| 51  | S1    | 2185 | MA6  |
| 51  | S1    | 2195 | G    |
| 51  | S1    | 2196 | G    |
| 51  | S1    | 2197 | G    |
| 51  | S1    | 2198 | A    |
| 51  | S1    | 2199 | C    |
| 51  | S1    | 2202 | PSU  |
| 51  | S1    | 2203 | U    |
| 52  | S2    | 34   | G    |
| 52  | S2    | 35   | A    |
| 52  | S2    | 76   | A    |
| 53  | S3    | 10   | G    |
| 53  | S3    | 16   | C    |
| 53  | S3    | 18   | U    |
| 53  | S3    | 23   | G    |
| 53  | S3    | 47   | A    |
| 53  | S3    | 48   | U    |
| 53  | S3    | 49   | C    |
| 53  | S3    | 50   | G    |
| 53  | S3    | 75   | C    |
| 53  | S3    | 77   | A    |
| 52  | S4    | 4    | C    |
| 52  | S4    | 8    | U    |
| 52  | S4    | 14   | A    |
| 52  | S4    | 15   | G    |
| 52  | S4    | 24   | G    |
| 52  | S4    | 25   | A    |
| 52  | S4    | 26   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | S4    | 27  | U    |
| 52  | S4    | 29  | A    |
| 52  | S4    | 30  | A    |
| 52  | S4    | 36  | G    |
| 52  | S4    | 37  | U    |
| 52  | S4    | 38  | G    |
| 52  | S4    | 41  | C    |
| 52  | S4    | 43  | U    |
| 52  | S4    | 46  | U    |
| 52  | S4    | 47  | U    |
| 52  | S4    | 48  | C    |
| 52  | S4    | 49  | G    |
| 52  | S4    | 51  | U    |
| 52  | S4    | 53  | C    |
| 52  | S4    | 57  | G    |
| 52  | S4    | 62  | C    |
| 52  | S4    | 68  | A    |
| 88  | S5    | 4   | C    |
| 88  | S5    | 8   | U    |
| 88  | S5    | 9   | U    |

All (48) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L1    | 157  | U    |
| 1   | L1    | 170  | U    |
| 1   | L1    | 208  | C    |
| 1   | L1    | 510  | U    |
| 1   | L1    | 574  | G    |
| 1   | L1    | 584  | U    |
| 1   | L1    | 835  | G    |
| 1   | L1    | 967  | G    |
| 1   | L1    | 1390 | G    |
| 1   | L1    | 1479 | A    |
| 1   | L1    | 1524 | OMG  |
| 1   | L1    | 1565 | A    |
| 1   | L1    | 1574 | C    |
| 1   | L1    | 1662 | G    |
| 2   | L2    | 748  | C    |
| 2   | L2    | 784  | U    |
| 2   | L2    | 786  | A    |
| 2   | L2    | 1052 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | L2    | 1136 | U    |
| 2   | L2    | 1512 | G    |
| 3   | L3    | 173  | U    |
| 3   | L3    | 174  | C    |
| 4   | L4    | 149  | U    |
| 7   | L7    | 71   | A    |
| 7   | L7    | 83   | A    |
| 7   | L7    | 93   | C    |
| 51  | S1    | 128  | C    |
| 51  | S1    | 276  | G    |
| 51  | S1    | 294  | G    |
| 51  | S1    | 328  | C    |
| 51  | S1    | 550  | C    |
| 51  | S1    | 743  | A    |
| 51  | S1    | 777  | A    |
| 51  | S1    | 889  | A    |
| 51  | S1    | 937  | C    |
| 51  | S1    | 958  | G    |
| 51  | S1    | 1209 | C    |
| 51  | S1    | 1360 | U    |
| 51  | S1    | 1608 | A    |
| 51  | S1    | 1672 | C    |
| 51  | S1    | 1799 | U    |
| 51  | S1    | 1889 | G    |
| 51  | S1    | 1915 | U    |
| 51  | S1    | 2119 | C    |
| 52  | S2    | 34   | G    |
| 52  | S4    | 13   | C    |
| 52  | S4    | 35   | C    |
| 52  | S4    | 37   | U    |

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

175 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 |
| 2   | PSU  | L2    | 1382 | 92,2,90 | 18,21,22     | 4.82 | 7 (38%)  | 21,30,33    | 2.05 | 6 (28%)  |
| 2   | A2M  | L2    | 570  | 1,2     | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.37 | 11 (36%) |
| 1   | OMG  | L1    | 959  | 1       | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.67 | 10 (31%) |
| 1   | A2M  | L1    | 681  | 1       | 22,25,26     | 3.43 | 9 (40%)  | 30,36,39    | 2.23 | 10 (33%) |
| 51  | PSU  | S1    | 104  | 51      | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 51  | MA6  | S1    | 2184 | 51      | 23,26,27     | 1.40 | 4 (17%)  | 33,38,41    | 3.59 | 12 (36%) |
| 2   | A2M  | L2    | 572  | 2       | 22,25,26     | 3.46 | 9 (40%)  | 30,36,39    | 2.38 | 11 (36%) |
| 1   | OMC  | L1    | 695  | 1       | 19,22,23     | 3.06 | 8 (42%)  | 25,31,34    | 0.70 | 0        |
| 1   | OMG  | L1    | 1626 | 1,92    | 23,26,27     | 2.38 | 8 (34%)  | 32,38,41    | 2.44 | 9 (28%)  |
| 2   | OMU  | L2    | 1077 | 2       | 19,22,23     | 3.13 | 8 (42%)  | 25,31,34    | 1.79 | 4 (16%)  |
| 51  | OMG  | S1    | 1647 | 51      | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.56 | 10 (31%) |
| 1   | OMG  | L1    | 1190 | 1       | 23,26,27     | 2.44 | 9 (39%)  | 32,38,41    | 2.47 | 15 (46%) |
| 51  | PSU  | S1    | 1841 | 51      | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 1   | PSU  | L1    | 1664 | 1       | 18,21,22     | 4.73 | 8 (44%)  | 21,30,33    | 1.85 | 5 (23%)  |
| 51  | 7MG  | S1    | 1995 | 51,53   | 23,26,27     | 4.00 | 11 (47%) | 27,39,42    | 2.19 | 9 (33%)  |
| 2   | A2M  | L2    | 1067 | 2       | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.37 | 12 (40%) |
| 2   | PSU  | L2    | 504  | 2       | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.95 | 6 (28%)  |
| 2   | OMG  | L2    | 1078 | 2       | 23,26,27     | 2.41 | 9 (39%)  | 32,38,41    | 2.45 | 12 (37%) |
| 51  | PSU  | S1    | 33   | 51      | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.93 | 5 (23%)  |
| 2   | OMU  | L2    | 667  | 2       | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 1   | PSU  | L1    | 1011 | 1,2     | 18,21,22     | 4.78 | 7 (38%)  | 21,30,33    | 1.76 | 4 (19%)  |
| 2   | PSU  | L2    | 512  | 2       | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 1   | A2M  | L1    | 697  | 1       | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.36 | 11 (36%) |
| 3   | OMU  | L3    | 13   | 3       | 19,22,23     | 3.08 | 8 (42%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 1   | OMU  | L1    | 1371 | 1       | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 1.78 | 4 (16%)  |
| 2   | OMG  | L2    | 71   | 2       | 23,26,27     | 2.38 | 8 (34%)  | 32,38,41    | 2.51 | 9 (28%)  |
| 2   | PSU  | L2    | 78   | 2       | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.89 | 5 (23%)  |
| 51  | PSU  | S1    | 1156 | 51      | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 51  | OMG  | S1    | 1623 | 51      | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.62 | 10 (31%) |
| 1   | PSU  | L1    | 1171 | 1,91,92 | 18,21,22     | 4.79 | 8 (44%)  | 21,30,33    | 2.05 | 5 (23%)  |
| 1   | OMC  | L1    | 1010 | 1,90    | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 0.77 | 1 (4%)   |
| 51  | OMG  | S1    | 1829 | 51,90   | 23,26,27     | 2.34 | 8 (34%)  | 32,38,41    | 2.35 | 9 (28%)  |
| 2   | OMG  | L2    | 1253 | 2       | 23,26,27     | 2.38 | 8 (34%)  | 32,38,41    | 2.46 | 9 (28%)  |
| 1   | 1MA  | L1    | 677  | 1,90    | 21,25,26     | 2.86 | 5 (23%)  | 30,37,40    | 1.59 | 5 (16%)  |
| 51  | OMG  | S1    | 2151 | 51      | 23,26,27     | 2.44 | 9 (39%)  | 32,38,41    | 2.52 | 11 (34%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 51  | OMG  | S1    | 2008 | 51    | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.51 | 13 (40%) |
| 1   | OMG  | L1    | 1524 | 1     | 23,26,27     | 2.39 | 8 (34%)  | 32,38,41    | 2.50 | 8 (25%)  |
| 51  | OMG  | S1    | 600  | 51    | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.60 | 10 (31%) |
| 2   | OMG  | L2    | 641  | 2     | 23,26,27     | 2.36 | 8 (34%)  | 32,38,41    | 2.28 | 8 (25%)  |
| 2   | A2M  | L2    | 665  | 2     | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.38 | 10 (33%) |
| 2   | OMG  | L2    | 1231 | 2     | 23,26,27     | 2.43 | 9 (39%)  | 32,38,41    | 2.59 | 11 (34%) |
| 1   | PSU  | L1    | 1533 | 1,2   | 18,21,22     | 4.71 | 7 (38%)  | 21,30,33    | 1.91 | 5 (23%)  |
| 51  | PSU  | S1    | 1657 | 51    | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.91 | 5 (23%)  |
| 2   | A2M  | L2    | 1185 | 2     | 22,25,26     | 3.50 | 9 (40%)  | 30,36,39    | 2.28 | 10 (33%) |
| 2   | 5MC  | L2    | 1308 | 2,90  | 18,21,23     | 4.96 | 13 (72%) | 26,30,35    | 1.39 | 3 (11%)  |
| 2   | PSU  | L2    | 1403 | 2     | 18,21,22     | 4.83 | 7 (38%)  | 21,30,33    | 1.93 | 6 (28%)  |
| 2   | OMU  | L2    | 1359 | 2,90  | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 1   | OMU  | L1    | 1659 | 1,90  | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 51  | OMU  | S1    | 29   | 51    | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 51  | PSU  | S1    | 1246 | 51    | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.96 | 5 (23%)  |
| 2   | PSU  | L2    | 1264 | 2     | 18,21,22     | 4.83 | 9 (50%)  | 21,30,33    | 1.93 | 5 (23%)  |
| 51  | OMC  | S1    | 2019 | 51    | 19,22,23     | 3.06 | 8 (42%)  | 25,31,34    | 0.71 | 0        |
| 2   | PSU  | L2    | 1284 | 2     | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 2   | A2M  | L2    | 628  | 2     | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.36 | 10 (33%) |
| 1   | PSU  | L1    | 1017 | 1,91  | 18,21,22     | 4.83 | 7 (38%)  | 21,30,33    | 2.00 | 5 (23%)  |
| 2   | OMU  | L2    | 560  | 2,90  | 19,22,23     | 3.15 | 8 (42%)  | 25,31,34    | 1.93 | 4 (16%)  |
| 51  | OMG  | S1    | 1865 | 51,91 | 23,26,27     | 2.47 | 9 (39%)  | 32,38,41    | 2.58 | 10 (31%) |
| 2   | OMG  | L2    | 686  | 2     | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.57 | 10 (31%) |
| 1   | PSU  | L1    | 422  | 1     | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.93 | 5 (23%)  |
| 1   | OMU  | L1    | 48   | 1     | 19,22,23     | 3.08 | 8 (42%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 1   | OMU  | L1    | 847  | 1     | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 1.79 | 4 (16%)  |
| 51  | OMG  | S1    | 1550 | 51    | 23,26,27     | 2.38 | 8 (34%)  | 32,38,41    | 2.40 | 9 (28%)  |
| 51  | A2M  | S1    | 479  | 51    | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.36 | 10 (33%) |
| 1   | PSU  | L1    | 940  | 1     | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.91 | 5 (23%)  |
| 51  | A2M  | S1    | 668  | 51,90 | 22,25,26     | 3.39 | 9 (40%)  | 30,36,39    | 2.22 | 11 (36%) |
| 2   | PSU  | L2    | 593  | 2     | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.91 | 5 (23%)  |
| 2   | PSU  | L2    | 1413 | 2     | 18,21,22     | 4.84 | 7 (38%)  | 21,30,33    | 2.04 | 5 (23%)  |
| 51  | OMC  | S1    | 2140 | 51    | 19,22,23     | 3.07 | 8 (42%)  | 25,31,34    | 0.74 | 0        |
| 2   | OMU  | L2    | 56   | 1,2   | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 51  | PSU  | S1    | 2202 | 51    | 18,21,22     | 4.72 | 8 (44%)  | 21,30,33    | 1.85 | 5 (23%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | PSU  | L1    | 1528 | 1,92  | 18,21,22     | 4.84 | 7 (38%)  | 21,30,33    | 1.96 | 5 (23%)  |
| 2   | PSU  | L2    | 506  | 2     | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 2   | OMG  | L2    | 1046 | 53,2  | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.64 | 10 (31%) |
| 51  | OMU  | S1    | 1833 | 51    | 19,22,23     | 3.11 | 8 (42%)  | 25,31,34    | 1.85 | 4 (16%)  |
| 2   | OMG  | L2    | 534  | 2     | 23,26,27     | 2.44 | 9 (39%)  | 32,38,41    | 2.57 | 10 (31%) |
| 2   | PSU  | L2    | 1361 | 52,2  | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 2.03 | 5 (23%)  |
| 2   | A2M  | L2    | 382  | 2     | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.17 | 10 (33%) |
| 1   | A2M  | L1    | 678  | 1,2   | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.37 | 11 (36%) |
| 2   | PSU  | L2    | 437  | 92,2  | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.91 | 5 (23%)  |
| 51  | PSU  | S1    | 12   | 51    | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 2   | A2M  | L2    | 1384 | 2,90  | 22,25,26     | 3.46 | 9 (40%)  | 30,36,39    | 2.23 | 12 (40%) |
| 2   | PSU  | L2    | 662  | 2,90  | 18,21,22     | 4.79 | 8 (44%)  | 21,30,33    | 2.03 | 5 (23%)  |
| 2   | PSU  | L2    | 1303 | 2     | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.98 | 6 (28%)  |
| 7   | OMG  | L7    | 75   | 7     | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.51 | 10 (31%) |
| 2   | PSU  | L2    | 1265 | 2,90  | 18,21,22     | 4.67 | 8 (44%)  | 21,30,33    | 1.83 | 5 (23%)  |
| 2   | PSU  | L2    | 500  | 2     | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 2   | OMU  | L2    | 1419 | 2     | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 1.76 | 4 (16%)  |
| 51  | OMC  | S1    | 2059 | 51,90 | 19,22,23     | 3.07 | 8 (42%)  | 25,31,34    | 0.77 | 0        |
| 51  | OMU  | S1    | 1621 | 51,90 | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 2   | PSU  | L2    | 1318 | 2     | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 4   | OMG  | L4    | 74   | 4     | 23,26,27     | 2.44 | 9 (39%)  | 32,38,41    | 2.54 | 11 (34%) |
| 51  | PSU  | S1    | 1292 | 51,90 | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.89 | 5 (23%)  |
| 1   | A2M  | L1    | 69   | 1     | 22,25,26     | 3.39 | 7 (31%)  | 30,36,39    | 2.32 | 11 (36%) |
| 51  | PSU  | S1    | 2046 | 51    | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 1   | A2M  | L1    | 235  | 1     | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.33 | 10 (33%) |
| 1   | A2M  | L1    | 955  | 1     | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.38 | 11 (36%) |
| 2   | PSU  | L2    | 626  | 2     | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 2   | A2M  | L2    | 527  | 2,90  | 22,25,26     | 3.33 | 8 (36%)  | 30,36,39    | 2.34 | 13 (43%) |
| 2   | OMU  | L2    | 73   | 2     | 19,22,23     | 3.07 | 8 (42%)  | 25,31,34    | 1.74 | 4 (16%)  |
| 51  | A2M  | S1    | 2021 | 51    | 22,25,26     | 3.46 | 9 (40%)  | 30,36,39    | 2.40 | 12 (40%) |
| 2   | OMG  | L2    | 655  | 92,2  | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.63 | 10 (31%) |
| 2   | PSU  | L2    | 510  | 2     | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.90 | 5 (23%)  |
| 2   | A2M  | L2    | 1372 | 2     | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.45 | 12 (40%) |
| 1   | PSU  | L1    | 672  | 1,90  | 18,21,22     | 4.80 | 7 (38%)  | 21,30,33    | 2.03 | 5 (23%)  |
| 52  | MIA  | S2    | 37   | 52    | 28,31,32     | 2.53 | 4 (14%)  | 38,44,47    | 4.82 | 19 (50%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | OMG  | L2    | 1360 | 52,2  | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.61 | 10 (31%) |
| 51  | OMC  | S1    | 38   | 51    | 19,22,23     | 3.07 | 8 (42%)  | 25,31,34    | 0.73 | 0        |
| 1   | A2M  | L1    | 858  | 1     | 22,25,26     | 3.51 | 9 (40%)  | 30,36,39    | 2.34 | 10 (33%) |
| 2   | OMC  | L2    | 1159 | 2     | 19,22,23     | 3.06 | 8 (42%)  | 25,31,34    | 0.76 | 0        |
| 1   | OMU  | L1    | 1039 | 1     | 19,22,23     | 3.13 | 8 (42%)  | 25,31,34    | 1.81 | 4 (16%)  |
| 2   | PSU  | L2    | 1213 | 2     | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.95 | 5 (23%)  |
| 51  | PSU  | S1    | 455  | 51    | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.87 | 5 (23%)  |
| 51  | B8N  | S1    | 1543 | 51    | 25,29,30     | 3.47 | 9 (36%)  | 28,42,45    | 1.96 | 7 (25%)  |
| 2   | OMC  | L2    | 443  | 91,2  | 19,22,23     | 3.03 | 8 (42%)  | 25,31,34    | 0.64 | 0        |
| 2   | PSU  | L2    | 472  | 2     | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.93 | 5 (23%)  |
| 7   | OMU  | L7    | 101  | 7     | 19,22,23     | 4.64 | 14 (73%) | 25,31,34    | 2.06 | 6 (24%)  |
| 1   | A2M  | L1    | 927  | 1,90  | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.28 | 11 (36%) |
| 51  | A2M  | S1    | 969  | 51    | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.40 | 12 (40%) |
| 2   | OMC  | L2    | 583  | 2     | 19,22,23     | 3.06 | 8 (42%)  | 25,31,34    | 0.75 | 0        |
| 51  | OMU  | S1    | 1979 | 51    | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 2   | PSU  | L2    | 597  | 2     | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 51  | PSU  | S1    | 1533 | 51    | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 1   | OMC  | L1    | 1527 | 1     | 19,22,23     | 3.10 | 8 (42%)  | 25,31,34    | 0.80 | 1 (4%)   |
| 2   | PSU  | L2    | 1194 | 2     | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.91 | 5 (23%)  |
| 51  | OMG  | S1    | 1478 | 51    | 23,26,27     | 2.43 | 9 (39%)  | 32,38,41    | 2.45 | 11 (34%) |
| 51  | MA6  | S1    | 2185 | 51    | 23,26,27     | 1.39 | 3 (13%)  | 33,38,41    | 3.66 | 12 (36%) |
| 1   | OMG  | L1    | 1540 | 1,2   | 23,26,27     | 2.37 | 8 (34%)  | 32,38,41    | 2.31 | 8 (25%)  |
| 51  | PSU  | S1    | 1539 | 51    | 18,21,22     | 4.84 | 7 (38%)  | 21,30,33    | 2.00 | 5 (23%)  |
| 2   | OMC  | L2    | 1248 | 2     | 19,22,23     | 3.08 | 8 (42%)  | 25,31,34    | 0.72 | 0        |
| 1   | OMU  | L1    | 1253 | 1     | 19,22,23     | 3.11 | 8 (42%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 2   | A2M  | L2    | 502  | 2,90  | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.36 | 11 (36%) |
| 51  | PSU  | S1    | 1192 | 51    | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.78 | 4 (19%)  |
| 1   | PSU  | L1    | 239  | 1     | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.91 | 5 (23%)  |
| 2   | 5MC  | L2    | 524  | 2,90  | 19,22,23     | 3.90 | 8 (42%)  | 26,32,35    | 1.02 | 1 (3%)   |
| 51  | A2M  | S1    | 512  | 51,90 | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.39 | 11 (36%) |
| 2   | PSU  | L2    | 1144 | 2     | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.95 | 5 (23%)  |
| 51  | PSU  | S1    | 609  | 51    | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 7   | PSU  | L7    | 69   | 90,7  | 18,21,22     | 4.79 | 8 (44%)  | 21,30,33    | 2.00 | 6 (28%)  |
| 1   | A2M  | L1    | 1373 | 1     | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.38 | 12 (40%) |
| 2   | OMC  | L2    | 1317 | 2     | 19,22,23     | 3.05 | 8 (42%)  | 25,31,34    | 0.67 | 0        |

| Mol | Type | Chain | Res  | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PSU  | L2    | 1058 | 2      | 18,21,22     | 4.81 | 7 (38%)  | 21,30,33    | 2.08 | 5 (23%)  |
| 51  | A2M  | S1    | 897  | 51     | 22,25,26     | 3.50 | 9 (40%)  | 30,36,39    | 2.40 | 12 (40%) |
| 1   | OMC  | L1    | 1552 | 1      | 19,22,23     | 3.06 | 8 (42%)  | 25,31,34    | 0.75 | 0        |
| 1   | A2M  | L1    | 1539 | 1,2,90 | 22,25,26     | 3.50 | 8 (36%)  | 30,36,39    | 2.20 | 10 (33%) |
| 7   | A2M  | L7    | 43   | 7      | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.40 | 12 (40%) |
| 51  | OMU  | S1    | 1662 | 51     | 19,22,23     | 3.11 | 8 (42%)  | 25,31,34    | 1.78 | 4 (16%)  |
| 51  | OMU  | S1    | 8    | 51     | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 1.85 | 5 (20%)  |
| 51  | A2M  | S1    | 98   | 51,90  | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.35 | 12 (40%) |
| 51  | OMC  | S1    | 1866 | 51     | 19,22,23     | 3.07 | 8 (42%)  | 25,31,34    | 0.76 | 0        |
| 1   | PSU  | L1    | 1093 | 1      | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 2   | A2M  | L2    | 604  | 1,2    | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.37 | 11 (36%) |
| 7   | PSU  | L7    | 74   | 7      | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.98 | 5 (23%)  |
| 2   | A2M  | L2    | 591  | 2      | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.31 | 11 (36%) |
| 51  | A2M  | S1    | 28   | 51,90  | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.36 | 10 (33%) |
| 1   | PSU  | L1    | 774  | 1      | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 1   | OMU  | L1    | 1107 | 1      | 19,22,23     | 3.06 | 8 (42%)  | 25,31,34    | 1.87 | 5 (20%)  |
| 2   | OMC  | L2    | 14   | 1,2    | 19,22,23     | 3.07 | 8 (42%)  | 25,31,34    | 0.73 | 0        |
| 51  | 5MC  | S1    | 1544 | 51     | 19,22,23     | 3.91 | 8 (42%)  | 26,32,35    | 1.01 | 1 (3%)   |
| 1   | OMU  | L1    | 845  | 1      | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 1.77 | 5 (20%)  |
| 51  | PSU  | S1    | 2048 | 51     | 18,21,22     | 4.72 | 7 (38%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 2   | PSU  | L2    | 1060 | 2      | 18,21,22     | 4.71 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 7   | A2M  | L7    | 162  | 1,7    | 22,25,26     | 3.48 | 9 (40%)  | 30,36,39    | 2.35 | 10 (33%) |
| 51  | OMC  | S1    | 18   | 51     | 19,22,23     | 3.04 | 8 (42%)  | 25,31,34    | 0.67 | 0        |
| 51  | OMU  | S1    | 661  | 51     | 19,22,23     | 3.16 | 8 (42%)  | 25,31,34    | 1.81 | 4 (16%)  |
| 1   | OMC  | L1    | 669  | 1      | 19,22,23     | 2.99 | 8 (42%)  | 25,31,34    | 0.60 | 0        |
| 2   | OMC  | L2    | 1397 | 2      | 19,22,23     | 3.08 | 8 (42%)  | 25,31,34    | 0.75 | 0        |
| 51  | 5MC  | S1    | 2061 | 51     | 19,22,23     | 3.89 | 8 (42%)  | 26,32,35    | 0.93 | 1 (3%)   |
| 1   | OMG  | L1    | 856  | 1      | 23,26,27     | 2.37 | 8 (34%)  | 32,38,41    | 2.50 | 9 (28%)  |
| 1   | PSU  | L1    | 1181 | 1      | 18,21,22     | 4.73 | 7 (38%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 1   | A2M  | L1    | 305  | 1      | 22,25,26     | 3.47 | 9 (40%)  | 30,36,39    | 2.38 | 11 (36%) |
| 2   | OMC  | L2    | 359  | 2      | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 0.68 | 0        |
| 2   | A2M  | L2    | 95   | 2      | 22,25,26     | 3.49 | 9 (40%)  | 30,36,39    | 2.38 | 11 (36%) |
| 51  | PSU  | S1    | 1566 | 51     | 18,21,22     | 4.74 | 7 (38%)  | 21,30,33    | 1.88 | 5 (23%)  |
| 51  | OMU  | S1    | 1777 | 51     | 19,22,23     | 3.11 | 8 (42%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 2   | OMG  | L2    | 1229 | 2      | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.57 | 10 (31%) |



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   |
|-----|------|-------|------|---------|---------|------------|---------|
| 2   | PSU  | L2    | 1382 | 92,2,90 | -       | 1/7/25/26  | 0/2/2/2 |
| 2   | A2M  | L2    | 570  | 1,2     | -       | 5/9/27/28  | 0/3/3/3 |
| 1   | OMG  | L1    | 959  | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | L1    | 681  | 1       | -       | 3/9/27/28  | 0/3/3/3 |
| 51  | PSU  | S1    | 104  | 51      | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | MA6  | S1    | 2184 | 51      | -       | 0/11/29/30 | 0/3/3/3 |
| 2   | A2M  | L2    | 572  | 2       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | L1    | 695  | 1       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | L1    | 1626 | 1,92    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMU  | L2    | 1077 | 2       | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | OMG  | S1    | 1647 | 51      | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | L1    | 1190 | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | PSU  | S1    | 1841 | 51      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | L1    | 1664 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | 7MG  | S1    | 1995 | 51,53   | -       | 2/7/37/38  | 0/3/3/3 |
| 2   | A2M  | L2    | 1067 | 2       | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 504  | 2       | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMG  | L2    | 1078 | 2       | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | PSU  | S1    | 33   | 51      | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMU  | L2    | 667  | 2       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | L1    | 1011 | 1,2     | -       | 4/7/25/26  | 0/2/2/2 |
| 2   | PSU  | L2    | 512  | 2       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | L1    | 697  | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMU  | L3    | 13   | 3       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMU  | L1    | 1371 | 1       | -       | 3/9/27/28  | 0/2/2/2 |
| 2   | OMG  | L2    | 71   | 2       | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 78   | 2       | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | PSU  | S1    | 1156 | 51      | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | OMG  | S1    | 1623 | 51      | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | PSU  | L1    | 1171 | 1,91,92 | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | OMC  | L1    | 1010 | 1,90    | -       | 3/9/27/28  | 0/2/2/2 |
| 51  | OMG  | S1    | 1829 | 51,90   | -       | 2/9/27/28  | 0/3/3/3 |
| 2   | OMG  | L2    | 1253 | 2       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 1MA  | L1    | 677  | 1,90    | -       | 2/7/25/26  | 0/3/3/3 |
| 51  | OMG  | S1    | 2151 | 51      | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | OMG  | S1    | 2008 | 51      | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | L1    | 1524 | 1       | -       | 3/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 51  | OMG  | S1    | 600  | 51    | -       | 2/9/27/28 | 0/3/3/3 |
| 2   | OMG  | L2    | 641  | 2     | -       | 0/9/27/28 | 0/3/3/3 |
| 2   | A2M  | L2    | 665  | 2     | -       | 3/9/27/28 | 0/3/3/3 |
| 2   | OMG  | L2    | 1231 | 2     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | L1    | 1533 | 1,2   | -       | 0/7/25/26 | 0/2/2/2 |
| 51  | PSU  | S1    | 1657 | 51    | -       | 1/7/25/26 | 0/2/2/2 |
| 2   | A2M  | L2    | 1185 | 2     | -       | 3/9/27/28 | 0/3/3/3 |
| 2   | 5MC  | L2    | 1308 | 2,90  | -       | 4/6/24/26 | 0/2/2/2 |
| 2   | PSU  | L2    | 1403 | 2     | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | OMU  | L2    | 1359 | 2,90  | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | L1    | 1659 | 1,90  | -       | 0/9/27/28 | 0/2/2/2 |
| 51  | OMU  | S1    | 29   | 51    | -       | 1/9/27/28 | 0/2/2/2 |
| 51  | PSU  | S1    | 1246 | 51    | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | PSU  | L2    | 1264 | 2     | -       | 2/7/25/26 | 0/2/2/2 |
| 51  | OMC  | S1    | 2019 | 51    | -       | 0/9/27/28 | 0/2/2/2 |
| 2   | PSU  | L2    | 1284 | 2     | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | A2M  | L2    | 628  | 2     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | L1    | 1017 | 1,91  | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | OMU  | L2    | 560  | 2,90  | -       | 1/9/27/28 | 0/2/2/2 |
| 51  | OMG  | S1    | 1865 | 51,91 | -       | 0/9/27/28 | 0/3/3/3 |
| 2   | OMG  | L2    | 686  | 2     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | L1    | 422  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMU  | L1    | 48   | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMU  | L1    | 847  | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 51  | OMG  | S1    | 1550 | 51    | -       | 0/9/27/28 | 0/3/3/3 |
| 51  | A2M  | S1    | 479  | 51    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | L1    | 940  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 51  | A2M  | S1    | 668  | 51,90 | -       | 6/9/27/28 | 0/3/3/3 |
| 2   | PSU  | L2    | 593  | 2     | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | PSU  | L2    | 1413 | 2     | -       | 0/7/25/26 | 0/2/2/2 |
| 51  | OMC  | S1    | 2140 | 51    | -       | 0/9/27/28 | 0/2/2/2 |
| 2   | OMU  | L2    | 56   | 1,2   | -       | 0/9/27/28 | 0/2/2/2 |
| 51  | PSU  | S1    | 2202 | 51    | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | PSU  | L1    | 1528 | 1,92  | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | PSU  | L2    | 506  | 2     | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | OMG  | L2    | 1046 | 53,2  | -       | 3/9/27/28 | 0/3/3/3 |
| 51  | OMU  | S1    | 1833 | 51    | -       | 1/9/27/28 | 0/2/2/2 |
| 2   | OMG  | L2    | 534  | 2     | -       | 2/9/27/28 | 0/3/3/3 |
| 2   | PSU  | L2    | 1361 | 52,2  | -       | 3/7/25/26 | 0/2/2/2 |
| 2   | A2M  | L2    | 382  | 2     | -       | 0/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | A2M  | L1    | 678  | 1,2   | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 437  | 92,2  | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | PSU  | S1    | 12   | 51    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | A2M  | L2    | 1384 | 2,90  | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 662  | 2,90  | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | PSU  | L2    | 1303 | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 7   | OMG  | L7    | 75   | 7     | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 1265 | 2,90  | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | PSU  | L2    | 500  | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMU  | L2    | 1419 | 2     | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | OMC  | S1    | 2059 | 51,90 | -       | 1/9/27/28  | 0/2/2/2 |
| 51  | OMU  | S1    | 1621 | 51,90 | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | PSU  | L2    | 1318 | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 4   | OMG  | L4    | 74   | 4     | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | PSU  | S1    | 1292 | 51,90 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | L1    | 69   | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | PSU  | S1    | 2046 | 51    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | L1    | 235  | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | L1    | 955  | 1     | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 626  | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | A2M  | L2    | 527  | 2,90  | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMU  | L2    | 73   | 2     | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | A2M  | S1    | 2021 | 51    | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | OMG  | L2    | 655  | 92,2  | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 510  | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | A2M  | L2    | 1372 | 2     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | L1    | 672  | 1,90  | -       | 0/7/25/26  | 0/2/2/2 |
| 52  | MIA  | S2    | 37   | 52    | -       | 4/15/33/34 | 0/3/3/3 |
| 2   | OMG  | L2    | 1360 | 52,2  | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | OMC  | S1    | 38   | 51    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | A2M  | L1    | 858  | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMC  | L2    | 1159 | 2     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMU  | L1    | 1039 | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | PSU  | L2    | 1213 | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | PSU  | S1    | 455  | 51    | -       | 2/7/25/26  | 0/2/2/2 |
| 51  | B8N  | S1    | 1543 | 51    | -       | 4/16/34/35 | 0/2/2/2 |
| 2   | OMC  | L2    | 443  | 91,2  | -       | 4/9/27/28  | 0/2/2/2 |
| 2   | PSU  | L2    | 472  | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 7   | OMU  | L7    | 101  | 7     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | A2M  | L1    | 927  | 1,90  | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | A2M  | S1    | 969  | 51    | -       | 4/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link   | Chirals | Torsions   | Rings   |
|-----|------|-------|------|--------|---------|------------|---------|
| 2   | OMC  | L2    | 583  | 2      | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | OMU  | S1    | 1979 | 51     | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | PSU  | L2    | 597  | 2      | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | PSU  | S1    | 1533 | 51     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | L1    | 1527 | 1      | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | PSU  | L2    | 1194 | 2      | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | OMG  | S1    | 1478 | 51     | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | MA6  | S1    | 2185 | 51     | -       | 1/11/29/30 | 0/3/3/3 |
| 1   | OMG  | L1    | 1540 | 1,2    | -       | 2/9/27/28  | 0/3/3/3 |
| 51  | PSU  | S1    | 1539 | 51     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMC  | L2    | 1248 | 2      | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMU  | L1    | 1253 | 1      | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | A2M  | L2    | 502  | 2,90   | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | PSU  | S1    | 1192 | 51     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | L1    | 239  | 1      | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 5MC  | L2    | 524  | 2,90   | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | A2M  | S1    | 512  | 51,90  | -       | 2/9/27/28  | 0/3/3/3 |
| 2   | PSU  | L2    | 1144 | 2      | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | PSU  | S1    | 609  | 51     | -       | 0/7/25/26  | 0/2/2/2 |
| 7   | PSU  | L7    | 69   | 90,7   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | L1    | 1373 | 1      | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMC  | L2    | 1317 | 2      | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | PSU  | L2    | 1058 | 2      | -       | 0/7/25/26  | 0/2/2/2 |
| 51  | A2M  | S1    | 897  | 51     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | L1    | 1552 | 1      | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | A2M  | L1    | 1539 | 1,2,90 | -       | 0/9/27/28  | 0/3/3/3 |
| 7   | A2M  | L7    | 43   | 7      | -       | 0/9/27/28  | 0/3/3/3 |
| 51  | OMU  | S1    | 1662 | 51     | -       | 1/9/27/28  | 0/2/2/2 |
| 51  | OMU  | S1    | 8    | 51     | -       | 4/9/27/28  | 0/2/2/2 |
| 51  | A2M  | S1    | 98   | 51,90  | -       | 2/9/27/28  | 0/3/3/3 |
| 51  | OMC  | S1    | 1866 | 51     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | L1    | 1093 | 1      | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | A2M  | L2    | 604  | 1,2    | -       | 1/9/27/28  | 0/3/3/3 |
| 7   | PSU  | L7    | 74   | 7      | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | A2M  | L2    | 591  | 2      | -       | 1/9/27/28  | 0/3/3/3 |
| 51  | A2M  | S1    | 28   | 51,90  | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | L1    | 774  | 1      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | L1    | 1107 | 1      | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMC  | L2    | 14   | 1,2    | -       | 0/9/27/28  | 0/2/2/2 |
| 51  | 5MC  | S1    | 1544 | 51     | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | OMU  | L1    | 845  | 1      | -       | 0/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 51  | PSU  | S1    | 2048 | 51   | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | PSU  | L2    | 1060 | 2    | -       | 0/7/25/26 | 0/2/2/2 |
| 7   | A2M  | L7    | 162  | 1,7  | -       | 1/9/27/28 | 0/3/3/3 |
| 51  | OMC  | S1    | 18   | 51   | -       | 0/9/27/28 | 0/2/2/2 |
| 51  | OMU  | S1    | 661  | 51   | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMC  | L1    | 669  | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 2   | OMC  | L2    | 1397 | 2    | -       | 0/9/27/28 | 0/2/2/2 |
| 51  | 5MC  | S1    | 2061 | 51   | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMG  | L1    | 856  | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | L1    | 1181 | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | A2M  | L1    | 305  | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 2   | OMC  | L2    | 359  | 2    | -       | 0/9/27/28 | 0/2/2/2 |
| 2   | A2M  | L2    | 95   | 2    | -       | 0/9/27/28 | 0/3/3/3 |
| 51  | PSU  | S1    | 1566 | 51   | -       | 0/7/25/26 | 0/2/2/2 |
| 51  | OMU  | S1    | 1777 | 51   | -       | 0/9/27/28 | 0/2/2/2 |
| 2   | OMG  | L2    | 1229 | 2    | -       | 2/9/27/28 | 0/3/3/3 |

All (1399) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | L2    | 1264 | PSU  | C6-C5 | 12.98 | 1.49        | 1.35     |
| 2   | L2    | 1413 | PSU  | C6-C5 | 12.85 | 1.49        | 1.35     |
| 1   | L1    | 1528 | PSU  | C6-C5 | 12.82 | 1.49        | 1.35     |
| 1   | L1    | 1011 | PSU  | C6-C5 | 12.79 | 1.49        | 1.35     |
| 51  | S1    | 1539 | PSU  | C6-C5 | 12.78 | 1.49        | 1.35     |
| 1   | L1    | 1017 | PSU  | C6-C5 | 12.72 | 1.49        | 1.35     |
| 1   | L1    | 672  | PSU  | C6-C5 | 12.71 | 1.49        | 1.35     |
| 2   | L2    | 1382 | PSU  | C6-C5 | 12.69 | 1.49        | 1.35     |
| 2   | L2    | 1058 | PSU  | C6-C5 | 12.67 | 1.49        | 1.35     |
| 2   | L2    | 1403 | PSU  | C6-C5 | 12.64 | 1.49        | 1.35     |
| 1   | L1    | 1171 | PSU  | C6-C5 | 12.61 | 1.49        | 1.35     |
| 51  | S1    | 455  | PSU  | C6-C5 | 12.61 | 1.49        | 1.35     |
| 51  | S1    | 1192 | PSU  | C6-C5 | 12.57 | 1.49        | 1.35     |
| 2   | L2    | 510  | PSU  | C6-C5 | 12.54 | 1.49        | 1.35     |
| 2   | L2    | 593  | PSU  | C6-C5 | 12.51 | 1.49        | 1.35     |
| 2   | L2    | 1194 | PSU  | C6-C5 | 12.51 | 1.49        | 1.35     |
| 2   | L2    | 662  | PSU  | C6-C5 | 12.51 | 1.49        | 1.35     |
| 1   | L1    | 422  | PSU  | C6-C5 | 12.51 | 1.49        | 1.35     |
| 51  | S1    | 1156 | PSU  | C6-C5 | 12.51 | 1.49        | 1.35     |
| 51  | S1    | 104  | PSU  | C6-C5 | 12.51 | 1.49        | 1.35     |
| 2   | L2    | 1318 | PSU  | C6-C5 | 12.50 | 1.49        | 1.35     |
| 51  | S1    | 33   | PSU  | C6-C5 | 12.49 | 1.49        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | L2    | 626  | PSU  | C6-C5 | 12.49 | 1.49        | 1.35     |
| 2   | L2    | 504  | PSU  | C6-C5 | 12.49 | 1.49        | 1.35     |
| 2   | L2    | 78   | PSU  | C6-C5 | 12.48 | 1.49        | 1.35     |
| 2   | L2    | 437  | PSU  | C6-C5 | 12.48 | 1.49        | 1.35     |
| 1   | L1    | 774  | PSU  | C6-C5 | 12.48 | 1.49        | 1.35     |
| 7   | L7    | 69   | PSU  | C6-C5 | 12.48 | 1.49        | 1.35     |
| 51  | S1    | 1292 | PSU  | C6-C5 | 12.48 | 1.49        | 1.35     |
| 1   | L1    | 940  | PSU  | C6-C5 | 12.48 | 1.49        | 1.35     |
| 51  | S1    | 1533 | PSU  | C6-C5 | 12.47 | 1.49        | 1.35     |
| 2   | L2    | 1303 | PSU  | C6-C5 | 12.47 | 1.49        | 1.35     |
| 1   | L1    | 1093 | PSU  | C6-C5 | 12.46 | 1.49        | 1.35     |
| 2   | L2    | 597  | PSU  | C6-C5 | 12.46 | 1.49        | 1.35     |
| 1   | L1    | 1181 | PSU  | C6-C5 | 12.46 | 1.49        | 1.35     |
| 51  | S1    | 609  | PSU  | C6-C5 | 12.46 | 1.49        | 1.35     |
| 51  | S1    | 2048 | PSU  | C6-C5 | 12.46 | 1.49        | 1.35     |
| 2   | L2    | 506  | PSU  | C6-C5 | 12.46 | 1.49        | 1.35     |
| 51  | S1    | 1566 | PSU  | C6-C5 | 12.45 | 1.49        | 1.35     |
| 51  | S1    | 2046 | PSU  | C6-C5 | 12.45 | 1.49        | 1.35     |
| 1   | L1    | 239  | PSU  | C6-C5 | 12.45 | 1.49        | 1.35     |
| 1   | L1    | 1664 | PSU  | C6-C5 | 12.45 | 1.49        | 1.35     |
| 2   | L2    | 1213 | PSU  | C6-C5 | 12.45 | 1.49        | 1.35     |
| 2   | L2    | 1284 | PSU  | C6-C5 | 12.44 | 1.49        | 1.35     |
| 7   | L7    | 74   | PSU  | C6-C5 | 12.44 | 1.49        | 1.35     |
| 51  | S1    | 12   | PSU  | C6-C5 | 12.43 | 1.49        | 1.35     |
| 51  | S1    | 2202 | PSU  | C6-C5 | 12.41 | 1.49        | 1.35     |
| 51  | S1    | 1246 | PSU  | C6-C5 | 12.41 | 1.49        | 1.35     |
| 1   | L1    | 1533 | PSU  | C6-C5 | 12.41 | 1.49        | 1.35     |
| 2   | L2    | 1144 | PSU  | C6-C5 | 12.41 | 1.49        | 1.35     |
| 2   | L2    | 1361 | PSU  | C6-C5 | 12.40 | 1.49        | 1.35     |
| 2   | L2    | 500  | PSU  | C6-C5 | 12.39 | 1.49        | 1.35     |
| 51  | S1    | 1841 | PSU  | C6-C5 | 12.38 | 1.49        | 1.35     |
| 2   | L2    | 1060 | PSU  | C6-C5 | 12.38 | 1.49        | 1.35     |
| 2   | L2    | 472  | PSU  | C6-C5 | 12.37 | 1.49        | 1.35     |
| 2   | L2    | 1265 | PSU  | C6-C5 | 12.37 | 1.49        | 1.35     |
| 2   | L2    | 512  | PSU  | C6-C5 | 12.36 | 1.49        | 1.35     |
| 51  | S1    | 1657 | PSU  | C6-C5 | 12.35 | 1.49        | 1.35     |
| 2   | L2    | 1403 | PSU  | C2-N1 | 10.58 | 1.50        | 1.36     |
| 51  | S1    | 1539 | PSU  | C2-N1 | 10.56 | 1.50        | 1.36     |
| 1   | L1    | 1017 | PSU  | C2-N1 | 10.55 | 1.50        | 1.36     |
| 2   | L2    | 1413 | PSU  | C2-N1 | 10.54 | 1.50        | 1.36     |
| 2   | L2    | 662  | PSU  | C2-N1 | 10.53 | 1.50        | 1.36     |
| 2   | L2    | 1058 | PSU  | C2-N1 | 10.52 | 1.50        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | L1    | 1528 | PSU  | C2-N1 | 10.52 | 1.50        | 1.36     |
| 1   | L1    | 672  | PSU  | C2-N1 | 10.52 | 1.50        | 1.36     |
| 2   | L2    | 1382 | PSU  | C2-N1 | 10.49 | 1.50        | 1.36     |
| 1   | L1    | 1171 | PSU  | C2-N1 | 10.43 | 1.50        | 1.36     |
| 7   | L7    | 69   | PSU  | C2-N1 | 10.43 | 1.50        | 1.36     |
| 2   | L2    | 1264 | PSU  | C2-N1 | 10.39 | 1.50        | 1.36     |
| 1   | L1    | 1011 | PSU  | C2-N1 | 10.37 | 1.50        | 1.36     |
| 51  | S1    | 1841 | PSU  | C2-N1 | 10.29 | 1.50        | 1.36     |
| 7   | L7    | 74   | PSU  | C2-N1 | 10.28 | 1.50        | 1.36     |
| 2   | L2    | 1213 | PSU  | C2-N1 | 10.28 | 1.50        | 1.36     |
| 51  | S1    | 1156 | PSU  | C2-N1 | 10.28 | 1.50        | 1.36     |
| 51  | S1    | 33   | PSU  | C2-N1 | 10.28 | 1.50        | 1.36     |
| 1   | L1    | 1093 | PSU  | C2-N1 | 10.27 | 1.50        | 1.36     |
| 2   | L2    | 500  | PSU  | C2-N1 | 10.27 | 1.50        | 1.36     |
| 2   | L2    | 78   | PSU  | C2-N1 | 10.27 | 1.50        | 1.36     |
| 2   | L2    | 1318 | PSU  | C2-N1 | 10.25 | 1.50        | 1.36     |
| 51  | S1    | 1566 | PSU  | C2-N1 | 10.25 | 1.50        | 1.36     |
| 2   | L2    | 510  | PSU  | C2-N1 | 10.25 | 1.50        | 1.36     |
| 1   | L1    | 774  | PSU  | C2-N1 | 10.25 | 1.50        | 1.36     |
| 2   | L2    | 1303 | PSU  | C2-N1 | 10.25 | 1.50        | 1.36     |
| 1   | L1    | 1181 | PSU  | C2-N1 | 10.24 | 1.50        | 1.36     |
| 51  | S1    | 1657 | PSU  | C2-N1 | 10.24 | 1.50        | 1.36     |
| 51  | S1    | 1533 | PSU  | C2-N1 | 10.24 | 1.50        | 1.36     |
| 2   | L2    | 1144 | PSU  | C2-N1 | 10.24 | 1.50        | 1.36     |
| 2   | L2    | 1284 | PSU  | C2-N1 | 10.23 | 1.50        | 1.36     |
| 2   | L2    | 437  | PSU  | C2-N1 | 10.22 | 1.50        | 1.36     |
| 2   | L2    | 506  | PSU  | C2-N1 | 10.22 | 1.50        | 1.36     |
| 1   | L1    | 422  | PSU  | C2-N1 | 10.22 | 1.50        | 1.36     |
| 51  | S1    | 2046 | PSU  | C2-N1 | 10.22 | 1.50        | 1.36     |
| 2   | L2    | 472  | PSU  | C2-N1 | 10.21 | 1.50        | 1.36     |
| 2   | L2    | 597  | PSU  | C2-N1 | 10.21 | 1.50        | 1.36     |
| 1   | L1    | 239  | PSU  | C2-N1 | 10.21 | 1.50        | 1.36     |
| 1   | L1    | 940  | PSU  | C2-N1 | 10.21 | 1.50        | 1.36     |
| 2   | L2    | 512  | PSU  | C2-N1 | 10.21 | 1.50        | 1.36     |
| 51  | S1    | 1246 | PSU  | C2-N1 | 10.21 | 1.50        | 1.36     |
| 1   | L1    | 1664 | PSU  | C2-N1 | 10.20 | 1.50        | 1.36     |
| 2   | L2    | 626  | PSU  | C2-N1 | 10.20 | 1.50        | 1.36     |
| 51  | S1    | 1292 | PSU  | C2-N1 | 10.20 | 1.50        | 1.36     |
| 51  | S1    | 12   | PSU  | C2-N1 | 10.19 | 1.50        | 1.36     |
| 2   | L2    | 1060 | PSU  | C2-N1 | 10.18 | 1.49        | 1.36     |
| 2   | L2    | 504  | PSU  | C2-N1 | 10.18 | 1.49        | 1.36     |
| 2   | L2    | 593  | PSU  | C2-N1 | 10.18 | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | S1    | 609  | PSU  | C2-N1   | 10.17 | 1.49        | 1.36     |
| 51  | S1    | 2202 | PSU  | C2-N1   | 10.17 | 1.49        | 1.36     |
| 51  | S1    | 104  | PSU  | C2-N1   | 10.16 | 1.49        | 1.36     |
| 1   | L1    | 1533 | PSU  | C2-N1   | 10.16 | 1.49        | 1.36     |
| 2   | L2    | 1194 | PSU  | C2-N1   | 10.16 | 1.49        | 1.36     |
| 51  | S1    | 1192 | PSU  | C2-N1   | 10.16 | 1.49        | 1.36     |
| 2   | L2    | 1361 | PSU  | C2-N1   | 10.15 | 1.49        | 1.36     |
| 51  | S1    | 2048 | PSU  | C2-N1   | 10.15 | 1.49        | 1.36     |
| 51  | S1    | 455  | PSU  | C2-N1   | 10.08 | 1.49        | 1.36     |
| 51  | S1    | 1995 | 7MG  | C8-N9   | 9.90  | 1.52        | 1.45     |
| 2   | L2    | 1265 | PSU  | C2-N1   | 9.84  | 1.49        | 1.36     |
| 51  | S1    | 1544 | 5MC  | C6-C5   | 9.30  | 1.49        | 1.34     |
| 2   | L2    | 524  | 5MC  | C6-C5   | 9.29  | 1.49        | 1.34     |
| 2   | L2    | 382  | A2M  | O4'-C1' | 9.24  | 1.63        | 1.42     |
| 2   | L2    | 1185 | A2M  | O4'-C1' | 9.20  | 1.63        | 1.42     |
| 51  | S1    | 2061 | 5MC  | C6-C5   | 9.17  | 1.49        | 1.34     |
| 1   | L1    | 1539 | A2M  | C2'-C1' | -9.15 | 1.30        | 1.53     |
| 2   | L2    | 1384 | A2M  | O4'-C1' | 9.13  | 1.63        | 1.42     |
| 1   | L1    | 927  | A2M  | O4'-C1' | 9.13  | 1.63        | 1.42     |
| 1   | L1    | 927  | A2M  | C2'-C1' | -9.11 | 1.30        | 1.53     |
| 1   | L1    | 305  | A2M  | C2'-C1' | -9.11 | 1.30        | 1.53     |
| 1   | L1    | 1539 | A2M  | O4'-C1' | 9.11  | 1.63        | 1.42     |
| 2   | L2    | 1308 | 5MC  | C6-C5   | 9.10  | 1.49        | 1.34     |
| 1   | L1    | 858  | A2M  | C2'-C1' | -9.08 | 1.30        | 1.53     |
| 1   | L1    | 858  | A2M  | O4'-C1' | 9.06  | 1.62        | 1.42     |
| 1   | L1    | 681  | A2M  | C2'-C1' | -9.01 | 1.30        | 1.53     |
| 52  | S2    | 37   | MIA  | C2-S10  | 9.01  | 1.83        | 1.75     |
| 2   | L2    | 382  | A2M  | C2'-C1' | -8.99 | 1.31        | 1.53     |
| 1   | L1    | 1373 | A2M  | C2'-C1' | -8.99 | 1.31        | 1.53     |
| 51  | S1    | 897  | A2M  | C2'-C1' | -8.99 | 1.31        | 1.53     |
| 51  | S1    | 98   | A2M  | C2'-C1' | -8.98 | 1.31        | 1.53     |
| 2   | L2    | 502  | A2M  | C2'-C1' | -8.98 | 1.31        | 1.53     |
| 51  | S1    | 512  | A2M  | C2'-C1' | -8.97 | 1.31        | 1.53     |
| 51  | S1    | 969  | A2M  | C2'-C1' | -8.97 | 1.31        | 1.53     |
| 1   | L1    | 69   | A2M  | C2'-C1' | -8.97 | 1.31        | 1.53     |
| 51  | S1    | 897  | A2M  | O4'-C1' | 8.96  | 1.62        | 1.42     |
| 2   | L2    | 604  | A2M  | C2'-C1' | -8.96 | 1.31        | 1.53     |
| 2   | L2    | 1067 | A2M  | C2'-C1' | -8.95 | 1.31        | 1.53     |
| 1   | L1    | 681  | A2M  | O4'-C1' | 8.95  | 1.62        | 1.42     |
| 2   | L2    | 570  | A2M  | O4'-C1' | 8.95  | 1.62        | 1.42     |
| 2   | L2    | 527  | A2M  | C2'-C1' | -8.94 | 1.31        | 1.53     |
| 2   | L2    | 1384 | A2M  | C2'-C1' | -8.94 | 1.31        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | L7    | 43   | A2M  | C2'-C1' | -8.94 | 1.31        | 1.53     |
| 51  | S1    | 28   | A2M  | O4'-C1' | 8.94  | 1.62        | 1.42     |
| 7   | L7    | 43   | A2M  | O4'-C1' | 8.94  | 1.62        | 1.42     |
| 1   | L1    | 678  | A2M  | C2'-C1' | -8.93 | 1.31        | 1.53     |
| 2   | L2    | 591  | A2M  | C2'-C1' | -8.93 | 1.31        | 1.53     |
| 2   | L2    | 1185 | A2M  | C2'-C1' | -8.93 | 1.31        | 1.53     |
| 2   | L2    | 572  | A2M  | C2'-C1' | -8.91 | 1.31        | 1.53     |
| 7   | L7    | 162  | A2M  | C2'-C1' | -8.91 | 1.31        | 1.53     |
| 2   | L2    | 1067 | A2M  | O4'-C1' | 8.91  | 1.62        | 1.42     |
| 2   | L2    | 95   | A2M  | C2'-C1' | -8.90 | 1.31        | 1.53     |
| 51  | S1    | 479  | A2M  | C2'-C1' | -8.90 | 1.31        | 1.53     |
| 1   | L1    | 235  | A2M  | C2'-C1' | -8.90 | 1.31        | 1.53     |
| 2   | L2    | 665  | A2M  | O4'-C1' | 8.90  | 1.62        | 1.42     |
| 1   | L1    | 697  | A2M  | O4'-C1' | 8.89  | 1.62        | 1.42     |
| 2   | L2    | 1308 | 5MC  | C3'-C4' | -8.89 | 1.30        | 1.53     |
| 1   | L1    | 1373 | A2M  | O4'-C1' | 8.89  | 1.62        | 1.42     |
| 51  | S1    | 98   | A2M  | O4'-C1' | 8.89  | 1.62        | 1.42     |
| 2   | L2    | 628  | A2M  | O4'-C1' | 8.89  | 1.62        | 1.42     |
| 51  | S1    | 28   | A2M  | C2'-C1' | -8.89 | 1.31        | 1.53     |
| 2   | L2    | 502  | A2M  | O4'-C1' | 8.89  | 1.62        | 1.42     |
| 2   | L2    | 604  | A2M  | O4'-C1' | 8.89  | 1.62        | 1.42     |
| 2   | L2    | 628  | A2M  | C2'-C1' | -8.88 | 1.31        | 1.53     |
| 51  | S1    | 479  | A2M  | O4'-C1' | 8.87  | 1.62        | 1.42     |
| 2   | L2    | 572  | A2M  | O4'-C1' | 8.87  | 1.62        | 1.42     |
| 2   | L2    | 95   | A2M  | O4'-C1' | 8.87  | 1.62        | 1.42     |
| 2   | L2    | 665  | A2M  | C2'-C1' | -8.86 | 1.31        | 1.53     |
| 51  | S1    | 512  | A2M  | O4'-C1' | 8.85  | 1.62        | 1.42     |
| 1   | L1    | 955  | A2M  | O4'-C1' | 8.85  | 1.62        | 1.42     |
| 1   | L1    | 697  | A2M  | C2'-C1' | -8.84 | 1.31        | 1.53     |
| 7   | L7    | 162  | A2M  | O4'-C1' | 8.83  | 1.62        | 1.42     |
| 1   | L1    | 235  | A2M  | O4'-C1' | 8.83  | 1.62        | 1.42     |
| 1   | L1    | 955  | A2M  | C2'-C1' | -8.82 | 1.31        | 1.53     |
| 2   | L2    | 591  | A2M  | O4'-C1' | 8.82  | 1.62        | 1.42     |
| 2   | L2    | 1372 | A2M  | C2'-C1' | -8.81 | 1.31        | 1.53     |
| 2   | L2    | 570  | A2M  | C2'-C1' | -8.81 | 1.31        | 1.53     |
| 1   | L1    | 678  | A2M  | O4'-C1' | 8.80  | 1.62        | 1.42     |
| 51  | S1    | 2021 | A2M  | O4'-C1' | 8.80  | 1.62        | 1.42     |
| 2   | L2    | 1372 | A2M  | O4'-C1' | 8.77  | 1.62        | 1.42     |
| 51  | S1    | 668  | A2M  | C2'-C1' | -8.77 | 1.31        | 1.53     |
| 51  | S1    | 2021 | A2M  | C2'-C1' | -8.71 | 1.31        | 1.53     |
| 51  | S1    | 969  | A2M  | O4'-C1' | 8.71  | 1.62        | 1.42     |
| 7   | L7    | 101  | OMU  | C3'-C2' | -8.70 | 1.34        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | L1    | 305  | A2M  | O4'-C1' | 8.66  | 1.62        | 1.42     |
| 51  | S1    | 1995 | 7MG  | C5-N7   | 8.62  | 1.46        | 1.35     |
| 1   | L1    | 69   | A2M  | O4'-C1' | 8.60  | 1.61        | 1.42     |
| 51  | S1    | 668  | A2M  | O4'-C1' | 8.56  | 1.61        | 1.42     |
| 1   | L1    | 677  | 1MA  | C2-N3   | 8.48  | 1.46        | 1.30     |
| 2   | L2    | 527  | A2M  | O4'-C1' | 8.17  | 1.60        | 1.42     |
| 51  | S1    | 1543 | B8N  | C6-N1   | 8.04  | 1.56        | 1.36     |
| 2   | L2    | 500  | PSU  | C2-N3   | 8.03  | 1.50        | 1.37     |
| 51  | S1    | 609  | PSU  | C2-N3   | 8.02  | 1.50        | 1.37     |
| 2   | L2    | 1361 | PSU  | C2-N3   | 8.01  | 1.50        | 1.37     |
| 1   | L1    | 1528 | PSU  | C2-N3   | 8.00  | 1.50        | 1.37     |
| 2   | L2    | 504  | PSU  | C2-N3   | 8.00  | 1.50        | 1.37     |
| 2   | L2    | 1303 | PSU  | C2-N3   | 8.00  | 1.50        | 1.37     |
| 51  | S1    | 1841 | PSU  | C2-N3   | 8.00  | 1.50        | 1.37     |
| 2   | L2    | 1264 | PSU  | C2-N3   | 7.99  | 1.50        | 1.37     |
| 2   | L2    | 506  | PSU  | C2-N3   | 7.99  | 1.50        | 1.37     |
| 51  | S1    | 1246 | PSU  | C2-N3   | 7.98  | 1.50        | 1.37     |
| 51  | S1    | 1566 | PSU  | C2-N3   | 7.98  | 1.50        | 1.37     |
| 51  | S1    | 1657 | PSU  | C2-N3   | 7.98  | 1.50        | 1.37     |
| 1   | L1    | 1533 | PSU  | C2-N3   | 7.97  | 1.50        | 1.37     |
| 2   | L2    | 472  | PSU  | C2-N3   | 7.97  | 1.50        | 1.37     |
| 51  | S1    | 1192 | PSU  | C2-N3   | 7.97  | 1.50        | 1.37     |
| 51  | S1    | 1543 | B8N  | C4-N3   | -7.96 | 1.26        | 1.40     |
| 51  | S1    | 1533 | PSU  | C2-N3   | 7.96  | 1.50        | 1.37     |
| 51  | S1    | 33   | PSU  | C2-N3   | 7.96  | 1.50        | 1.37     |
| 2   | L2    | 512  | PSU  | C2-N3   | 7.96  | 1.50        | 1.37     |
| 51  | S1    | 2046 | PSU  | C2-N3   | 7.96  | 1.50        | 1.37     |
| 7   | L7    | 74   | PSU  | C2-N3   | 7.95  | 1.50        | 1.37     |
| 51  | S1    | 455  | PSU  | C2-N3   | 7.95  | 1.50        | 1.37     |
| 2   | L2    | 1284 | PSU  | C2-N3   | 7.95  | 1.50        | 1.37     |
| 1   | L1    | 774  | PSU  | C2-N3   | 7.95  | 1.50        | 1.37     |
| 2   | L2    | 593  | PSU  | C2-N3   | 7.95  | 1.50        | 1.37     |
| 51  | S1    | 2048 | PSU  | C2-N3   | 7.94  | 1.50        | 1.37     |
| 2   | L2    | 1213 | PSU  | C2-N3   | 7.94  | 1.50        | 1.37     |
| 1   | L1    | 1093 | PSU  | C2-N3   | 7.94  | 1.50        | 1.37     |
| 51  | S1    | 104  | PSU  | C2-N3   | 7.94  | 1.50        | 1.37     |
| 1   | L1    | 1181 | PSU  | C2-N3   | 7.94  | 1.50        | 1.37     |
| 51  | S1    | 1292 | PSU  | C2-N3   | 7.94  | 1.50        | 1.37     |
| 2   | L2    | 560  | OMU  | C2-N1   | 7.94  | 1.50        | 1.38     |
| 1   | L1    | 239  | PSU  | C2-N3   | 7.93  | 1.50        | 1.37     |
| 2   | L2    | 626  | PSU  | C2-N3   | 7.93  | 1.50        | 1.37     |
| 51  | S1    | 2202 | PSU  | C2-N3   | 7.93  | 1.50        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 52  | S2    | 37   | MIA  | C6-N6   | 7.93 | 1.46        | 1.34     |
| 1   | L1    | 940  | PSU  | C2-N3   | 7.93 | 1.50        | 1.37     |
| 2   | L2    | 1194 | PSU  | C2-N3   | 7.92 | 1.50        | 1.37     |
| 2   | L2    | 1413 | PSU  | C2-N3   | 7.92 | 1.50        | 1.37     |
| 1   | L1    | 1664 | PSU  | C2-N3   | 7.92 | 1.50        | 1.37     |
| 51  | S1    | 12   | PSU  | C2-N3   | 7.92 | 1.50        | 1.37     |
| 2   | L2    | 597  | PSU  | C2-N3   | 7.92 | 1.50        | 1.37     |
| 1   | L1    | 1017 | PSU  | C2-N3   | 7.91 | 1.50        | 1.37     |
| 2   | L2    | 437  | PSU  | C2-N3   | 7.91 | 1.50        | 1.37     |
| 2   | L2    | 510  | PSU  | C2-N3   | 7.91 | 1.50        | 1.37     |
| 1   | L1    | 422  | PSU  | C2-N3   | 7.90 | 1.50        | 1.37     |
| 51  | S1    | 1156 | PSU  | C2-N3   | 7.89 | 1.50        | 1.37     |
| 2   | L2    | 1060 | PSU  | C2-N3   | 7.89 | 1.50        | 1.37     |
| 1   | L1    | 1011 | PSU  | C2-N3   | 7.88 | 1.50        | 1.37     |
| 2   | L2    | 1058 | PSU  | C2-N3   | 7.88 | 1.50        | 1.37     |
| 2   | L2    | 1144 | PSU  | C2-N3   | 7.88 | 1.50        | 1.37     |
| 2   | L2    | 1318 | PSU  | C2-N3   | 7.87 | 1.50        | 1.37     |
| 7   | L7    | 69   | PSU  | C2-N3   | 7.86 | 1.50        | 1.37     |
| 51  | S1    | 1539 | PSU  | C2-N3   | 7.85 | 1.50        | 1.37     |
| 2   | L2    | 78   | PSU  | C2-N3   | 7.85 | 1.50        | 1.37     |
| 2   | L2    | 1382 | PSU  | C2-N3   | 7.84 | 1.50        | 1.37     |
| 2   | L2    | 1077 | OMU  | C2-N1   | 7.84 | 1.50        | 1.38     |
| 2   | L2    | 1403 | PSU  | C2-N3   | 7.83 | 1.50        | 1.37     |
| 51  | S1    | 661  | OMU  | C2-N1   | 7.83 | 1.50        | 1.38     |
| 2   | L2    | 662  | PSU  | C2-N3   | 7.81 | 1.50        | 1.37     |
| 2   | L2    | 1265 | PSU  | C2-N3   | 7.79 | 1.50        | 1.37     |
| 1   | L1    | 1039 | OMU  | C2-N1   | 7.79 | 1.50        | 1.38     |
| 1   | L1    | 1171 | PSU  | C2-N3   | 7.75 | 1.50        | 1.37     |
| 1   | L1    | 672  | PSU  | C2-N3   | 7.72 | 1.50        | 1.37     |
| 7   | L7    | 101  | OMU  | O4'-C1' | 7.61 | 1.59        | 1.42     |
| 51  | S1    | 1543 | B8N  | C4-C5   | 7.52 | 1.64        | 1.47     |
| 2   | L2    | 1308 | 5MC  | O4'-C4' | 7.42 | 1.61        | 1.45     |
| 7   | L7    | 101  | OMU  | C2-N1   | 7.41 | 1.50        | 1.38     |
| 51  | S1    | 1833 | OMU  | C2-N1   | 7.38 | 1.50        | 1.38     |
| 51  | S1    | 1662 | OMU  | C2-N1   | 7.29 | 1.49        | 1.38     |
| 51  | S1    | 1777 | OMU  | C2-N1   | 7.27 | 1.49        | 1.38     |
| 1   | L1    | 847  | OMU  | C2-N1   | 7.27 | 1.49        | 1.38     |
| 2   | L2    | 667  | OMU  | C2-N1   | 7.26 | 1.49        | 1.38     |
| 1   | L1    | 1253 | OMU  | C2-N1   | 7.24 | 1.49        | 1.38     |
| 51  | S1    | 1979 | OMU  | C2-N1   | 7.24 | 1.49        | 1.38     |
| 1   | L1    | 1659 | OMU  | C2-N1   | 7.23 | 1.49        | 1.38     |
| 2   | L2    | 1419 | OMU  | C2-N1   | 7.23 | 1.49        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | L1    | 845  | OMU  | C2-N1 | 7.23 | 1.49        | 1.38     |
| 1   | L1    | 677  | 1MA  | C4-N3 | 7.22 | 1.50        | 1.35     |
| 51  | S1    | 1995 | 7MG  | C4-N9 | 7.22 | 1.46        | 1.37     |
| 2   | L2    | 56   | OMU  | C2-N1 | 7.22 | 1.49        | 1.38     |
| 51  | S1    | 1621 | OMU  | C2-N1 | 7.20 | 1.49        | 1.38     |
| 1   | L1    | 1371 | OMU  | C2-N1 | 7.19 | 1.49        | 1.38     |
| 51  | S1    | 8    | OMU  | C2-N1 | 7.18 | 1.49        | 1.38     |
| 51  | S1    | 29   | OMU  | C2-N1 | 7.18 | 1.49        | 1.38     |
| 2   | L2    | 1359 | OMU  | C2-N1 | 7.17 | 1.49        | 1.38     |
| 1   | L1    | 48   | OMU  | C2-N1 | 7.14 | 1.49        | 1.38     |
| 2   | L2    | 1308 | 5MC  | C5-C4 | 7.13 | 1.49        | 1.44     |
| 2   | L2    | 73   | OMU  | C2-N1 | 7.12 | 1.49        | 1.38     |
| 3   | L3    | 13   | OMU  | C2-N1 | 7.11 | 1.49        | 1.38     |
| 2   | L2    | 524  | 5MC  | C5-C4 | 7.10 | 1.49        | 1.44     |
| 51  | S1    | 1777 | OMU  | C2-N3 | 7.10 | 1.50        | 1.38     |
| 1   | L1    | 1253 | OMU  | C2-N3 | 7.09 | 1.50        | 1.38     |
| 1   | L1    | 1107 | OMU  | C2-N1 | 7.08 | 1.49        | 1.38     |
| 51  | S1    | 661  | OMU  | C2-N3 | 7.05 | 1.50        | 1.38     |
| 1   | L1    | 1659 | OMU  | C2-N3 | 7.04 | 1.50        | 1.38     |
| 2   | L2    | 1359 | OMU  | C2-N3 | 7.04 | 1.50        | 1.38     |
| 51  | S1    | 1662 | OMU  | C2-N3 | 7.04 | 1.50        | 1.38     |
| 51  | S1    | 1979 | OMU  | C2-N3 | 7.04 | 1.50        | 1.38     |
| 51  | S1    | 1621 | OMU  | C2-N3 | 7.03 | 1.50        | 1.38     |
| 2   | L2    | 56   | OMU  | C2-N3 | 7.01 | 1.50        | 1.38     |
| 2   | L2    | 667  | OMU  | C2-N3 | 7.01 | 1.50        | 1.38     |
| 51  | S1    | 8    | OMU  | C2-N3 | 7.00 | 1.50        | 1.38     |
| 1   | L1    | 845  | OMU  | C2-N3 | 7.00 | 1.50        | 1.38     |
| 51  | S1    | 29   | OMU  | C2-N3 | 6.99 | 1.50        | 1.38     |
| 1   | L1    | 847  | OMU  | C2-N3 | 6.98 | 1.50        | 1.38     |
| 3   | L3    | 13   | OMU  | C2-N3 | 6.97 | 1.50        | 1.38     |
| 2   | L2    | 1419 | OMU  | C2-N3 | 6.96 | 1.50        | 1.38     |
| 7   | L7    | 101  | OMU  | C2-N3 | 6.96 | 1.50        | 1.38     |
| 1   | L1    | 1371 | OMU  | C2-N3 | 6.95 | 1.50        | 1.38     |
| 1   | L1    | 48   | OMU  | C2-N3 | 6.95 | 1.50        | 1.38     |
| 1   | L1    | 1039 | OMU  | C2-N3 | 6.92 | 1.50        | 1.38     |
| 2   | L2    | 73   | OMU  | C2-N3 | 6.91 | 1.50        | 1.38     |
| 51  | S1    | 2061 | 5MC  | C4-N3 | 6.91 | 1.45        | 1.34     |
| 1   | L1    | 1107 | OMU  | C2-N3 | 6.90 | 1.50        | 1.38     |
| 51  | S1    | 1544 | 5MC  | C5-C4 | 6.88 | 1.49        | 1.44     |
| 2   | L2    | 1077 | OMU  | C2-N3 | 6.88 | 1.50        | 1.38     |
| 51  | S1    | 2061 | 5MC  | C5-C4 | 6.88 | 1.49        | 1.44     |
| 2   | L2    | 560  | OMU  | C2-N3 | 6.86 | 1.49        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | S1    | 1544 | 5MC  | C4-N3   | 6.86  | 1.45        | 1.34     |
| 51  | S1    | 1833 | OMU  | C2-N3   | 6.73  | 1.49        | 1.38     |
| 2   | L2    | 524  | 5MC  | C4-N3   | 6.72  | 1.44        | 1.34     |
| 51  | S1    | 1865 | OMG  | C4-N3   | 6.66  | 1.49        | 1.34     |
| 2   | L2    | 359  | OMC  | C2-N3   | 6.63  | 1.49        | 1.36     |
| 51  | S1    | 1623 | OMG  | C4-N3   | 6.63  | 1.49        | 1.34     |
| 1   | L1    | 959  | OMG  | C4-N3   | 6.62  | 1.49        | 1.34     |
| 2   | L2    | 1046 | OMG  | C4-N3   | 6.61  | 1.49        | 1.34     |
| 51  | S1    | 1647 | OMG  | C4-N3   | 6.61  | 1.49        | 1.34     |
| 2   | L2    | 1229 | OMG  | C4-N3   | 6.60  | 1.49        | 1.34     |
| 2   | L2    | 655  | OMG  | C4-N3   | 6.60  | 1.49        | 1.34     |
| 7   | L7    | 75   | OMG  | C4-N3   | 6.59  | 1.49        | 1.34     |
| 2   | L2    | 686  | OMG  | C4-N3   | 6.58  | 1.49        | 1.34     |
| 2   | L2    | 1360 | OMG  | C4-N3   | 6.58  | 1.49        | 1.34     |
| 51  | S1    | 600  | OMG  | C4-N3   | 6.57  | 1.49        | 1.34     |
| 1   | L1    | 856  | OMG  | C4-N3   | 6.55  | 1.49        | 1.34     |
| 1   | L1    | 858  | A2M  | O4'-C4' | -6.54 | 1.30        | 1.45     |
| 2   | L2    | 71   | OMG  | C4-N3   | 6.54  | 1.49        | 1.34     |
| 51  | S1    | 2008 | OMG  | C4-N3   | 6.53  | 1.49        | 1.34     |
| 51  | S1    | 2140 | OMC  | C2-N3   | 6.53  | 1.49        | 1.36     |
| 51  | S1    | 2151 | OMG  | C4-N3   | 6.53  | 1.49        | 1.34     |
| 2   | L2    | 1253 | OMG  | C4-N3   | 6.52  | 1.49        | 1.34     |
| 1   | L1    | 1626 | OMG  | C4-N3   | 6.52  | 1.49        | 1.34     |
| 51  | S1    | 2059 | OMC  | C2-N3   | 6.51  | 1.49        | 1.36     |
| 1   | L1    | 1552 | OMC  | C2-N3   | 6.51  | 1.49        | 1.36     |
| 51  | S1    | 18   | OMC  | C2-N3   | 6.50  | 1.49        | 1.36     |
| 1   | L1    | 695  | OMC  | C2-N3   | 6.50  | 1.49        | 1.36     |
| 2   | L2    | 1317 | OMC  | C2-N3   | 6.50  | 1.49        | 1.36     |
| 2   | L2    | 14   | OMC  | C2-N3   | 6.49  | 1.49        | 1.36     |
| 1   | L1    | 1540 | OMG  | C4-N3   | 6.49  | 1.49        | 1.34     |
| 2   | L2    | 534  | OMG  | C4-N3   | 6.49  | 1.49        | 1.34     |
| 51  | S1    | 1866 | OMC  | C2-N3   | 6.49  | 1.49        | 1.36     |
| 51  | S1    | 1550 | OMG  | C4-N3   | 6.48  | 1.49        | 1.34     |
| 51  | S1    | 38   | OMC  | C2-N3   | 6.48  | 1.49        | 1.36     |
| 2   | L2    | 1159 | OMC  | C2-N3   | 6.48  | 1.49        | 1.36     |
| 1   | L1    | 1524 | OMG  | C4-N3   | 6.47  | 1.49        | 1.34     |
| 2   | L2    | 1231 | OMG  | C4-N3   | 6.47  | 1.49        | 1.34     |
| 4   | L4    | 74   | OMG  | C4-N3   | 6.47  | 1.49        | 1.34     |
| 2   | L2    | 641  | OMG  | C4-N3   | 6.46  | 1.49        | 1.34     |
| 2   | L2    | 1185 | A2M  | O4'-C4' | -6.46 | 1.30        | 1.45     |
| 1   | L1    | 1010 | OMC  | C2-N3   | 6.46  | 1.49        | 1.36     |
| 51  | S1    | 2019 | OMC  | C2-N3   | 6.46  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | L2    | 443  | OMC  | C2-N3   | 6.45  | 1.49        | 1.36     |
| 51  | S1    | 668  | A2M  | O4'-C4' | -6.44 | 1.30        | 1.45     |
| 2   | L2    | 583  | OMC  | C2-N3   | 6.44  | 1.49        | 1.36     |
| 51  | S1    | 1829 | OMG  | C4-N3   | 6.42  | 1.48        | 1.34     |
| 1   | L1    | 1190 | OMG  | C4-N3   | 6.41  | 1.48        | 1.34     |
| 1   | L1    | 1527 | OMC  | C2-N3   | 6.41  | 1.49        | 1.36     |
| 51  | S1    | 1478 | OMG  | C4-N3   | 6.41  | 1.48        | 1.34     |
| 2   | L2    | 1248 | OMC  | C2-N3   | 6.40  | 1.49        | 1.36     |
| 2   | L2    | 1397 | OMC  | C2-N3   | 6.39  | 1.49        | 1.36     |
| 1   | L1    | 235  | A2M  | O4'-C4' | -6.38 | 1.30        | 1.45     |
| 1   | L1    | 669  | OMC  | C2-N3   | 6.38  | 1.49        | 1.36     |
| 51  | S1    | 1995 | 7MG  | C2-N3   | 6.35  | 1.48        | 1.33     |
| 2   | L2    | 443  | OMC  | C6-C5   | 6.33  | 1.49        | 1.35     |
| 2   | L2    | 1372 | A2M  | O4'-C4' | -6.33 | 1.30        | 1.45     |
| 2   | L2    | 628  | A2M  | O4'-C4' | -6.32 | 1.30        | 1.45     |
| 1   | L1    | 1010 | OMC  | C6-C5   | 6.32  | 1.49        | 1.35     |
| 51  | S1    | 969  | A2M  | O4'-C4' | -6.32 | 1.30        | 1.45     |
| 2   | L2    | 665  | A2M  | O4'-C4' | -6.32 | 1.30        | 1.45     |
| 1   | L1    | 1527 | OMC  | C6-C5   | 6.32  | 1.49        | 1.35     |
| 1   | L1    | 1539 | A2M  | O4'-C4' | -6.32 | 1.31        | 1.45     |
| 51  | S1    | 2021 | A2M  | O4'-C4' | -6.31 | 1.31        | 1.45     |
| 51  | S1    | 1544 | 5MC  | C2-N3   | 6.30  | 1.48        | 1.36     |
| 2   | L2    | 1397 | OMC  | C6-C5   | 6.30  | 1.49        | 1.35     |
| 51  | S1    | 1543 | B8N  | C6-C5   | 6.28  | 1.44        | 1.35     |
| 7   | L7    | 162  | A2M  | O4'-C4' | -6.26 | 1.31        | 1.45     |
| 1   | L1    | 678  | A2M  | O4'-C4' | -6.26 | 1.31        | 1.45     |
| 51  | S1    | 2061 | 5MC  | C2-N3   | 6.25  | 1.48        | 1.36     |
| 1   | L1    | 955  | A2M  | O4'-C4' | -6.25 | 1.31        | 1.45     |
| 51  | S1    | 98   | A2M  | O4'-C4' | -6.25 | 1.31        | 1.45     |
| 2   | L2    | 95   | A2M  | O4'-C4' | -6.25 | 1.31        | 1.45     |
| 2   | L2    | 591  | A2M  | O4'-C4' | -6.24 | 1.31        | 1.45     |
| 2   | L2    | 1248 | OMC  | C6-C5   | 6.24  | 1.49        | 1.35     |
| 1   | L1    | 69   | A2M  | O4'-C4' | -6.23 | 1.31        | 1.45     |
| 2   | L2    | 1078 | OMG  | C4-N3   | 6.23  | 1.48        | 1.34     |
| 51  | S1    | 28   | A2M  | O4'-C4' | -6.23 | 1.31        | 1.45     |
| 1   | L1    | 927  | A2M  | O4'-C4' | -6.22 | 1.31        | 1.45     |
| 51  | S1    | 479  | A2M  | O4'-C4' | -6.22 | 1.31        | 1.45     |
| 1   | L1    | 697  | A2M  | O4'-C4' | -6.21 | 1.31        | 1.45     |
| 51  | S1    | 897  | A2M  | O4'-C4' | -6.21 | 1.31        | 1.45     |
| 1   | L1    | 1373 | A2M  | O4'-C4' | -6.21 | 1.31        | 1.45     |
| 7   | L7    | 101  | OMU  | O4'-C4' | -6.20 | 1.31        | 1.45     |
| 7   | L7    | 43   | A2M  | O4'-C4' | -6.20 | 1.31        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | L1    | 669  | OMC  | C6-C5   | 6.19  | 1.49        | 1.35     |
| 2   | L2    | 570  | A2M  | O4'-C4' | -6.19 | 1.31        | 1.45     |
| 2   | L2    | 1067 | A2M  | O4'-C4' | -6.19 | 1.31        | 1.45     |
| 2   | L2    | 502  | A2M  | O4'-C4' | -6.18 | 1.31        | 1.45     |
| 2   | L2    | 604  | A2M  | O4'-C4' | -6.18 | 1.31        | 1.45     |
| 2   | L2    | 524  | 5MC  | C2-N3   | 6.17  | 1.48        | 1.36     |
| 2   | L2    | 1384 | A2M  | O4'-C4' | -6.16 | 1.31        | 1.45     |
| 2   | L2    | 527  | A2M  | O4'-C4' | -6.16 | 1.31        | 1.45     |
| 51  | S1    | 512  | A2M  | O4'-C4' | -6.15 | 1.31        | 1.45     |
| 51  | S1    | 1543 | B8N  | C2-N1   | 6.15  | 1.57        | 1.39     |
| 51  | S1    | 2019 | OMC  | C6-C5   | 6.14  | 1.49        | 1.35     |
| 51  | S1    | 38   | OMC  | C6-C5   | 6.13  | 1.49        | 1.35     |
| 1   | L1    | 305  | A2M  | O4'-C4' | -6.13 | 1.31        | 1.45     |
| 2   | L2    | 359  | OMC  | C6-C5   | 6.12  | 1.49        | 1.35     |
| 2   | L2    | 572  | A2M  | O4'-C4' | -6.12 | 1.31        | 1.45     |
| 1   | L1    | 1552 | OMC  | C6-C5   | 6.11  | 1.49        | 1.35     |
| 51  | S1    | 1866 | OMC  | C6-C5   | 6.11  | 1.49        | 1.35     |
| 2   | L2    | 14   | OMC  | C6-C5   | 6.10  | 1.49        | 1.35     |
| 2   | L2    | 1159 | OMC  | C6-C5   | 6.10  | 1.49        | 1.35     |
| 51  | S1    | 2140 | OMC  | C6-C5   | 6.09  | 1.49        | 1.35     |
| 2   | L2    | 583  | OMC  | C6-C5   | 6.08  | 1.49        | 1.35     |
| 2   | L2    | 1308 | 5MC  | C4-N3   | 6.07  | 1.43        | 1.34     |
| 51  | S1    | 2059 | OMC  | C6-C5   | 6.07  | 1.49        | 1.35     |
| 2   | L2    | 382  | A2M  | O4'-C4' | -6.07 | 1.31        | 1.45     |
| 1   | L1    | 695  | OMC  | C6-C5   | 6.06  | 1.49        | 1.35     |
| 2   | L2    | 1317 | OMC  | C6-C5   | 6.05  | 1.49        | 1.35     |
| 51  | S1    | 18   | OMC  | C6-C5   | 6.03  | 1.49        | 1.35     |
| 2   | L2    | 1403 | PSU  | C6-N1   | 6.00  | 1.46        | 1.36     |
| 1   | L1    | 681  | A2M  | O4'-C4' | -6.00 | 1.31        | 1.45     |
| 2   | L2    | 1308 | 5MC  | C2-N3   | 5.95  | 1.48        | 1.36     |
| 51  | S1    | 1539 | PSU  | C6-N1   | 5.89  | 1.45        | 1.36     |
| 7   | L7    | 69   | PSU  | C6-N1   | 5.84  | 1.45        | 1.36     |
| 1   | L1    | 1017 | PSU  | C6-N1   | 5.83  | 1.45        | 1.36     |
| 51  | S1    | 1833 | OMU  | C6-C5   | 5.82  | 1.48        | 1.35     |
| 1   | L1    | 1171 | PSU  | C6-N1   | 5.79  | 1.45        | 1.36     |
| 2   | L2    | 1382 | PSU  | C6-N1   | 5.79  | 1.45        | 1.36     |
| 7   | L7    | 101  | OMU  | C6-C5   | 5.78  | 1.48        | 1.35     |
| 1   | L1    | 672  | PSU  | C6-N1   | 5.77  | 1.45        | 1.36     |
| 1   | L1    | 1011 | PSU  | C6-N1   | 5.76  | 1.45        | 1.36     |
| 1   | L1    | 1371 | OMU  | C6-C5   | 5.75  | 1.48        | 1.35     |
| 51  | S1    | 8    | OMU  | C6-C5   | 5.75  | 1.48        | 1.35     |
| 51  | S1    | 1662 | OMU  | C6-C5   | 5.75  | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 51  | S1    | 1979 | OMU  | C6-C5 | 5.75 | 1.48        | 1.35     |
| 51  | S1    | 1621 | OMU  | C6-C5 | 5.74 | 1.48        | 1.35     |
| 2   | L2    | 662  | PSU  | C6-N1 | 5.74 | 1.45        | 1.36     |
| 2   | L2    | 1359 | OMU  | C6-C5 | 5.74 | 1.48        | 1.35     |
| 51  | S1    | 1995 | 7MG  | C4-N3 | 5.74 | 1.47        | 1.34     |
| 1   | L1    | 48   | OMU  | C6-C5 | 5.73 | 1.48        | 1.35     |
| 1   | L1    | 847  | OMU  | C6-C5 | 5.73 | 1.48        | 1.35     |
| 2   | L2    | 56   | OMU  | C6-C5 | 5.73 | 1.48        | 1.35     |
| 2   | L2    | 667  | OMU  | C6-C5 | 5.73 | 1.48        | 1.35     |
| 1   | L1    | 1253 | OMU  | C6-C5 | 5.73 | 1.48        | 1.35     |
| 2   | L2    | 1058 | PSU  | C6-N1 | 5.73 | 1.45        | 1.36     |
| 51  | S1    | 29   | OMU  | C6-C5 | 5.72 | 1.48        | 1.35     |
| 2   | L2    | 1413 | PSU  | C6-N1 | 5.72 | 1.45        | 1.36     |
| 1   | L1    | 845  | OMU  | C6-C5 | 5.72 | 1.48        | 1.35     |
| 1   | L1    | 1659 | OMU  | C6-C5 | 5.71 | 1.48        | 1.35     |
| 51  | S1    | 1777 | OMU  | C6-C5 | 5.71 | 1.48        | 1.35     |
| 2   | L2    | 1419 | OMU  | C6-C5 | 5.71 | 1.48        | 1.35     |
| 2   | L2    | 73   | OMU  | C6-C5 | 5.70 | 1.48        | 1.35     |
| 3   | L3    | 13   | OMU  | C6-C5 | 5.68 | 1.48        | 1.35     |
| 1   | L1    | 1528 | PSU  | C6-N1 | 5.66 | 1.45        | 1.36     |
| 1   | L1    | 1107 | OMU  | C6-C5 | 5.66 | 1.48        | 1.35     |
| 2   | L2    | 78   | PSU  | C6-N1 | 5.54 | 1.45        | 1.36     |
| 51  | S1    | 1566 | PSU  | C6-N1 | 5.52 | 1.45        | 1.36     |
| 2   | L2    | 560  | OMU  | C6-C5 | 5.52 | 1.47        | 1.35     |
| 1   | L1    | 1664 | PSU  | C6-N1 | 5.51 | 1.45        | 1.36     |
| 1   | L1    | 1039 | OMU  | C6-C5 | 5.51 | 1.47        | 1.35     |
| 51  | S1    | 1841 | PSU  | C6-N1 | 5.51 | 1.45        | 1.36     |
| 51  | S1    | 661  | OMU  | C6-C5 | 5.50 | 1.47        | 1.35     |
| 2   | L2    | 510  | PSU  | C6-N1 | 5.50 | 1.45        | 1.36     |
| 51  | S1    | 1156 | PSU  | C6-N1 | 5.50 | 1.45        | 1.36     |
| 51  | S1    | 2046 | PSU  | C6-N1 | 5.49 | 1.45        | 1.36     |
| 2   | L2    | 437  | PSU  | C6-N1 | 5.48 | 1.45        | 1.36     |
| 51  | S1    | 33   | PSU  | C6-N1 | 5.48 | 1.45        | 1.36     |
| 1   | L1    | 1093 | PSU  | C6-N1 | 5.47 | 1.45        | 1.36     |
| 2   | L2    | 506  | PSU  | C6-N1 | 5.47 | 1.45        | 1.36     |
| 2   | L2    | 1284 | PSU  | C6-N1 | 5.47 | 1.45        | 1.36     |
| 2   | L2    | 1318 | PSU  | C6-N1 | 5.47 | 1.45        | 1.36     |
| 51  | S1    | 1623 | OMG  | C2-N3 | 5.47 | 1.46        | 1.33     |
| 1   | L1    | 422  | PSU  | C6-N1 | 5.47 | 1.45        | 1.36     |
| 7   | L7    | 74   | PSU  | C6-N1 | 5.47 | 1.45        | 1.36     |
| 2   | L2    | 500  | PSU  | C6-N1 | 5.47 | 1.45        | 1.36     |
| 2   | L2    | 1077 | OMU  | C6-C5 | 5.47 | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | L1    | 239  | PSU  | C6-N1 | 5.46 | 1.45        | 1.36     |
| 1   | L1    | 940  | PSU  | C6-N1 | 5.46 | 1.45        | 1.36     |
| 51  | S1    | 12   | PSU  | C6-N1 | 5.46 | 1.45        | 1.36     |
| 2   | L2    | 1213 | PSU  | C6-N1 | 5.46 | 1.45        | 1.36     |
| 51  | S1    | 1533 | PSU  | C6-N1 | 5.46 | 1.45        | 1.36     |
| 1   | L1    | 774  | PSU  | C6-N1 | 5.46 | 1.45        | 1.36     |
| 1   | L1    | 1181 | PSU  | C6-N1 | 5.44 | 1.45        | 1.36     |
| 51  | S1    | 1657 | PSU  | C6-N1 | 5.44 | 1.45        | 1.36     |
| 51  | S1    | 1865 | OMG  | C2-N3 | 5.44 | 1.46        | 1.33     |
| 2   | L2    | 1265 | PSU  | C6-N1 | 5.44 | 1.45        | 1.36     |
| 2   | L2    | 1060 | PSU  | C6-N1 | 5.44 | 1.45        | 1.36     |
| 1   | L1    | 959  | OMG  | C2-N3 | 5.44 | 1.46        | 1.33     |
| 2   | L2    | 472  | PSU  | C6-N1 | 5.44 | 1.45        | 1.36     |
| 2   | L2    | 504  | PSU  | C6-N1 | 5.44 | 1.45        | 1.36     |
| 2   | L2    | 626  | PSU  | C6-N1 | 5.43 | 1.45        | 1.36     |
| 2   | L2    | 597  | PSU  | C6-N1 | 5.43 | 1.45        | 1.36     |
| 51  | S1    | 1292 | PSU  | C6-N1 | 5.43 | 1.45        | 1.36     |
| 2   | L2    | 512  | PSU  | C6-N1 | 5.42 | 1.45        | 1.36     |
| 2   | L2    | 1144 | PSU  | C6-N1 | 5.42 | 1.45        | 1.36     |
| 51  | S1    | 2202 | PSU  | C6-N1 | 5.42 | 1.45        | 1.36     |
| 51  | S1    | 609  | PSU  | C6-N1 | 5.41 | 1.45        | 1.36     |
| 2   | L2    | 1303 | PSU  | C6-N1 | 5.41 | 1.45        | 1.36     |
| 1   | L1    | 1533 | PSU  | C6-N1 | 5.40 | 1.45        | 1.36     |
| 51  | S1    | 1192 | PSU  | C6-N1 | 5.40 | 1.45        | 1.36     |
| 51  | S1    | 600  | OMG  | C2-N3 | 5.39 | 1.46        | 1.33     |
| 51  | S1    | 1246 | PSU  | C6-N1 | 5.39 | 1.45        | 1.36     |
| 2   | L2    | 1360 | OMG  | C2-N3 | 5.39 | 1.46        | 1.33     |
| 2   | L2    | 1046 | OMG  | C2-N3 | 5.39 | 1.46        | 1.33     |
| 2   | L2    | 1264 | PSU  | C6-N1 | 5.39 | 1.45        | 1.36     |
| 51  | S1    | 104  | PSU  | C6-N1 | 5.39 | 1.45        | 1.36     |
| 2   | L2    | 1229 | OMG  | C2-N3 | 5.39 | 1.46        | 1.33     |
| 2   | L2    | 593  | PSU  | C6-N1 | 5.39 | 1.45        | 1.36     |
| 2   | L2    | 1194 | PSU  | C6-N1 | 5.38 | 1.45        | 1.36     |
| 2   | L2    | 359  | OMC  | C4-N3 | 5.38 | 1.45        | 1.34     |
| 51  | S1    | 1647 | OMG  | C2-N3 | 5.38 | 1.46        | 1.33     |
| 51  | S1    | 455  | PSU  | C6-N1 | 5.38 | 1.45        | 1.36     |
| 2   | L2    | 686  | OMG  | C2-N3 | 5.37 | 1.46        | 1.33     |
| 51  | S1    | 2048 | PSU  | C6-N1 | 5.37 | 1.45        | 1.36     |
| 2   | L2    | 655  | OMG  | C2-N3 | 5.37 | 1.46        | 1.33     |
| 2   | L2    | 1361 | PSU  | C6-N1 | 5.37 | 1.45        | 1.36     |
| 1   | L1    | 695  | OMC  | C4-N3 | 5.32 | 1.45        | 1.34     |
| 2   | L2    | 534  | OMG  | C2-N3 | 5.32 | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | L2    | 1159 | OMC  | C4-N3  | 5.32  | 1.45        | 1.34     |
| 7   | L7    | 75   | OMG  | C2-N3  | 5.31  | 1.46        | 1.33     |
| 1   | L1    | 1552 | OMC  | C4-N3  | 5.31  | 1.45        | 1.34     |
| 51  | S1    | 2151 | OMG  | C2-N3  | 5.31  | 1.46        | 1.33     |
| 51  | S1    | 2059 | OMC  | C4-N3  | 5.31  | 1.45        | 1.34     |
| 51  | S1    | 2140 | OMC  | C4-N3  | 5.31  | 1.45        | 1.34     |
| 51  | S1    | 2019 | OMC  | C4-N3  | 5.31  | 1.45        | 1.34     |
| 51  | S1    | 38   | OMC  | C4-N3  | 5.30  | 1.45        | 1.34     |
| 51  | S1    | 1866 | OMC  | C4-N3  | 5.30  | 1.45        | 1.34     |
| 2   | L2    | 14   | OMC  | C4-N3  | 5.30  | 1.45        | 1.34     |
| 51  | S1    | 18   | OMC  | C4-N3  | 5.29  | 1.45        | 1.34     |
| 7   | L7    | 101  | OMU  | C1'-N1 | -5.29 | 1.32        | 1.47     |
| 51  | S1    | 2008 | OMG  | C2-N3  | 5.29  | 1.46        | 1.33     |
| 2   | L2    | 1231 | OMG  | C2-N3  | 5.28  | 1.46        | 1.33     |
| 2   | L2    | 583  | OMC  | C4-N3  | 5.26  | 1.44        | 1.34     |
| 4   | L4    | 74   | OMG  | C2-N3  | 5.26  | 1.45        | 1.33     |
| 2   | L2    | 1317 | OMC  | C4-N3  | 5.25  | 1.44        | 1.34     |
| 51  | S1    | 1478 | OMG  | C2-N3  | 5.17  | 1.45        | 1.33     |
| 2   | L2    | 71   | OMG  | C2-N3  | 5.17  | 1.45        | 1.33     |
| 1   | L1    | 1190 | OMG  | C2-N3  | 5.15  | 1.45        | 1.33     |
| 1   | L1    | 1527 | OMC  | C2-N1  | 5.15  | 1.50        | 1.40     |
| 2   | L2    | 1248 | OMC  | C4-N3  | 5.11  | 1.44        | 1.34     |
| 1   | L1    | 1524 | OMG  | C2-N3  | 5.10  | 1.45        | 1.33     |
| 1   | L1    | 1527 | OMC  | C4-N3  | 5.10  | 1.44        | 1.34     |
| 2   | L2    | 1253 | OMG  | C2-N3  | 5.08  | 1.45        | 1.33     |
| 1   | L1    | 1626 | OMG  | C2-N3  | 5.04  | 1.45        | 1.33     |
| 1   | L1    | 856  | OMG  | C2-N3  | 5.04  | 1.45        | 1.33     |
| 51  | S1    | 1550 | OMG  | C2-N3  | 5.02  | 1.45        | 1.33     |
| 1   | L1    | 669  | OMC  | C4-N3  | 5.02  | 1.44        | 1.34     |
| 2   | L2    | 1078 | OMG  | C2-N3  | 5.01  | 1.45        | 1.33     |
| 1   | L1    | 1010 | OMC  | C4-N3  | 5.01  | 1.44        | 1.34     |
| 2   | L2    | 1397 | OMC  | C4-N3  | 5.01  | 1.44        | 1.34     |
| 2   | L2    | 443  | OMC  | C4-N3  | 5.00  | 1.44        | 1.34     |
| 1   | L1    | 1540 | OMG  | C2-N3  | 5.00  | 1.45        | 1.33     |
| 2   | L2    | 641  | OMG  | C2-N3  | 4.96  | 1.45        | 1.33     |
| 2   | L2    | 1308 | 5MC  | C4-N4  | 4.94  | 1.46        | 1.34     |
| 51  | S1    | 1829 | OMG  | C2-N3  | 4.93  | 1.45        | 1.33     |
| 2   | L2    | 359  | OMC  | C4-N4  | 4.92  | 1.45        | 1.33     |
| 2   | L2    | 1248 | OMC  | C2-N1  | 4.92  | 1.50        | 1.40     |
| 51  | S1    | 2140 | OMC  | C4-N4  | 4.92  | 1.45        | 1.33     |
| 2   | L2    | 1397 | OMC  | C2-N1  | 4.90  | 1.50        | 1.40     |
| 1   | L1    | 1010 | OMC  | C4-N4  | 4.90  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | L2    | 583  | OMC  | C4-N4  | 4.89  | 1.45        | 1.33     |
| 51  | S1    | 2059 | OMC  | C4-N4  | 4.88  | 1.45        | 1.33     |
| 51  | S1    | 1866 | OMC  | C4-N4  | 4.87  | 1.45        | 1.33     |
| 51  | S1    | 38   | OMC  | C4-N4  | 4.87  | 1.45        | 1.33     |
| 1   | L1    | 695  | OMC  | C4-N4  | 4.87  | 1.45        | 1.33     |
| 1   | L1    | 1552 | OMC  | C4-N4  | 4.86  | 1.45        | 1.33     |
| 2   | L2    | 14   | OMC  | C4-N4  | 4.86  | 1.45        | 1.33     |
| 51  | S1    | 2019 | OMC  | C4-N4  | 4.86  | 1.45        | 1.33     |
| 2   | L2    | 1159 | OMC  | C4-N4  | 4.85  | 1.45        | 1.33     |
| 2   | L2    | 1360 | OMG  | C2-N2  | 4.84  | 1.45        | 1.34     |
| 51  | S1    | 1647 | OMG  | C2-N2  | 4.84  | 1.45        | 1.34     |
| 1   | L1    | 959  | OMG  | C2-N2  | 4.84  | 1.45        | 1.34     |
| 7   | L7    | 75   | OMG  | C2-N2  | 4.83  | 1.45        | 1.34     |
| 2   | L2    | 1229 | OMG  | C2-N2  | 4.83  | 1.45        | 1.34     |
| 51  | S1    | 1865 | OMG  | C2-N2  | 4.83  | 1.45        | 1.34     |
| 2   | L2    | 1317 | OMC  | C4-N4  | 4.83  | 1.45        | 1.33     |
| 51  | S1    | 18   | OMC  | C4-N4  | 4.83  | 1.45        | 1.33     |
| 2   | L2    | 655  | OMG  | C2-N2  | 4.82  | 1.45        | 1.34     |
| 2   | L2    | 686  | OMG  | C2-N2  | 4.82  | 1.45        | 1.34     |
| 51  | S1    | 1623 | OMG  | C2-N2  | 4.82  | 1.45        | 1.34     |
| 2   | L2    | 1046 | OMG  | C2-N2  | 4.81  | 1.45        | 1.34     |
| 51  | S1    | 2008 | OMG  | C2-N2  | 4.81  | 1.45        | 1.34     |
| 51  | S1    | 600  | OMG  | C2-N2  | 4.78  | 1.45        | 1.34     |
| 4   | L4    | 74   | OMG  | C2-N2  | 4.77  | 1.45        | 1.34     |
| 51  | S1    | 2151 | OMG  | C2-N2  | 4.76  | 1.45        | 1.34     |
| 51  | S1    | 2061 | 5MC  | C6-N1  | 4.76  | 1.46        | 1.38     |
| 1   | L1    | 1190 | OMG  | C2-N2  | 4.76  | 1.45        | 1.34     |
| 1   | L1    | 1010 | OMC  | C2-N1  | 4.73  | 1.50        | 1.40     |
| 2   | L2    | 534  | OMG  | C2-N2  | 4.73  | 1.45        | 1.34     |
| 2   | L2    | 1231 | OMG  | C2-N2  | 4.73  | 1.45        | 1.34     |
| 51  | S1    | 1478 | OMG  | C2-N2  | 4.72  | 1.45        | 1.34     |
| 2   | L2    | 14   | OMC  | C2-N1  | 4.72  | 1.50        | 1.40     |
| 7   | L7    | 69   | PSU  | C1'-C5 | -4.71 | 1.39        | 1.50     |
| 51  | S1    | 2140 | OMC  | C2-N1  | 4.71  | 1.49        | 1.40     |
| 51  | S1    | 1866 | OMC  | C2-N1  | 4.70  | 1.49        | 1.40     |
| 2   | L2    | 1397 | OMC  | C4-N4  | 4.69  | 1.45        | 1.33     |
| 2   | L2    | 583  | OMC  | C2-N1  | 4.69  | 1.49        | 1.40     |
| 51  | S1    | 2059 | OMC  | C2-N1  | 4.69  | 1.49        | 1.40     |
| 2   | L2    | 524  | 5MC  | C6-N1  | 4.69  | 1.46        | 1.38     |
| 2   | L2    | 1078 | OMG  | C2-N2  | 4.69  | 1.45        | 1.34     |
| 2   | L2    | 1382 | PSU  | C1'-C5 | -4.68 | 1.39        | 1.50     |
| 51  | S1    | 1544 | 5MC  | C6-N1  | 4.67  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | L1    | 669  | OMC  | C4-N4  | 4.65  | 1.45        | 1.33     |
| 2   | L2    | 443  | OMC  | C2-N1  | 4.65  | 1.49        | 1.40     |
| 2   | L2    | 1248 | OMC  | C4-N4  | 4.65  | 1.45        | 1.33     |
| 2   | L2    | 1058 | PSU  | C1'-C5 | -4.65 | 1.39        | 1.50     |
| 1   | L1    | 1552 | OMC  | C2-N1  | 4.65  | 1.49        | 1.40     |
| 2   | L2    | 359  | OMC  | C2-N1  | 4.65  | 1.49        | 1.40     |
| 51  | S1    | 2019 | OMC  | C2-N1  | 4.64  | 1.49        | 1.40     |
| 2   | L2    | 1159 | OMC  | C2-N1  | 4.64  | 1.49        | 1.40     |
| 1   | L1    | 1527 | OMC  | C4-N4  | 4.64  | 1.45        | 1.33     |
| 2   | L2    | 662  | PSU  | C1'-C5 | -4.64 | 1.39        | 1.50     |
| 51  | S1    | 38   | OMC  | C2-N1  | 4.64  | 1.49        | 1.40     |
| 1   | L1    | 672  | PSU  | C1'-C5 | -4.63 | 1.39        | 1.50     |
| 2   | L2    | 1317 | OMC  | C2-N1  | 4.63  | 1.49        | 1.40     |
| 51  | S1    | 1539 | PSU  | C1'-C5 | -4.63 | 1.39        | 1.50     |
| 1   | L1    | 695  | OMC  | C2-N1  | 4.62  | 1.49        | 1.40     |
| 51  | S1    | 18   | OMC  | C2-N1  | 4.59  | 1.49        | 1.40     |
| 2   | L2    | 1413 | PSU  | C1'-C5 | -4.59 | 1.39        | 1.50     |
| 2   | L2    | 1403 | PSU  | C1'-C5 | -4.58 | 1.39        | 1.50     |
| 1   | L1    | 1017 | PSU  | C1'-C5 | -4.58 | 1.39        | 1.50     |
| 1   | L1    | 1171 | PSU  | C1'-C5 | -4.55 | 1.40        | 1.50     |
| 2   | L2    | 443  | OMC  | C4-N4  | 4.54  | 1.44        | 1.33     |
| 1   | L1    | 1528 | PSU  | C1'-C5 | -4.52 | 1.40        | 1.50     |
| 1   | L1    | 1540 | OMG  | C2-N2  | 4.46  | 1.44        | 1.34     |
| 51  | S1    | 1544 | 5MC  | C4-N4  | 4.46  | 1.45        | 1.34     |
| 1   | L1    | 669  | OMC  | C2-N1  | 4.45  | 1.49        | 1.40     |
| 51  | S1    | 1841 | PSU  | C1'-C5 | -4.45 | 1.40        | 1.50     |
| 51  | S1    | 1657 | PSU  | C1'-C5 | -4.45 | 1.40        | 1.50     |
| 2   | L2    | 502  | A2M  | C6-N6  | 4.45  | 1.45        | 1.34     |
| 2   | L2    | 1253 | OMG  | C2-N2  | 4.44  | 1.44        | 1.34     |
| 1   | L1    | 1626 | OMG  | C2-N2  | 4.42  | 1.44        | 1.34     |
| 2   | L2    | 1060 | PSU  | C1'-C5 | -4.42 | 1.40        | 1.50     |
| 51  | S1    | 28   | A2M  | C6-N6  | 4.42  | 1.45        | 1.34     |
| 51  | S1    | 1544 | 5MC  | C2-N1  | 4.42  | 1.49        | 1.40     |
| 1   | L1    | 1181 | PSU  | C1'-C5 | -4.42 | 1.40        | 1.50     |
| 51  | S1    | 1550 | OMG  | C2-N2  | 4.42  | 1.44        | 1.34     |
| 2   | L2    | 71   | OMG  | C2-N2  | 4.41  | 1.44        | 1.34     |
| 2   | L2    | 1361 | PSU  | C1'-C5 | -4.41 | 1.40        | 1.50     |
| 2   | L2    | 591  | A2M  | C6-N6  | 4.41  | 1.45        | 1.34     |
| 51  | S1    | 479  | A2M  | C6-N6  | 4.41  | 1.45        | 1.34     |
| 51  | S1    | 2061 | 5MC  | C4-N4  | 4.41  | 1.45        | 1.34     |
| 2   | L2    | 1372 | A2M  | C6-N6  | 4.40  | 1.45        | 1.34     |
| 1   | L1    | 235  | A2M  | C6-N6  | 4.40  | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 51  | S1    | 512  | A2M  | C6-N6  | 4.40  | 1.45        | 1.34     |
| 1   | L1    | 774  | PSU  | C1'-C5 | -4.40 | 1.40        | 1.50     |
| 1   | L1    | 1524 | OMG  | C2-N2  | 4.40  | 1.44        | 1.34     |
| 7   | L7    | 162  | A2M  | C6-N6  | 4.40  | 1.45        | 1.34     |
| 51  | S1    | 98   | A2M  | C6-N6  | 4.40  | 1.45        | 1.34     |
| 2   | L2    | 1144 | PSU  | C1'-C5 | -4.39 | 1.40        | 1.50     |
| 2   | L2    | 500  | PSU  | C1'-C5 | -4.39 | 1.40        | 1.50     |
| 2   | L2    | 1213 | PSU  | C1'-C5 | -4.39 | 1.40        | 1.50     |
| 51  | S1    | 2046 | PSU  | C1'-C5 | -4.39 | 1.40        | 1.50     |
| 51  | S1    | 897  | A2M  | C6-N6  | 4.39  | 1.45        | 1.34     |
| 2   | L2    | 665  | A2M  | C6-N6  | 4.39  | 1.45        | 1.34     |
| 51  | S1    | 2021 | A2M  | C6-N6  | 4.39  | 1.45        | 1.34     |
| 2   | L2    | 524  | 5MC  | C4-N4  | 4.39  | 1.45        | 1.34     |
| 2   | L2    | 570  | A2M  | C6-N6  | 4.39  | 1.45        | 1.34     |
| 1   | L1    | 239  | PSU  | C1'-C5 | -4.38 | 1.40        | 1.50     |
| 1   | L1    | 1373 | A2M  | C6-N6  | 4.38  | 1.45        | 1.34     |
| 2   | L2    | 1067 | A2M  | C6-N6  | 4.38  | 1.45        | 1.34     |
| 2   | L2    | 95   | A2M  | C6-N6  | 4.38  | 1.45        | 1.34     |
| 2   | L2    | 628  | A2M  | C6-N6  | 4.38  | 1.45        | 1.34     |
| 1   | L1    | 955  | A2M  | C6-N6  | 4.38  | 1.45        | 1.34     |
| 51  | S1    | 1246 | PSU  | C1'-C5 | -4.38 | 1.40        | 1.50     |
| 2   | L2    | 593  | PSU  | C1'-C5 | -4.38 | 1.40        | 1.50     |
| 51  | S1    | 1777 | OMU  | C4-N3  | 4.38  | 1.46        | 1.38     |
| 1   | L1    | 305  | A2M  | C6-N6  | 4.38  | 1.45        | 1.34     |
| 2   | L2    | 604  | A2M  | C6-N6  | 4.37  | 1.45        | 1.34     |
| 51  | S1    | 33   | PSU  | C1'-C5 | -4.37 | 1.40        | 1.50     |
| 7   | L7    | 43   | A2M  | C6-N6  | 4.37  | 1.45        | 1.34     |
| 1   | L1    | 678  | A2M  | C6-N6  | 4.37  | 1.45        | 1.34     |
| 51  | S1    | 2048 | PSU  | C1'-C5 | -4.37 | 1.40        | 1.50     |
| 1   | L1    | 940  | PSU  | C1'-C5 | -4.37 | 1.40        | 1.50     |
| 2   | L2    | 472  | PSU  | C1'-C5 | -4.37 | 1.40        | 1.50     |
| 51  | S1    | 104  | PSU  | C1'-C5 | -4.37 | 1.40        | 1.50     |
| 2   | L2    | 1303 | PSU  | C1'-C5 | -4.36 | 1.40        | 1.50     |
| 2   | L2    | 512  | PSU  | C1'-C5 | -4.36 | 1.40        | 1.50     |
| 2   | L2    | 1194 | PSU  | C1'-C5 | -4.36 | 1.40        | 1.50     |
| 51  | S1    | 1829 | OMG  | C2-N2  | 4.36  | 1.44        | 1.34     |
| 2   | L2    | 626  | PSU  | C1'-C5 | -4.36 | 1.40        | 1.50     |
| 51  | S1    | 1533 | PSU  | C1'-C5 | -4.36 | 1.40        | 1.50     |
| 51  | S1    | 1292 | PSU  | C1'-C5 | -4.35 | 1.40        | 1.50     |
| 7   | L7    | 74   | PSU  | C1'-C5 | -4.35 | 1.40        | 1.50     |
| 2   | L2    | 506  | PSU  | C1'-C5 | -4.35 | 1.40        | 1.50     |
| 2   | L2    | 524  | 5MC  | C2-N1  | 4.35  | 1.49        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | L1    | 1107 | OMU  | C4-N3   | 4.35  | 1.46        | 1.38     |
| 1   | L1    | 1093 | PSU  | C1'-C5  | -4.35 | 1.40        | 1.50     |
| 51  | S1    | 1156 | PSU  | C1'-C5  | -4.35 | 1.40        | 1.50     |
| 2   | L2    | 597  | PSU  | C1'-C5  | -4.34 | 1.40        | 1.50     |
| 2   | L2    | 572  | A2M  | C6-N6   | 4.34  | 1.45        | 1.34     |
| 1   | L1    | 422  | PSU  | C1'-C5  | -4.34 | 1.40        | 1.50     |
| 2   | L2    | 1419 | OMU  | C4-N3   | 4.33  | 1.46        | 1.38     |
| 1   | L1    | 1253 | OMU  | C4-N3   | 4.33  | 1.46        | 1.38     |
| 2   | L2    | 1308 | 5MC  | O4'-C1' | -4.33 | 1.32        | 1.42     |
| 2   | L2    | 641  | OMG  | C2-N2   | 4.33  | 1.44        | 1.34     |
| 51  | S1    | 1621 | OMU  | C4-N3   | 4.33  | 1.46        | 1.38     |
| 1   | L1    | 697  | A2M  | C6-N6   | 4.33  | 1.45        | 1.34     |
| 2   | L2    | 1318 | PSU  | C1'-C5  | -4.33 | 1.40        | 1.50     |
| 51  | S1    | 1979 | OMU  | C4-N3   | 4.33  | 1.46        | 1.38     |
| 1   | L1    | 856  | OMG  | C2-N2   | 4.32  | 1.44        | 1.34     |
| 2   | L2    | 510  | PSU  | C1'-C5  | -4.32 | 1.40        | 1.50     |
| 3   | L3    | 13   | OMU  | C4-N3   | 4.32  | 1.46        | 1.38     |
| 51  | S1    | 609  | PSU  | C1'-C5  | -4.32 | 1.40        | 1.50     |
| 1   | L1    | 1659 | OMU  | C4-N3   | 4.32  | 1.46        | 1.38     |
| 51  | S1    | 29   | OMU  | C4-N3   | 4.31  | 1.46        | 1.38     |
| 2   | L2    | 504  | PSU  | C1'-C5  | -4.31 | 1.40        | 1.50     |
| 51  | S1    | 969  | A2M  | C6-N6   | 4.31  | 1.45        | 1.34     |
| 51  | S1    | 1662 | OMU  | C4-N3   | 4.31  | 1.46        | 1.38     |
| 1   | L1    | 1533 | PSU  | C1'-C5  | -4.30 | 1.40        | 1.50     |
| 2   | L2    | 56   | OMU  | C4-N3   | 4.30  | 1.46        | 1.38     |
| 2   | L2    | 1359 | OMU  | C4-N3   | 4.29  | 1.46        | 1.38     |
| 2   | L2    | 78   | PSU  | C1'-C5  | -4.29 | 1.40        | 1.50     |
| 51  | S1    | 661  | OMU  | C4-N3   | 4.29  | 1.46        | 1.38     |
| 1   | L1    | 845  | OMU  | C4-N3   | 4.29  | 1.46        | 1.38     |
| 51  | S1    | 1566 | PSU  | C1'-C5  | -4.28 | 1.40        | 1.50     |
| 2   | L2    | 1284 | PSU  | C1'-C5  | -4.28 | 1.40        | 1.50     |
| 51  | S1    | 2061 | 5MC  | C2-N1   | 4.28  | 1.49        | 1.40     |
| 51  | S1    | 2202 | PSU  | C1'-C5  | -4.28 | 1.40        | 1.50     |
| 7   | L7    | 101  | OMU  | C4-N3   | 4.27  | 1.45        | 1.38     |
| 51  | S1    | 12   | PSU  | C1'-C5  | -4.26 | 1.40        | 1.50     |
| 2   | L2    | 437  | PSU  | C1'-C5  | -4.26 | 1.40        | 1.50     |
| 1   | L1    | 48   | OMU  | C4-N3   | 4.26  | 1.45        | 1.38     |
| 2   | L2    | 667  | OMU  | C4-N3   | 4.25  | 1.45        | 1.38     |
| 1   | L1    | 847  | OMU  | C4-N3   | 4.25  | 1.45        | 1.38     |
| 1   | L1    | 1371 | OMU  | C4-N3   | 4.25  | 1.45        | 1.38     |
| 1   | L1    | 1664 | PSU  | C1'-C5  | -4.23 | 1.40        | 1.50     |
| 51  | S1    | 8    | OMU  | C4-N3   | 4.23  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | L2    | 1308 | 5MC  | C2-N1   | 4.23  | 1.48        | 1.40     |
| 2   | L2    | 1265 | PSU  | C1'-C5  | -4.22 | 1.40        | 1.50     |
| 2   | L2    | 560  | OMU  | C4-N3   | 4.21  | 1.45        | 1.38     |
| 2   | L2    | 73   | OMU  | C4-N3   | 4.20  | 1.45        | 1.38     |
| 7   | L7    | 101  | OMU  | C3'-C4' | 4.20  | 1.63        | 1.53     |
| 51  | S1    | 455  | PSU  | C1'-C5  | -4.19 | 1.40        | 1.50     |
| 2   | L2    | 1308 | 5MC  | C6-N1   | 4.18  | 1.45        | 1.38     |
| 1   | L1    | 677  | 1MA  | C2-N1   | 4.17  | 1.44        | 1.35     |
| 2   | L2    | 1077 | OMU  | C4-N3   | 4.16  | 1.45        | 1.38     |
| 2   | L2    | 1264 | PSU  | C1'-C5  | -4.16 | 1.40        | 1.50     |
| 51  | S1    | 1192 | PSU  | C1'-C5  | -4.14 | 1.40        | 1.50     |
| 2   | L2    | 1185 | A2M  | C6-N6   | 4.13  | 1.44        | 1.34     |
| 51  | S1    | 1833 | OMU  | C4-N3   | 4.10  | 1.45        | 1.38     |
| 1   | L1    | 1039 | OMU  | C4-N3   | 4.09  | 1.45        | 1.38     |
| 51  | S1    | 668  | A2M  | C6-N6   | 4.08  | 1.44        | 1.34     |
| 1   | L1    | 1011 | PSU  | C1'-C5  | -4.05 | 1.41        | 1.50     |
| 2   | L2    | 504  | PSU  | C4-N3   | 4.04  | 1.46        | 1.38     |
| 51  | S1    | 2185 | MA6  | C6-N6   | 4.02  | 1.47        | 1.36     |
| 51  | S1    | 1192 | PSU  | C4-N3   | 4.01  | 1.46        | 1.38     |
| 2   | L2    | 512  | PSU  | C4-N3   | 4.01  | 1.46        | 1.38     |
| 51  | S1    | 2184 | MA6  | C6-N6   | 4.00  | 1.47        | 1.36     |
| 51  | S1    | 609  | PSU  | C4-N3   | 3.99  | 1.46        | 1.38     |
| 51  | S1    | 1566 | PSU  | C4-N3   | 3.99  | 1.46        | 1.38     |
| 2   | L2    | 500  | PSU  | C4-N3   | 3.99  | 1.46        | 1.38     |
| 1   | L1    | 858  | A2M  | C6-N6   | 3.98  | 1.44        | 1.34     |
| 1   | L1    | 69   | A2M  | C6-N6   | 3.98  | 1.44        | 1.34     |
| 2   | L2    | 1284 | PSU  | C4-N3   | 3.97  | 1.46        | 1.38     |
| 51  | S1    | 455  | PSU  | C4-N3   | 3.97  | 1.46        | 1.38     |
| 2   | L2    | 437  | PSU  | C4-N3   | 3.97  | 1.46        | 1.38     |
| 1   | L1    | 1533 | PSU  | C4-N3   | 3.97  | 1.46        | 1.38     |
| 51  | S1    | 1533 | PSU  | C4-N3   | 3.96  | 1.46        | 1.38     |
| 51  | S1    | 33   | PSU  | C4-N3   | 3.96  | 1.46        | 1.38     |
| 2   | L2    | 506  | PSU  | C4-N3   | 3.96  | 1.46        | 1.38     |
| 2   | L2    | 472  | PSU  | C4-N3   | 3.95  | 1.46        | 1.38     |
| 51  | S1    | 1657 | PSU  | C4-N3   | 3.95  | 1.46        | 1.38     |
| 51  | S1    | 2046 | PSU  | C4-N3   | 3.95  | 1.46        | 1.38     |
| 2   | L2    | 1303 | PSU  | C4-N3   | 3.95  | 1.46        | 1.38     |
| 51  | S1    | 1292 | PSU  | C4-N3   | 3.95  | 1.46        | 1.38     |
| 7   | L7    | 74   | PSU  | C4-N3   | 3.95  | 1.46        | 1.38     |
| 51  | S1    | 1841 | PSU  | C4-N3   | 3.94  | 1.46        | 1.38     |
| 51  | S1    | 2048 | PSU  | C4-N3   | 3.94  | 1.46        | 1.38     |
| 51  | S1    | 12   | PSU  | C4-N3   | 3.94  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 51  | S1    | 1246 | PSU  | C4-N3  | 3.94 | 1.46        | 1.38     |
| 51  | S1    | 2202 | PSU  | C4-N3  | 3.94 | 1.46        | 1.38     |
| 1   | L1    | 1539 | A2M  | C6-N6  | 3.94 | 1.44        | 1.34     |
| 1   | L1    | 1664 | PSU  | C4-N3  | 3.93 | 1.46        | 1.38     |
| 1   | L1    | 1093 | PSU  | C4-N3  | 3.93 | 1.46        | 1.38     |
| 2   | L2    | 593  | PSU  | C4-N3  | 3.93 | 1.46        | 1.38     |
| 2   | L2    | 1318 | PSU  | C4-N3  | 3.92 | 1.46        | 1.38     |
| 51  | S1    | 104  | PSU  | C4-N3  | 3.92 | 1.46        | 1.38     |
| 1   | L1    | 239  | PSU  | C4-N3  | 3.92 | 1.46        | 1.38     |
| 2   | L2    | 626  | PSU  | C4-N3  | 3.92 | 1.46        | 1.38     |
| 2   | L2    | 597  | PSU  | C4-N3  | 3.92 | 1.46        | 1.38     |
| 1   | L1    | 422  | PSU  | C4-N3  | 3.92 | 1.46        | 1.38     |
| 2   | L2    | 1213 | PSU  | C4-N3  | 3.91 | 1.46        | 1.38     |
| 2   | L2    | 1194 | PSU  | C4-N3  | 3.91 | 1.46        | 1.38     |
| 1   | L1    | 927  | A2M  | C6-N6  | 3.90 | 1.44        | 1.34     |
| 2   | L2    | 510  | PSU  | C4-N3  | 3.89 | 1.46        | 1.38     |
| 2   | L2    | 1361 | PSU  | C4-N3  | 3.89 | 1.46        | 1.38     |
| 1   | L1    | 681  | A2M  | C6-N6  | 3.88 | 1.44        | 1.34     |
| 1   | L1    | 774  | PSU  | C4-N3  | 3.88 | 1.46        | 1.38     |
| 2   | L2    | 527  | A2M  | C6-N6  | 3.88 | 1.44        | 1.34     |
| 2   | L2    | 1384 | A2M  | C6-N6  | 3.88 | 1.44        | 1.34     |
| 1   | L1    | 940  | PSU  | C4-N3  | 3.87 | 1.46        | 1.38     |
| 2   | L2    | 78   | PSU  | C4-N3  | 3.87 | 1.46        | 1.38     |
| 51  | S1    | 1156 | PSU  | C4-N3  | 3.87 | 1.46        | 1.38     |
| 2   | L2    | 382  | A2M  | C6-N6  | 3.87 | 1.44        | 1.34     |
| 1   | L1    | 1181 | PSU  | C4-N3  | 3.86 | 1.46        | 1.38     |
| 2   | L2    | 1060 | PSU  | C4-N3  | 3.85 | 1.46        | 1.38     |
| 2   | L2    | 1144 | PSU  | C4-N3  | 3.85 | 1.46        | 1.38     |
| 2   | L2    | 1265 | PSU  | C4-N3  | 3.83 | 1.46        | 1.38     |
| 1   | L1    | 1011 | PSU  | C4-N3  | 3.75 | 1.45        | 1.38     |
| 2   | L2    | 1264 | PSU  | C4-N3  | 3.74 | 1.45        | 1.38     |
| 2   | L2    | 1397 | OMC  | C6-N1  | 3.73 | 1.47        | 1.38     |
| 2   | L2    | 1248 | OMC  | C6-N1  | 3.71 | 1.46        | 1.38     |
| 1   | L1    | 1527 | OMC  | C6-N1  | 3.70 | 1.46        | 1.38     |
| 1   | L1    | 1528 | PSU  | C4-N3  | 3.69 | 1.45        | 1.38     |
| 7   | L7    | 69   | PSU  | C4-N3  | 3.69 | 1.45        | 1.38     |
| 1   | L1    | 1017 | PSU  | C4-N3  | 3.67 | 1.45        | 1.38     |
| 2   | L2    | 1403 | PSU  | C4-N3  | 3.64 | 1.45        | 1.38     |
| 51  | S1    | 1995 | 7MG  | C2-N1  | 3.64 | 1.46        | 1.37     |
| 51  | S1    | 1995 | 7MG  | C5-C6  | 3.64 | 1.52        | 1.43     |
| 1   | L1    | 1171 | PSU  | C4-N3  | 3.63 | 1.45        | 1.38     |
| 51  | S1    | 1543 | B8N  | C1'-C5 | 3.62 | 1.58        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | L2    | 662  | PSU  | C4-N3   | 3.61  | 1.45        | 1.38     |
| 51  | S1    | 1995 | 7MG  | C6-N1   | 3.60  | 1.45        | 1.38     |
| 2   | L2    | 1382 | PSU  | C4-N3   | 3.60  | 1.45        | 1.38     |
| 51  | S1    | 1539 | PSU  | C4-N3   | 3.60  | 1.45        | 1.38     |
| 2   | L2    | 1413 | PSU  | C4-N3   | 3.59  | 1.45        | 1.38     |
| 1   | L1    | 677  | 1MA  | C5-C6   | 3.56  | 1.53        | 1.43     |
| 2   | L2    | 1058 | PSU  | C4-N3   | 3.54  | 1.45        | 1.38     |
| 1   | L1    | 672  | PSU  | C4-N3   | 3.46  | 1.45        | 1.38     |
| 1   | L1    | 1010 | OMC  | C6-N1   | 3.45  | 1.46        | 1.38     |
| 1   | L1    | 1524 | OMG  | C5-N7   | -3.44 | 1.32        | 1.39     |
| 51  | S1    | 1995 | 7MG  | C2-N2   | 3.41  | 1.42        | 1.34     |
| 2   | L2    | 71   | OMG  | C5-N7   | -3.40 | 1.32        | 1.39     |
| 1   | L1    | 695  | OMC  | C6-N1   | 3.35  | 1.46        | 1.38     |
| 2   | L2    | 359  | OMC  | C6-N1   | 3.34  | 1.46        | 1.38     |
| 2   | L2    | 583  | OMC  | C6-N1   | 3.34  | 1.46        | 1.38     |
| 51  | S1    | 2140 | OMC  | C6-N1   | 3.33  | 1.46        | 1.38     |
| 2   | L2    | 1317 | OMC  | C6-N1   | 3.33  | 1.46        | 1.38     |
| 1   | L1    | 856  | OMG  | C5-N7   | -3.32 | 1.32        | 1.39     |
| 51  | S1    | 1866 | OMC  | C6-N1   | 3.32  | 1.46        | 1.38     |
| 2   | L2    | 1159 | OMC  | C6-N1   | 3.30  | 1.46        | 1.38     |
| 51  | S1    | 38   | OMC  | C6-N1   | 3.30  | 1.46        | 1.38     |
| 1   | L1    | 1626 | OMG  | C5-N7   | -3.29 | 1.32        | 1.39     |
| 1   | L1    | 1039 | OMU  | C6-N1   | 3.29  | 1.45        | 1.38     |
| 51  | S1    | 2019 | OMC  | C6-N1   | 3.29  | 1.45        | 1.38     |
| 51  | S1    | 661  | OMU  | C6-N1   | 3.29  | 1.45        | 1.38     |
| 1   | L1    | 1552 | OMC  | C6-N1   | 3.28  | 1.45        | 1.38     |
| 51  | S1    | 1550 | OMG  | C5-N7   | -3.27 | 1.32        | 1.39     |
| 2   | L2    | 14   | OMC  | C6-N1   | 3.26  | 1.45        | 1.38     |
| 51  | S1    | 2059 | OMC  | C6-N1   | 3.26  | 1.45        | 1.38     |
| 2   | L2    | 1253 | OMG  | C5-N7   | -3.26 | 1.32        | 1.39     |
| 51  | S1    | 18   | OMC  | C6-N1   | 3.26  | 1.45        | 1.38     |
| 51  | S1    | 2021 | A2M  | O2'-C2' | 3.24  | 1.50        | 1.42     |
| 2   | L2    | 1077 | OMU  | C6-N1   | 3.21  | 1.45        | 1.38     |
| 1   | L1    | 927  | A2M  | O3'-C3' | -3.18 | 1.35        | 1.43     |
| 2   | L2    | 443  | OMC  | C6-N1   | 3.18  | 1.45        | 1.38     |
| 1   | L1    | 1539 | A2M  | O3'-C3' | -3.17 | 1.35        | 1.43     |
| 2   | L2    | 1185 | A2M  | O2'-C2' | 3.16  | 1.50        | 1.42     |
| 2   | L2    | 382  | A2M  | O3'-C3' | -3.15 | 1.35        | 1.43     |
| 2   | L2    | 641  | OMG  | C5-N7   | -3.13 | 1.32        | 1.39     |
| 2   | L2    | 1185 | A2M  | O3'-C3' | -3.13 | 1.35        | 1.43     |
| 1   | L1    | 681  | A2M  | O2'-C2' | 3.11  | 1.50        | 1.42     |
| 51  | S1    | 1833 | OMU  | C6-N1   | 3.10  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | L1    | 1540 | OMG  | C5-N7   | -3.10 | 1.32        | 1.39     |
| 1   | L1    | 1539 | A2M  | O2'-C2' | 3.10  | 1.50        | 1.42     |
| 51  | S1    | 1829 | OMG  | C5-N7   | -3.10 | 1.32        | 1.39     |
| 2   | L2    | 382  | A2M  | O2'-C2' | 3.09  | 1.50        | 1.42     |
| 2   | L2    | 570  | A2M  | O2'-C2' | 3.07  | 1.50        | 1.42     |
| 1   | L1    | 681  | A2M  | O3'-C3' | -3.07 | 1.35        | 1.43     |
| 2   | L2    | 604  | A2M  | O2'-C2' | 3.06  | 1.50        | 1.42     |
| 1   | L1    | 669  | OMC  | C6-N1   | 3.06  | 1.45        | 1.38     |
| 2   | L2    | 1384 | A2M  | O2'-C2' | 3.05  | 1.50        | 1.42     |
| 1   | L1    | 927  | A2M  | O2'-C2' | 3.05  | 1.50        | 1.42     |
| 7   | L7    | 162  | A2M  | O2'-C2' | 3.04  | 1.50        | 1.42     |
| 1   | L1    | 955  | A2M  | O2'-C2' | 3.04  | 1.50        | 1.42     |
| 51  | S1    | 1995 | 7MG  | O6-C6   | -3.03 | 1.17        | 1.23     |
| 1   | L1    | 858  | A2M  | O3'-C3' | -3.03 | 1.35        | 1.43     |
| 2   | L2    | 665  | A2M  | O2'-C2' | 3.02  | 1.50        | 1.42     |
| 51  | S1    | 8    | OMU  | O4-C4   | -3.02 | 1.18        | 1.24     |
| 2   | L2    | 95   | A2M  | O2'-C2' | 3.02  | 1.50        | 1.42     |
| 2   | L2    | 1384 | A2M  | O3'-C3' | -3.02 | 1.35        | 1.43     |
| 1   | L1    | 235  | A2M  | O2'-C2' | 3.01  | 1.50        | 1.42     |
| 2   | L2    | 560  | OMU  | C6-N1   | 3.01  | 1.45        | 1.38     |
| 2   | L2    | 591  | A2M  | O2'-C2' | 3.01  | 1.50        | 1.42     |
| 2   | L2    | 73   | OMU  | O4-C4   | -3.00 | 1.18        | 1.24     |
| 1   | L1    | 48   | OMU  | O4-C4   | -3.00 | 1.18        | 1.24     |
| 51  | S1    | 1833 | OMU  | O4-C4   | -3.00 | 1.18        | 1.24     |
| 51  | S1    | 479  | A2M  | O2'-C2' | 3.00  | 1.50        | 1.42     |
| 1   | L1    | 858  | A2M  | O2'-C2' | 3.00  | 1.50        | 1.42     |
| 2   | L2    | 1372 | A2M  | O2'-C2' | 2.99  | 1.50        | 1.42     |
| 51  | S1    | 668  | A2M  | O2'-C2' | 2.99  | 1.50        | 1.42     |
| 1   | L1    | 235  | A2M  | C5-C4   | -2.99 | 1.33        | 1.39     |
| 1   | L1    | 1373 | A2M  | C5-C4   | -2.99 | 1.33        | 1.39     |
| 2   | L2    | 95   | A2M  | C5-C4   | -2.98 | 1.33        | 1.39     |
| 7   | L7    | 101  | OMU  | O4-C4   | -2.97 | 1.18        | 1.24     |
| 2   | L2    | 1372 | A2M  | C5-C4   | -2.97 | 1.33        | 1.39     |
| 7   | L7    | 43   | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 1   | L1    | 697  | A2M  | O2'-C2' | 2.97  | 1.49        | 1.42     |
| 51  | S1    | 969  | A2M  | O2'-C2' | 2.97  | 1.49        | 1.42     |
| 2   | L2    | 1078 | OMG  | C2-N1   | 2.97  | 1.44        | 1.37     |
| 2   | L2    | 604  | A2M  | C5-C4   | -2.96 | 1.33        | 1.39     |
| 51  | S1    | 98   | A2M  | O2'-C2' | 2.96  | 1.49        | 1.42     |
| 1   | L1    | 1107 | OMU  | O4-C4   | -2.96 | 1.18        | 1.24     |
| 2   | L2    | 572  | A2M  | O2'-C2' | 2.95  | 1.49        | 1.42     |
| 2   | L2    | 628  | A2M  | O2'-C2' | 2.95  | 1.49        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | L2    | 570  | A2M  | C5-C4   | -2.95 | 1.33        | 1.39     |
| 1   | L1    | 1371 | OMU  | O4-C4   | -2.95 | 1.18        | 1.24     |
| 3   | L3    | 13   | OMU  | O4-C4   | -2.95 | 1.18        | 1.24     |
| 2   | L2    | 56   | OMU  | O4-C4   | -2.95 | 1.18        | 1.24     |
| 1   | L1    | 677  | 1MA  | C5-N7   | -2.95 | 1.33        | 1.39     |
| 51  | S1    | 897  | A2M  | C5-C4   | -2.95 | 1.33        | 1.39     |
| 2   | L2    | 1419 | OMU  | O4-C4   | -2.95 | 1.18        | 1.24     |
| 2   | L2    | 572  | A2M  | C5-C4   | -2.95 | 1.33        | 1.39     |
| 51  | S1    | 512  | A2M  | O2'-C2' | 2.95  | 1.49        | 1.42     |
| 51  | S1    | 897  | A2M  | O3'-C3' | -2.95 | 1.35        | 1.43     |
| 1   | L1    | 1190 | OMG  | C2-N1   | 2.95  | 1.44        | 1.37     |
| 1   | L1    | 847  | OMU  | O4-C4   | -2.95 | 1.18        | 1.24     |
| 7   | L7    | 101  | OMU  | C6-N1   | 2.95  | 1.45        | 1.38     |
| 2   | L2    | 502  | A2M  | O2'-C2' | 2.94  | 1.49        | 1.42     |
| 1   | L1    | 678  | A2M  | C5-C4   | -2.94 | 1.33        | 1.39     |
| 51  | S1    | 969  | A2M  | C5-C4   | -2.94 | 1.33        | 1.39     |
| 1   | L1    | 1373 | A2M  | O2'-C2' | 2.94  | 1.49        | 1.42     |
| 1   | L1    | 847  | OMU  | C6-N1   | 2.94  | 1.45        | 1.38     |
| 51  | S1    | 29   | OMU  | O4-C4   | -2.94 | 1.18        | 1.24     |
| 2   | L2    | 527  | A2M  | O2'-C2' | 2.93  | 1.49        | 1.42     |
| 2   | L2    | 1419 | OMU  | C6-N1   | 2.93  | 1.45        | 1.38     |
| 51  | S1    | 28   | A2M  | O2'-C2' | 2.93  | 1.49        | 1.42     |
| 2   | L2    | 56   | OMU  | C6-N1   | 2.93  | 1.45        | 1.38     |
| 2   | L2    | 667  | OMU  | O4-C4   | -2.93 | 1.18        | 1.24     |
| 2   | L2    | 1308 | 5MC  | O3'-C3' | 2.93  | 1.50        | 1.43     |
| 2   | L2    | 73   | OMU  | C6-N1   | 2.93  | 1.45        | 1.38     |
| 7   | L7    | 43   | A2M  | C5-C4   | -2.93 | 1.33        | 1.39     |
| 1   | L1    | 678  | A2M  | O2'-C2' | 2.93  | 1.49        | 1.42     |
| 1   | L1    | 305  | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 2   | L2    | 1067 | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 2   | L2    | 591  | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 1   | L1    | 697  | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 2   | L2    | 502  | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 2   | L2    | 1067 | A2M  | O2'-C2' | 2.92  | 1.49        | 1.42     |
| 1   | L1    | 845  | OMU  | C6-N1   | 2.92  | 1.45        | 1.38     |
| 51  | S1    | 2021 | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 2   | L2    | 665  | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 7   | L7    | 162  | A2M  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 3   | L3    | 13   | OMU  | C6-N1   | 2.91  | 1.45        | 1.38     |
| 51  | S1    | 1478 | OMG  | C2-N1   | 2.91  | 1.44        | 1.37     |
| 1   | L1    | 48   | OMU  | C6-N1   | 2.91  | 1.45        | 1.38     |
| 2   | L2    | 1231 | OMG  | C2-N1   | 2.91  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | S1    | 98   | A2M  | C5-C4   | -2.91 | 1.33        | 1.39     |
| 51  | S1    | 1662 | OMU  | O4-C4   | -2.91 | 1.18        | 1.24     |
| 2   | L2    | 1359 | OMU  | C6-N1   | 2.90  | 1.45        | 1.38     |
| 2   | L2    | 1067 | A2M  | O3'-C3' | -2.90 | 1.35        | 1.43     |
| 2   | L2    | 1359 | OMU  | O4-C4   | -2.90 | 1.18        | 1.24     |
| 51  | S1    | 1979 | OMU  | C6-N1   | 2.90  | 1.45        | 1.38     |
| 2   | L2    | 686  | OMG  | C2-N1   | 2.90  | 1.44        | 1.37     |
| 1   | L1    | 1659 | OMU  | O4-C4   | -2.90 | 1.18        | 1.24     |
| 51  | S1    | 1662 | OMU  | C6-N1   | 2.90  | 1.45        | 1.38     |
| 1   | L1    | 1371 | OMU  | C6-N1   | 2.90  | 1.45        | 1.38     |
| 51  | S1    | 1777 | OMU  | O4-C4   | -2.90 | 1.18        | 1.24     |
| 51  | S1    | 512  | A2M  | O3'-C3' | -2.90 | 1.35        | 1.43     |
| 51  | S1    | 28   | A2M  | C5-C4   | -2.89 | 1.33        | 1.39     |
| 2   | L2    | 628  | A2M  | C5-C4   | -2.89 | 1.33        | 1.39     |
| 51  | S1    | 1979 | OMU  | O4-C4   | -2.89 | 1.18        | 1.24     |
| 51  | S1    | 1621 | OMU  | O4-C4   | -2.89 | 1.18        | 1.24     |
| 7   | L7    | 75   | OMG  | C2-N1   | 2.89  | 1.44        | 1.37     |
| 1   | L1    | 845  | OMU  | O4-C4   | -2.89 | 1.18        | 1.24     |
| 2   | L2    | 1308 | 5MC  | O2'-C2' | -2.89 | 1.35        | 1.43     |
| 51  | S1    | 668  | A2M  | O3'-C3' | -2.89 | 1.35        | 1.43     |
| 7   | L7    | 43   | A2M  | O3'-C3' | -2.89 | 1.35        | 1.43     |
| 51  | S1    | 1777 | OMU  | C6-N1   | 2.89  | 1.45        | 1.38     |
| 51  | S1    | 600  | OMG  | C2-N1   | 2.89  | 1.44        | 1.37     |
| 2   | L2    | 534  | OMG  | C2-N1   | 2.89  | 1.44        | 1.37     |
| 51  | S1    | 897  | A2M  | O2'-C2' | 2.88  | 1.49        | 1.42     |
| 51  | S1    | 1647 | OMG  | C2-N1   | 2.88  | 1.44        | 1.37     |
| 2   | L2    | 667  | OMU  | C6-N1   | 2.88  | 1.45        | 1.38     |
| 4   | L4    | 74   | OMG  | C2-N1   | 2.88  | 1.44        | 1.37     |
| 1   | L1    | 955  | A2M  | C5-C4   | -2.88 | 1.34        | 1.39     |
| 51  | S1    | 512  | A2M  | C5-C4   | -2.88 | 1.34        | 1.39     |
| 2   | L2    | 1046 | OMG  | C2-N1   | 2.88  | 1.44        | 1.37     |
| 1   | L1    | 1659 | OMU  | C6-N1   | 2.87  | 1.44        | 1.38     |
| 51  | S1    | 479  | A2M  | C5-C4   | -2.87 | 1.34        | 1.39     |
| 51  | S1    | 1621 | OMU  | C6-N1   | 2.86  | 1.44        | 1.38     |
| 1   | L1    | 959  | OMG  | C2-N1   | 2.86  | 1.44        | 1.37     |
| 51  | S1    | 8    | OMU  | C6-N1   | 2.86  | 1.44        | 1.38     |
| 51  | S1    | 2151 | OMG  | C2-N1   | 2.86  | 1.44        | 1.37     |
| 2   | L2    | 95   | A2M  | O3'-C3' | -2.86 | 1.35        | 1.43     |
| 51  | S1    | 28   | A2M  | O3'-C3' | -2.86 | 1.35        | 1.43     |
| 1   | L1    | 69   | A2M  | O2'-C2' | 2.86  | 1.49        | 1.42     |
| 1   | L1    | 955  | A2M  | O3'-C3' | -2.86 | 1.35        | 1.43     |
| 51  | S1    | 29   | OMU  | C6-N1   | 2.85  | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | L1    | 235  | A2M  | O3'-C3' | -2.85 | 1.35        | 1.43     |
| 51  | S1    | 1865 | OMG  | C2-N1   | 2.85  | 1.44        | 1.37     |
| 1   | L1    | 1107 | OMU  | C6-N1   | 2.85  | 1.44        | 1.38     |
| 1   | L1    | 305  | A2M  | O2'-C2' | 2.85  | 1.49        | 1.42     |
| 51  | S1    | 1623 | OMG  | C2-N1   | 2.85  | 1.44        | 1.37     |
| 2   | L2    | 1229 | OMG  | C2-N1   | 2.85  | 1.44        | 1.37     |
| 2   | L2    | 665  | A2M  | O3'-C3' | -2.85 | 1.35        | 1.43     |
| 2   | L2    | 570  | A2M  | O3'-C3' | -2.85 | 1.35        | 1.43     |
| 1   | L1    | 1253 | OMU  | C6-N1   | 2.85  | 1.44        | 1.38     |
| 7   | L7    | 162  | A2M  | O3'-C3' | -2.84 | 1.35        | 1.43     |
| 1   | L1    | 1253 | OMU  | O4-C4   | -2.84 | 1.19        | 1.24     |
| 51  | S1    | 2008 | OMG  | C2-N1   | 2.84  | 1.44        | 1.37     |
| 2   | L2    | 502  | A2M  | O3'-C3' | -2.83 | 1.35        | 1.43     |
| 1   | L1    | 69   | A2M  | O3'-C3' | -2.83 | 1.35        | 1.43     |
| 1   | L1    | 697  | A2M  | O3'-C3' | -2.83 | 1.35        | 1.43     |
| 2   | L2    | 604  | A2M  | O3'-C3' | -2.83 | 1.36        | 1.43     |
| 2   | L2    | 1046 | OMG  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 2   | L2    | 1360 | OMG  | C2-N1   | 2.82  | 1.44        | 1.37     |
| 2   | L2    | 655  | OMG  | C2-N1   | 2.82  | 1.44        | 1.37     |
| 1   | L1    | 959  | OMG  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 1   | L1    | 856  | OMG  | O6-C6   | -2.82 | 1.18        | 1.23     |
| 51  | S1    | 98   | A2M  | O3'-C3' | -2.81 | 1.36        | 1.43     |
| 2   | L2    | 628  | A2M  | O3'-C3' | -2.81 | 1.36        | 1.43     |
| 1   | L1    | 1373 | A2M  | O3'-C3' | -2.81 | 1.36        | 1.43     |
| 2   | L2    | 591  | A2M  | O3'-C3' | -2.81 | 1.36        | 1.43     |
| 1   | L1    | 1039 | OMU  | O4-C4   | -2.80 | 1.19        | 1.24     |
| 2   | L2    | 1360 | OMG  | C5-N7   | -2.80 | 1.33        | 1.39     |
| 51  | S1    | 2021 | A2M  | O3'-C3' | -2.78 | 1.36        | 1.43     |
| 2   | L2    | 1253 | OMG  | O6-C6   | -2.78 | 1.18        | 1.23     |
| 2   | L2    | 1231 | OMG  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 2   | L2    | 572  | A2M  | O3'-C3' | -2.77 | 1.36        | 1.43     |
| 51  | S1    | 2059 | OMC  | O2-C2   | -2.77 | 1.18        | 1.23     |
| 51  | S1    | 969  | A2M  | O3'-C3' | -2.76 | 1.36        | 1.43     |
| 2   | L2    | 534  | OMG  | C5-N7   | -2.76 | 1.33        | 1.39     |
| 1   | L1    | 305  | A2M  | O3'-C3' | -2.76 | 1.36        | 1.43     |
| 1   | L1    | 1524 | OMG  | O6-C6   | -2.75 | 1.18        | 1.23     |
| 51  | S1    | 661  | OMU  | O4-C4   | -2.75 | 1.19        | 1.24     |
| 2   | L2    | 560  | OMU  | O4-C4   | -2.75 | 1.19        | 1.24     |
| 2   | L2    | 1372 | A2M  | C5-N7   | -2.74 | 1.34        | 1.39     |
| 51  | S1    | 600  | OMG  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 2   | L2    | 1372 | A2M  | O3'-C3' | -2.74 | 1.36        | 1.43     |
| 51  | S1    | 1623 | OMG  | C5-N7   | -2.73 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | L2    | 1077 | OMU  | O4-C4   | -2.73 | 1.19        | 1.24     |
| 51  | S1    | 479  | A2M  | O3'-C3' | -2.73 | 1.36        | 1.43     |
| 2   | L2    | 443  | OMC  | C5-C4   | 2.72  | 1.49        | 1.42     |
| 2   | L2    | 1067 | A2M  | C5-N7   | -2.72 | 1.34        | 1.39     |
| 2   | L2    | 570  | A2M  | C5-N7   | -2.72 | 1.34        | 1.39     |
| 2   | L2    | 1229 | OMG  | C5-N7   | -2.72 | 1.33        | 1.39     |
| 2   | L2    | 641  | OMG  | O6-C6   | -2.72 | 1.18        | 1.23     |
| 1   | L1    | 1190 | OMG  | C6-N1   | 2.71  | 1.43        | 1.38     |
| 51  | S1    | 1865 | OMG  | C5-N7   | -2.71 | 1.33        | 1.39     |
| 51  | S1    | 2184 | MA6  | C5-C4   | -2.71 | 1.34        | 1.39     |
| 2   | L2    | 1078 | OMG  | C6-N1   | 2.71  | 1.43        | 1.38     |
| 1   | L1    | 1010 | OMC  | C5-C4   | 2.71  | 1.49        | 1.42     |
| 2   | L2    | 591  | A2M  | C5-N7   | -2.70 | 1.34        | 1.39     |
| 51  | S1    | 38   | OMC  | O2-C2   | -2.70 | 1.18        | 1.23     |
| 2   | L2    | 665  | A2M  | C5-N7   | -2.70 | 1.34        | 1.39     |
| 1   | L1    | 305  | A2M  | C5-N7   | -2.69 | 1.34        | 1.39     |
| 2   | L2    | 71   | OMG  | O6-C6   | -2.69 | 1.18        | 1.23     |
| 52  | S2    | 37   | MIA  | C5-C4   | -2.69 | 1.34        | 1.39     |
| 51  | S1    | 2061 | 5MC  | O2-C2   | -2.69 | 1.18        | 1.23     |
| 1   | L1    | 678  | A2M  | O3'-C3' | -2.68 | 1.36        | 1.43     |
| 2   | L2    | 572  | A2M  | C5-N7   | -2.68 | 1.34        | 1.39     |
| 2   | L2    | 583  | OMC  | O2-C2   | -2.68 | 1.18        | 1.23     |
| 1   | L1    | 1373 | A2M  | C5-N7   | -2.68 | 1.34        | 1.39     |
| 4   | L4    | 74   | OMG  | C5-N7   | -2.67 | 1.33        | 1.39     |
| 51  | S1    | 479  | A2M  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 2   | L2    | 686  | OMG  | C5-N7   | -2.67 | 1.33        | 1.39     |
| 1   | L1    | 678  | A2M  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 1   | L1    | 695  | OMC  | O2-C2   | -2.67 | 1.18        | 1.23     |
| 1   | L1    | 235  | A2M  | C5-N7   | -2.66 | 1.34        | 1.39     |
| 7   | L7    | 75   | OMG  | C5-N7   | -2.66 | 1.33        | 1.39     |
| 7   | L7    | 43   | A2M  | C5-N7   | -2.66 | 1.34        | 1.39     |
| 2   | L2    | 1078 | OMG  | C4-N9   | -2.65 | 1.31        | 1.38     |
| 51  | S1    | 98   | A2M  | C5-N7   | -2.65 | 1.34        | 1.39     |
| 51  | S1    | 1647 | OMG  | C5-N7   | -2.65 | 1.33        | 1.39     |
| 1   | L1    | 1540 | OMG  | O6-C6   | -2.65 | 1.18        | 1.23     |
| 2   | L2    | 628  | A2M  | C5-N7   | -2.65 | 1.34        | 1.39     |
| 51  | S1    | 2185 | MA6  | C5-C4   | -2.65 | 1.34        | 1.39     |
| 2   | L2    | 604  | A2M  | C5-N7   | -2.65 | 1.34        | 1.39     |
| 1   | L1    | 1524 | OMG  | C2-N1   | 2.65  | 1.44        | 1.37     |
| 51  | S1    | 1833 | OMU  | O2-C2   | -2.65 | 1.18        | 1.23     |
| 1   | L1    | 1626 | OMG  | O6-C6   | -2.65 | 1.18        | 1.23     |
| 2   | L2    | 1159 | OMC  | O2-C2   | -2.64 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 51  | S1    | 1550 | OMG  | C2-N1 | 2.64  | 1.44        | 1.37     |
| 1   | L1    | 669  | OMC  | C5-C4 | 2.64  | 1.49        | 1.42     |
| 2   | L2    | 78   | PSU  | O4-C4 | -2.64 | 1.18        | 1.23     |
| 51  | S1    | 1478 | OMG  | C5-N7 | -2.64 | 1.33        | 1.39     |
| 1   | L1    | 697  | A2M  | C5-N7 | -2.64 | 1.34        | 1.39     |
| 2   | L2    | 95   | A2M  | C5-N7 | -2.64 | 1.34        | 1.39     |
| 2   | L2    | 14   | OMC  | O2-C2 | -2.64 | 1.18        | 1.23     |
| 51  | S1    | 897  | A2M  | C5-N7 | -2.64 | 1.34        | 1.39     |
| 7   | L7    | 162  | A2M  | C5-N7 | -2.64 | 1.34        | 1.39     |
| 51  | S1    | 2151 | OMG  | C5-N7 | -2.63 | 1.33        | 1.39     |
| 2   | L2    | 655  | OMG  | C5-N7 | -2.63 | 1.33        | 1.39     |
| 51  | S1    | 18   | OMC  | O2-C2 | -2.63 | 1.18        | 1.23     |
| 2   | L2    | 524  | 5MC  | O2-C2 | -2.63 | 1.18        | 1.23     |
| 51  | S1    | 512  | A2M  | C5-N7 | -2.62 | 1.34        | 1.39     |
| 51  | S1    | 1866 | OMC  | O2-C2 | -2.62 | 1.18        | 1.23     |
| 2   | L2    | 1248 | OMC  | C5-C4 | 2.62  | 1.49        | 1.42     |
| 1   | L1    | 1626 | OMG  | C2-N1 | 2.62  | 1.44        | 1.37     |
| 51  | S1    | 2021 | A2M  | C5-N7 | -2.61 | 1.34        | 1.39     |
| 2   | L2    | 1284 | PSU  | O4-C4 | -2.61 | 1.18        | 1.23     |
| 2   | L2    | 1361 | PSU  | O4-C4 | -2.61 | 1.18        | 1.23     |
| 51  | S1    | 2019 | OMC  | O2-C2 | -2.61 | 1.18        | 1.23     |
| 51  | S1    | 2151 | OMG  | C5-C6 | 2.61  | 1.54        | 1.44     |
| 51  | S1    | 2008 | OMG  | O6-C6 | -2.61 | 1.18        | 1.23     |
| 2   | L2    | 1317 | OMC  | O2-C2 | -2.60 | 1.18        | 1.23     |
| 51  | S1    | 1829 | OMG  | O6-C6 | -2.60 | 1.18        | 1.23     |
| 51  | S1    | 1829 | OMG  | C2-N1 | 2.60  | 1.43        | 1.37     |
| 2   | L2    | 71   | OMG  | C2-N1 | 2.60  | 1.43        | 1.37     |
| 51  | S1    | 1544 | 5MC  | O2-C2 | -2.60 | 1.18        | 1.23     |
| 1   | L1    | 1540 | OMG  | C2-N1 | 2.60  | 1.43        | 1.37     |
| 51  | S1    | 2140 | OMC  | O2-C2 | -2.60 | 1.18        | 1.23     |
| 4   | L4    | 74   | OMG  | O6-C6 | -2.59 | 1.18        | 1.23     |
| 2   | L2    | 655  | OMG  | C5-C6 | 2.59  | 1.54        | 1.44     |
| 1   | L1    | 955  | A2M  | C5-N7 | -2.59 | 1.34        | 1.39     |
| 2   | L2    | 359  | OMC  | O2-C2 | -2.59 | 1.18        | 1.23     |
| 2   | L2    | 502  | A2M  | C5-N7 | -2.59 | 1.34        | 1.39     |
| 51  | S1    | 28   | A2M  | C5-N7 | -2.59 | 1.34        | 1.39     |
| 51  | S1    | 1478 | OMG  | O6-C6 | -2.59 | 1.18        | 1.23     |
| 2   | L2    | 1078 | OMG  | C5-C6 | 2.58  | 1.54        | 1.44     |
| 1   | L1    | 669  | OMC  | O2-C2 | -2.58 | 1.18        | 1.23     |
| 2   | L2    | 1194 | PSU  | O4-C4 | -2.58 | 1.18        | 1.23     |
| 1   | L1    | 1190 | OMG  | C5-C6 | 2.58  | 1.54        | 1.44     |
| 2   | L2    | 686  | OMG  | C6-N1 | 2.58  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | L1    | 1010 | OMC  | O2-C2 | -2.58 | 1.18        | 1.23     |
| 51  | S1    | 1829 | OMG  | C5-C6 | 2.58  | 1.54        | 1.44     |
| 4   | L4    | 74   | OMG  | C6-N1 | 2.58  | 1.43        | 1.38     |
| 2   | L2    | 686  | OMG  | C5-C6 | 2.58  | 1.54        | 1.44     |
| 2   | L2    | 1397 | OMC  | C5-C4 | 2.58  | 1.48        | 1.42     |
| 2   | L2    | 626  | PSU  | O4-C4 | -2.58 | 1.18        | 1.23     |
| 2   | L2    | 1213 | PSU  | O4-C4 | -2.58 | 1.18        | 1.23     |
| 1   | L1    | 1552 | OMC  | O2-C2 | -2.58 | 1.18        | 1.23     |
| 1   | L1    | 422  | PSU  | O4-C4 | -2.57 | 1.18        | 1.23     |
| 51  | S1    | 1550 | OMG  | O6-C6 | -2.57 | 1.18        | 1.23     |
| 51  | S1    | 12   | PSU  | O4-C4 | -2.57 | 1.18        | 1.23     |
| 51  | S1    | 2008 | OMG  | C5-N7 | -2.57 | 1.33        | 1.39     |
| 2   | L2    | 1046 | OMG  | O6-C6 | -2.57 | 1.18        | 1.23     |
| 2   | L2    | 1318 | PSU  | O4-C4 | -2.57 | 1.18        | 1.23     |
| 1   | L1    | 940  | PSU  | O4-C4 | -2.57 | 1.18        | 1.23     |
| 51  | S1    | 1292 | PSU  | O4-C4 | -2.57 | 1.18        | 1.23     |
| 51  | S1    | 1156 | PSU  | O4-C4 | -2.57 | 1.18        | 1.23     |
| 51  | S1    | 1478 | OMG  | C6-N1 | 2.56  | 1.43        | 1.38     |
| 2   | L2    | 437  | PSU  | O4-C4 | -2.56 | 1.18        | 1.23     |
| 51  | S1    | 2048 | PSU  | O4-C4 | -2.56 | 1.18        | 1.23     |
| 1   | L1    | 1527 | OMC  | C5-C4 | 2.56  | 1.48        | 1.42     |
| 51  | S1    | 1657 | PSU  | O4-C4 | -2.56 | 1.18        | 1.23     |
| 1   | L1    | 1664 | PSU  | O4-C4 | -2.56 | 1.18        | 1.23     |
| 51  | S1    | 2019 | OMC  | C5-C4 | 2.55  | 1.48        | 1.42     |
| 7   | L7    | 75   | OMG  | C5-C6 | 2.55  | 1.53        | 1.44     |
| 51  | S1    | 2008 | OMG  | C5-C6 | 2.55  | 1.53        | 1.44     |
| 2   | L2    | 1253 | OMG  | C2-N1 | 2.55  | 1.43        | 1.37     |
| 2   | L2    | 655  | OMG  | O6-C6 | -2.55 | 1.18        | 1.23     |
| 51  | S1    | 1647 | OMG  | C6-N1 | 2.55  | 1.43        | 1.38     |
| 1   | L1    | 1190 | OMG  | C5-N7 | -2.55 | 1.34        | 1.39     |
| 51  | S1    | 609  | PSU  | O4-C4 | -2.55 | 1.18        | 1.23     |
| 2   | L2    | 443  | OMC  | O2-C2 | -2.55 | 1.19        | 1.23     |
| 51  | S1    | 38   | OMC  | C5-C4 | 2.55  | 1.48        | 1.42     |
| 1   | L1    | 1181 | PSU  | O4-C4 | -2.55 | 1.18        | 1.23     |
| 2   | L2    | 506  | PSU  | O4-C4 | -2.55 | 1.18        | 1.23     |
| 1   | L1    | 1093 | PSU  | O4-C4 | -2.55 | 1.18        | 1.23     |
| 51  | S1    | 2008 | OMG  | C6-N1 | 2.55  | 1.43        | 1.38     |
| 51  | S1    | 1647 | OMG  | C5-C6 | 2.55  | 1.53        | 1.44     |
| 1   | L1    | 239  | PSU  | O4-C4 | -2.54 | 1.18        | 1.23     |
| 51  | S1    | 1192 | PSU  | O4-C4 | -2.54 | 1.18        | 1.23     |
| 1   | L1    | 959  | OMG  | O6-C6 | -2.54 | 1.18        | 1.23     |
| 51  | S1    | 2202 | PSU  | O4-C4 | -2.54 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | S1    | 1623 | OMG  | C5-C6   | 2.54  | 1.53        | 1.44     |
| 51  | S1    | 1865 | OMG  | C5-C6   | 2.54  | 1.53        | 1.44     |
| 1   | L1    | 774  | PSU  | O4-C4   | -2.54 | 1.18        | 1.23     |
| 2   | L2    | 534  | OMG  | C5-C6   | 2.54  | 1.53        | 1.44     |
| 51  | S1    | 2140 | OMC  | C5-C4   | 2.54  | 1.48        | 1.42     |
| 51  | S1    | 1833 | OMU  | C5-C4   | 2.53  | 1.49        | 1.43     |
| 51  | S1    | 1246 | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 2   | L2    | 14   | OMC  | C5-C4   | 2.53  | 1.48        | 1.42     |
| 2   | L2    | 597  | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 2   | L2    | 1078 | OMG  | C5-N7   | -2.53 | 1.34        | 1.39     |
| 2   | L2    | 527  | A2M  | O3'-C3' | -2.53 | 1.36        | 1.43     |
| 51  | S1    | 1478 | OMG  | C4-N9   | -2.53 | 1.31        | 1.38     |
| 51  | S1    | 600  | OMG  | C5-C6   | 2.53  | 1.53        | 1.44     |
| 2   | L2    | 1144 | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 2   | L2    | 1159 | OMC  | C5-C4   | 2.53  | 1.48        | 1.42     |
| 7   | L7    | 74   | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 51  | S1    | 2059 | OMC  | C5-C4   | 2.53  | 1.48        | 1.42     |
| 51  | S1    | 2151 | OMG  | O6-C6   | -2.53 | 1.18        | 1.23     |
| 51  | S1    | 104  | PSU  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 51  | S1    | 969  | A2M  | C5-N7   | -2.53 | 1.34        | 1.39     |
| 2   | L2    | 641  | OMG  | C2-N1   | 2.53  | 1.43        | 1.37     |
| 2   | L2    | 641  | OMG  | C5-C6   | 2.52  | 1.53        | 1.44     |
| 4   | L4    | 74   | OMG  | C5-C6   | 2.52  | 1.53        | 1.44     |
| 51  | S1    | 2046 | PSU  | O4-C4   | -2.52 | 1.18        | 1.23     |
| 51  | S1    | 1478 | OMG  | C5-C6   | 2.52  | 1.53        | 1.44     |
| 2   | L2    | 534  | OMG  | O6-C6   | -2.52 | 1.18        | 1.23     |
| 2   | L2    | 512  | PSU  | O4-C4   | -2.52 | 1.18        | 1.23     |
| 2   | L2    | 1360 | OMG  | O6-C6   | -2.52 | 1.18        | 1.23     |
| 2   | L2    | 1317 | OMC  | C5-C4   | 2.52  | 1.48        | 1.42     |
| 1   | L1    | 1552 | OMC  | C5-C4   | 2.52  | 1.48        | 1.42     |
| 2   | L2    | 500  | PSU  | O4-C4   | -2.52 | 1.18        | 1.23     |
| 1   | L1    | 1190 | OMG  | O6-C6   | -2.51 | 1.18        | 1.23     |
| 51  | S1    | 600  | OMG  | C6-N1   | 2.51  | 1.43        | 1.38     |
| 2   | L2    | 510  | PSU  | O4-C4   | -2.51 | 1.18        | 1.23     |
| 51  | S1    | 2151 | OMG  | C6-N1   | 2.51  | 1.43        | 1.38     |
| 2   | L2    | 583  | OMC  | C5-C4   | 2.51  | 1.48        | 1.42     |
| 51  | S1    | 1865 | OMG  | O6-C6   | -2.51 | 1.18        | 1.23     |
| 1   | L1    | 1533 | PSU  | O4-C4   | -2.51 | 1.18        | 1.23     |
| 2   | L2    | 1248 | OMC  | O2-C2   | -2.51 | 1.19        | 1.23     |
| 51  | S1    | 1866 | OMC  | C5-C4   | 2.51  | 1.48        | 1.42     |
| 51  | S1    | 33   | PSU  | O4-C4   | -2.51 | 1.18        | 1.23     |
| 2   | L2    | 1078 | OMG  | O6-C6   | -2.51 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 51  | S1    | 1841 | PSU  | O4-C4 | -2.51 | 1.18        | 1.23     |
| 2   | L2    | 472  | PSU  | O4-C4 | -2.51 | 1.18        | 1.23     |
| 1   | L1    | 856  | OMG  | C2-N1 | 2.51  | 1.43        | 1.37     |
| 2   | L2    | 1231 | OMG  | O6-C6 | -2.51 | 1.18        | 1.23     |
| 2   | L2    | 1060 | PSU  | O4-C4 | -2.50 | 1.18        | 1.23     |
| 51  | S1    | 1566 | PSU  | O4-C4 | -2.50 | 1.18        | 1.23     |
| 7   | L7    | 75   | OMG  | C6-N1 | 2.50  | 1.43        | 1.38     |
| 2   | L2    | 1229 | OMG  | O6-C6 | -2.50 | 1.18        | 1.23     |
| 1   | L1    | 1540 | OMG  | C5-C6 | 2.50  | 1.53        | 1.44     |
| 2   | L2    | 1397 | OMC  | O2-C2 | -2.50 | 1.19        | 1.23     |
| 51  | S1    | 455  | PSU  | O4-C4 | -2.50 | 1.18        | 1.23     |
| 1   | L1    | 959  | OMG  | C5-C6 | 2.50  | 1.53        | 1.44     |
| 2   | L2    | 359  | OMC  | C5-C4 | 2.50  | 1.48        | 1.42     |
| 51  | S1    | 1647 | OMG  | O6-C6 | -2.50 | 1.18        | 1.23     |
| 2   | L2    | 534  | OMG  | C6-N1 | 2.49  | 1.43        | 1.38     |
| 51  | S1    | 1533 | PSU  | O4-C4 | -2.49 | 1.18        | 1.23     |
| 2   | L2    | 504  | PSU  | O4-C4 | -2.49 | 1.18        | 1.23     |
| 2   | L2    | 1229 | OMG  | C5-C6 | 2.49  | 1.53        | 1.44     |
| 2   | L2    | 1253 | OMG  | C5-C6 | 2.49  | 1.53        | 1.44     |
| 1   | L1    | 695  | OMC  | C5-C4 | 2.49  | 1.48        | 1.42     |
| 51  | S1    | 2184 | MA6  | C5-N7 | -2.48 | 1.34        | 1.39     |
| 2   | L2    | 1360 | OMG  | C5-C6 | 2.48  | 1.53        | 1.44     |
| 2   | L2    | 1231 | OMG  | C5-C6 | 2.48  | 1.53        | 1.44     |
| 51  | S1    | 1623 | OMG  | C6-N1 | 2.48  | 1.43        | 1.38     |
| 2   | L2    | 1303 | PSU  | O4-C4 | -2.48 | 1.18        | 1.23     |
| 2   | L2    | 1231 | OMG  | C6-N1 | 2.48  | 1.43        | 1.38     |
| 2   | L2    | 1046 | OMG  | C5-C6 | 2.48  | 1.53        | 1.44     |
| 7   | L7    | 75   | OMG  | O6-C6 | -2.48 | 1.18        | 1.23     |
| 2   | L2    | 593  | PSU  | O4-C4 | -2.48 | 1.18        | 1.23     |
| 51  | S1    | 600  | OMG  | O6-C6 | -2.48 | 1.18        | 1.23     |
| 2   | L2    | 527  | A2M  | C5-C4 | -2.47 | 1.34        | 1.39     |
| 51  | S1    | 1865 | OMG  | C6-N1 | 2.47  | 1.43        | 1.38     |
| 2   | L2    | 560  | OMU  | C5-C4 | 2.47  | 1.49        | 1.43     |
| 2   | L2    | 1265 | PSU  | O4-C4 | -2.47 | 1.18        | 1.23     |
| 51  | S1    | 1623 | OMG  | O6-C6 | -2.46 | 1.18        | 1.23     |
| 2   | L2    | 667  | OMU  | O2-C2 | -2.46 | 1.18        | 1.23     |
| 3   | L3    | 13   | OMU  | O2-C2 | -2.46 | 1.18        | 1.23     |
| 2   | L2    | 1046 | OMG  | C6-N1 | 2.46  | 1.43        | 1.38     |
| 1   | L1    | 858  | A2M  | C5-C4 | -2.46 | 1.34        | 1.39     |
| 51  | S1    | 2185 | MA6  | C5-N7 | -2.45 | 1.34        | 1.39     |
| 1   | L1    | 48   | OMU  | C5-C4 | 2.45  | 1.49        | 1.43     |
| 2   | L2    | 686  | OMG  | O6-C6 | -2.45 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | L1    | 48   | OMU  | O2-C2 | -2.45 | 1.18        | 1.23     |
| 2   | L2    | 1229 | OMG  | C6-N1 | 2.45  | 1.43        | 1.38     |
| 51  | S1    | 18   | OMC  | C5-C4 | 2.45  | 1.48        | 1.42     |
| 1   | L1    | 1626 | OMG  | C5-C6 | 2.44  | 1.53        | 1.44     |
| 1   | L1    | 1190 | OMG  | C4-N9 | -2.44 | 1.31        | 1.38     |
| 2   | L2    | 71   | OMG  | C5-C6 | 2.44  | 1.53        | 1.44     |
| 1   | L1    | 1253 | OMU  | O2-C2 | -2.44 | 1.18        | 1.23     |
| 2   | L2    | 1359 | OMU  | O2-C2 | -2.44 | 1.18        | 1.23     |
| 2   | L2    | 641  | OMG  | C4-N9 | -2.43 | 1.31        | 1.38     |
| 51  | S1    | 1550 | OMG  | C4-N9 | -2.43 | 1.31        | 1.38     |
| 1   | L1    | 845  | OMU  | O2-C2 | -2.43 | 1.18        | 1.23     |
| 1   | L1    | 1171 | PSU  | O4-C4 | -2.43 | 1.19        | 1.23     |
| 2   | L2    | 1413 | PSU  | O4-C4 | -2.43 | 1.19        | 1.23     |
| 1   | L1    | 1659 | OMU  | O2-C2 | -2.43 | 1.18        | 1.23     |
| 51  | S1    | 8    | OMU  | O2-C2 | -2.43 | 1.18        | 1.23     |
| 2   | L2    | 1419 | OMU  | O2-C2 | -2.43 | 1.18        | 1.23     |
| 1   | L1    | 1107 | OMU  | C5-C4 | 2.42  | 1.49        | 1.43     |
| 2   | L2    | 1360 | OMG  | C6-N1 | 2.42  | 1.43        | 1.38     |
| 2   | L2    | 56   | OMU  | O2-C2 | -2.42 | 1.18        | 1.23     |
| 2   | L2    | 1359 | OMU  | C5-C4 | 2.42  | 1.48        | 1.43     |
| 1   | L1    | 847  | OMU  | O2-C2 | -2.42 | 1.18        | 1.23     |
| 1   | L1    | 1527 | OMC  | O2-C2 | -2.42 | 1.19        | 1.23     |
| 1   | L1    | 959  | OMG  | C6-N1 | 2.41  | 1.43        | 1.38     |
| 51  | S1    | 8    | OMU  | C5-C4 | 2.41  | 1.48        | 1.43     |
| 51  | S1    | 1550 | OMG  | C5-C6 | 2.41  | 1.53        | 1.44     |
| 1   | L1    | 1253 | OMU  | C5-C4 | 2.41  | 1.48        | 1.43     |
| 1   | L1    | 1371 | OMU  | O2-C2 | -2.40 | 1.18        | 1.23     |
| 2   | L2    | 667  | OMU  | C5-C4 | 2.40  | 1.48        | 1.43     |
| 51  | S1    | 1621 | OMU  | O2-C2 | -2.40 | 1.18        | 1.23     |
| 2   | L2    | 655  | OMG  | C6-N1 | 2.40  | 1.43        | 1.38     |
| 2   | L2    | 1382 | PSU  | O4-C4 | -2.40 | 1.19        | 1.23     |
| 51  | S1    | 29   | OMU  | C5-C4 | 2.40  | 1.48        | 1.43     |
| 1   | L1    | 1371 | OMU  | C5-C4 | 2.40  | 1.48        | 1.43     |
| 7   | L7    | 101  | OMU  | C5-C4 | 2.40  | 1.48        | 1.43     |
| 2   | L2    | 73   | OMU  | O2-C2 | -2.40 | 1.18        | 1.23     |
| 2   | L2    | 1077 | OMU  | C5-C4 | 2.40  | 1.48        | 1.43     |
| 7   | L7    | 101  | OMU  | O2-C2 | -2.39 | 1.18        | 1.23     |
| 51  | S1    | 1979 | OMU  | O2-C2 | -2.39 | 1.18        | 1.23     |
| 51  | S1    | 1662 | OMU  | C5-C4 | 2.39  | 1.48        | 1.43     |
| 3   | L3    | 13   | OMU  | C5-C4 | 2.39  | 1.48        | 1.43     |
| 51  | S1    | 2008 | OMG  | C4-N9 | -2.39 | 1.32        | 1.38     |
| 51  | S1    | 29   | OMU  | O2-C2 | -2.39 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | S1    | 1621 | OMU  | C5-C4   | 2.39  | 1.48        | 1.43     |
| 51  | S1    | 1662 | OMU  | O2-C2   | -2.38 | 1.18        | 1.23     |
| 1   | L1    | 1659 | OMU  | C5-C4   | 2.38  | 1.48        | 1.43     |
| 51  | S1    | 1979 | OMU  | C5-C4   | 2.38  | 1.48        | 1.43     |
| 2   | L2    | 56   | OMU  | C5-C4   | 2.38  | 1.48        | 1.43     |
| 1   | L1    | 1107 | OMU  | O2-C2   | -2.38 | 1.18        | 1.23     |
| 1   | L1    | 845  | OMU  | C5-C4   | 2.37  | 1.48        | 1.43     |
| 1   | L1    | 672  | PSU  | O4-C4   | -2.37 | 1.19        | 1.23     |
| 2   | L2    | 1419 | OMU  | C5-C4   | 2.37  | 1.48        | 1.43     |
| 2   | L2    | 1384 | A2M  | C5-C4   | -2.37 | 1.34        | 1.39     |
| 1   | L1    | 1017 | PSU  | O4-C4   | -2.37 | 1.19        | 1.23     |
| 51  | S1    | 1777 | OMU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 2   | L2    | 662  | PSU  | O4-C4   | -2.37 | 1.19        | 1.23     |
| 1   | L1    | 847  | OMU  | C5-C4   | 2.37  | 1.48        | 1.43     |
| 1   | L1    | 1528 | PSU  | O4-C4   | -2.37 | 1.19        | 1.23     |
| 2   | L2    | 1264 | PSU  | O4-C4   | -2.36 | 1.19        | 1.23     |
| 2   | L2    | 73   | OMU  | C5-C4   | 2.36  | 1.48        | 1.43     |
| 51  | S1    | 661  | OMU  | C5-C4   | 2.36  | 1.48        | 1.43     |
| 51  | S1    | 1777 | OMU  | C5-C4   | 2.36  | 1.48        | 1.43     |
| 1   | L1    | 1539 | A2M  | C5-C4   | -2.35 | 1.34        | 1.39     |
| 1   | L1    | 1524 | OMG  | C5-C6   | 2.35  | 1.53        | 1.44     |
| 2   | L2    | 1058 | PSU  | O4-C4   | -2.35 | 1.19        | 1.23     |
| 51  | S1    | 1539 | PSU  | O4-C4   | -2.35 | 1.19        | 1.23     |
| 4   | L4    | 74   | OMG  | C4-N9   | -2.34 | 1.32        | 1.38     |
| 1   | L1    | 856  | OMG  | C5-C6   | 2.34  | 1.53        | 1.44     |
| 1   | L1    | 1524 | OMG  | C4-N9   | -2.34 | 1.32        | 1.38     |
| 2   | L2    | 1264 | PSU  | O4'-C1' | -2.34 | 1.40        | 1.43     |
| 2   | L2    | 560  | OMU  | O2-C2   | -2.33 | 1.18        | 1.23     |
| 1   | L1    | 69   | A2M  | C5-C4   | -2.33 | 1.34        | 1.39     |
| 51  | S1    | 1829 | OMG  | C4-N9   | -2.32 | 1.32        | 1.38     |
| 51  | S1    | 668  | A2M  | C5-C4   | -2.32 | 1.35        | 1.39     |
| 1   | L1    | 681  | A2M  | C5-C4   | -2.31 | 1.35        | 1.39     |
| 2   | L2    | 382  | A2M  | C5-N7   | -2.30 | 1.34        | 1.39     |
| 1   | L1    | 1011 | PSU  | O4-C4   | -2.30 | 1.19        | 1.23     |
| 2   | L2    | 1077 | OMU  | O2-C2   | -2.30 | 1.19        | 1.23     |
| 51  | S1    | 661  | OMU  | O2-C2   | -2.30 | 1.19        | 1.23     |
| 2   | L2    | 1403 | PSU  | O4-C4   | -2.30 | 1.19        | 1.23     |
| 1   | L1    | 1039 | OMU  | C5-C4   | 2.30  | 1.48        | 1.43     |
| 2   | L2    | 382  | A2M  | C5-C4   | -2.29 | 1.35        | 1.39     |
| 1   | L1    | 1540 | OMG  | C4-N9   | -2.28 | 1.32        | 1.38     |
| 7   | L7    | 69   | PSU  | O4-C4   | -2.28 | 1.19        | 1.23     |
| 2   | L2    | 1384 | A2M  | C8-N9   | -2.26 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | L1    | 1626 | OMG  | C4-N9   | -2.26 | 1.32        | 1.38     |
| 1   | L1    | 927  | A2M  | C5-C4   | -2.26 | 1.35        | 1.39     |
| 2   | L2    | 534  | OMG  | C4-N9   | -2.24 | 1.32        | 1.38     |
| 51  | S1    | 1543 | B8N  | O4-C4   | -2.24 | 1.18        | 1.23     |
| 1   | L1    | 1039 | OMU  | O2-C2   | -2.24 | 1.19        | 1.23     |
| 2   | L2    | 1372 | A2M  | C8-N9   | -2.22 | 1.33        | 1.37     |
| 2   | L2    | 1384 | A2M  | C5-N7   | -2.21 | 1.35        | 1.39     |
| 51  | S1    | 1543 | B8N  | O2-C2   | -2.21 | 1.18        | 1.22     |
| 1   | L1    | 678  | A2M  | C8-N9   | -2.21 | 1.33        | 1.37     |
| 7   | L7    | 75   | OMG  | C4-N9   | -2.21 | 1.32        | 1.38     |
| 2   | L2    | 1253 | OMG  | C4-N9   | -2.21 | 1.32        | 1.38     |
| 51  | S1    | 2151 | OMG  | C4-N9   | -2.20 | 1.32        | 1.38     |
| 51  | S1    | 668  | A2M  | C8-N9   | -2.20 | 1.33        | 1.37     |
| 2   | L2    | 1229 | OMG  | C4-N9   | -2.20 | 1.32        | 1.38     |
| 2   | L2    | 686  | OMG  | C4-N9   | -2.20 | 1.32        | 1.38     |
| 1   | L1    | 305  | A2M  | C8-N9   | -2.19 | 1.33        | 1.37     |
| 2   | L2    | 1265 | PSU  | C4-C5   | 2.19  | 1.50        | 1.44     |
| 2   | L2    | 1231 | OMG  | C4-N9   | -2.19 | 1.32        | 1.38     |
| 2   | L2    | 382  | A2M  | C8-N9   | -2.19 | 1.33        | 1.37     |
| 2   | L2    | 665  | A2M  | C8-N9   | -2.18 | 1.33        | 1.37     |
| 7   | L7    | 101  | OMU  | O2'-C2' | 2.17  | 1.48        | 1.42     |
| 2   | L2    | 1067 | A2M  | C8-N9   | -2.17 | 1.33        | 1.37     |
| 51  | S1    | 1647 | OMG  | C4-N9   | -2.17 | 1.32        | 1.38     |
| 1   | L1    | 927  | A2M  | C5-N7   | -2.17 | 1.35        | 1.39     |
| 52  | S2    | 37   | MIA  | C5-N7   | -2.16 | 1.35        | 1.39     |
| 1   | L1    | 856  | OMG  | C4-N9   | -2.16 | 1.32        | 1.38     |
| 2   | L2    | 591  | A2M  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 51  | S1    | 479  | A2M  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 2   | L2    | 95   | A2M  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 7   | L7    | 43   | A2M  | C8-N9   | -2.16 | 1.33        | 1.37     |
| 2   | L2    | 655  | OMG  | C4-N9   | -2.15 | 1.32        | 1.38     |
| 51  | S1    | 2021 | A2M  | C8-N9   | -2.15 | 1.33        | 1.37     |
| 2   | L2    | 502  | A2M  | C8-N9   | -2.15 | 1.33        | 1.37     |
| 7   | L7    | 162  | A2M  | C8-N9   | -2.15 | 1.33        | 1.37     |
| 51  | S1    | 1543 | B8N  | C2-N3   | 2.14  | 1.42        | 1.38     |
| 2   | L2    | 1360 | OMG  | C4-N9   | -2.13 | 1.32        | 1.38     |
| 51  | S1    | 600  | OMG  | C4-N9   | -2.13 | 1.32        | 1.38     |
| 1   | L1    | 1373 | A2M  | C8-N9   | -2.13 | 1.33        | 1.37     |
| 2   | L2    | 628  | A2M  | C8-N9   | -2.12 | 1.33        | 1.37     |
| 51  | S1    | 28   | A2M  | C8-N9   | -2.12 | 1.33        | 1.37     |
| 1   | L1    | 1539 | A2M  | C5-N7   | -2.12 | 1.35        | 1.39     |
| 1   | L1    | 858  | A2M  | C8-N9   | -2.12 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | L1    | 235  | A2M  | C8-N9   | -2.11 | 1.34        | 1.37     |
| 51  | S1    | 1865 | OMG  | C4-N9   | -2.10 | 1.32        | 1.38     |
| 51  | S1    | 98   | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 2   | L2    | 604  | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 2   | L2    | 1185 | A2M  | C5-C4   | -2.09 | 1.35        | 1.39     |
| 1   | L1    | 858  | A2M  | C5-N7   | -2.09 | 1.35        | 1.39     |
| 51  | S1    | 897  | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 1   | L1    | 955  | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 1   | L1    | 681  | A2M  | C5-N7   | -2.09 | 1.35        | 1.39     |
| 2   | L2    | 1185 | A2M  | C5-N7   | -2.09 | 1.35        | 1.39     |
| 2   | L2    | 527  | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 51  | S1    | 512  | A2M  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 2   | L2    | 1308 | 5MC  | O2-C2   | -2.09 | 1.19        | 1.23     |
| 2   | L2    | 1185 | A2M  | C8-N9   | -2.08 | 1.34        | 1.37     |
| 51  | S1    | 969  | A2M  | C8-N9   | -2.08 | 1.34        | 1.37     |
| 1   | L1    | 927  | A2M  | C8-N9   | -2.08 | 1.34        | 1.37     |
| 2   | L2    | 1046 | OMG  | C4-N9   | -2.07 | 1.32        | 1.38     |
| 51  | S1    | 1995 | 7MG  | C8-N7   | 2.07  | 1.52        | 1.42     |
| 1   | L1    | 697  | A2M  | C8-N9   | -2.06 | 1.34        | 1.37     |
| 2   | L2    | 570  | A2M  | C8-N9   | -2.06 | 1.34        | 1.37     |
| 2   | L2    | 662  | PSU  | C4-C5   | 2.06  | 1.50        | 1.44     |
| 1   | L1    | 681  | A2M  | C8-N9   | -2.05 | 1.34        | 1.37     |
| 1   | L1    | 959  | OMG  | C4-N9   | -2.05 | 1.32        | 1.38     |
| 51  | S1    | 2184 | MA6  | C8-N9   | -2.04 | 1.34        | 1.37     |
| 51  | S1    | 1623 | OMG  | C4-N9   | -2.04 | 1.32        | 1.38     |
| 1   | L1    | 1171 | PSU  | C4-C5   | 2.04  | 1.50        | 1.44     |
| 2   | L2    | 1264 | PSU  | C4-C5   | 2.03  | 1.50        | 1.44     |
| 2   | L2    | 572  | A2M  | C8-N9   | -2.03 | 1.34        | 1.37     |
| 2   | L2    | 71   | OMG  | C4-N9   | -2.02 | 1.32        | 1.38     |
| 51  | S1    | 668  | A2M  | C5-N7   | -2.01 | 1.35        | 1.39     |
| 51  | S1    | 2202 | PSU  | C4-C5   | 2.01  | 1.49        | 1.44     |
| 1   | L1    | 1664 | PSU  | C4-C5   | 2.01  | 1.49        | 1.44     |
| 7   | L7    | 69   | PSU  | O4'-C1' | -2.00 | 1.41        | 1.43     |

All (1148) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 52  | S2    | 37   | MIA  | C1'-N9-C8  | -15.53 | 92.62       | 127.09   |
| 51  | S1    | 2185 | MA6  | N1-C6-N6   | -14.03 | 99.76       | 116.86   |
| 52  | S2    | 37   | MIA  | C4-N9-C1'  | 14.01  | 159.40      | 126.63   |
| 51  | S1    | 2184 | MA6  | N1-C6-N6   | -13.60 | 100.28      | 116.86   |
| 52  | S2    | 37   | MIA  | C11-S10-C2 | 9.87   | 109.66      | 102.25   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 51  | S1    | 2185 | MA6  | C5-C6-N6  | 9.70  | 140.69      | 125.33   |
| 52  | S2    | 37   | MIA  | S10-C2-N3 | 9.53  | 148.89      | 116.04   |
| 51  | S1    | 2184 | MA6  | C5-C6-N6  | 9.32  | 140.08      | 125.33   |
| 1   | L1    | 959  | OMG  | C1'-N9-C8 | -8.29 | 103.18      | 126.73   |
| 1   | L1    | 1524 | OMG  | C1'-N9-C8 | -8.21 | 103.39      | 126.73   |
| 1   | L1    | 856  | OMG  | C1'-N9-C8 | -8.21 | 103.42      | 126.73   |
| 2   | L2    | 1046 | OMG  | C1'-N9-C8 | -8.09 | 103.74      | 126.73   |
| 2   | L2    | 1360 | OMG  | C1'-N9-C8 | -7.99 | 104.03      | 126.73   |
| 51  | S1    | 1623 | OMG  | C1'-N9-C8 | -7.94 | 104.19      | 126.73   |
| 2   | L2    | 655  | OMG  | C1'-N9-C8 | -7.92 | 104.23      | 126.73   |
| 1   | L1    | 1626 | OMG  | C1'-N9-C8 | -7.89 | 104.32      | 126.73   |
| 2   | L2    | 71   | OMG  | C1'-N9-C8 | -7.85 | 104.42      | 126.73   |
| 2   | L2    | 1231 | OMG  | C1'-N9-C8 | -7.85 | 104.44      | 126.73   |
| 51  | S1    | 600  | OMG  | C1'-N9-C8 | -7.83 | 104.48      | 126.73   |
| 51  | S1    | 1550 | OMG  | C1'-N9-C8 | -7.80 | 104.56      | 126.73   |
| 2   | L2    | 534  | OMG  | C1'-N9-C8 | -7.76 | 104.67      | 126.73   |
| 2   | L2    | 1253 | OMG  | C1'-N9-C8 | -7.76 | 104.70      | 126.73   |
| 2   | L2    | 1229 | OMG  | C1'-N9-C8 | -7.75 | 104.70      | 126.73   |
| 51  | S1    | 1865 | OMG  | C1'-N9-C8 | -7.64 | 105.04      | 126.73   |
| 2   | L2    | 686  | OMG  | C1'-N9-C8 | -7.57 | 105.21      | 126.73   |
| 4   | L4    | 74   | OMG  | C1'-N9-C8 | -7.54 | 105.32      | 126.73   |
| 1   | L1    | 1524 | OMG  | C1'-N9-C4 | 7.52  | 148.69      | 126.49   |
| 51  | S1    | 1829 | OMG  | C1'-N9-C8 | -7.45 | 105.57      | 126.73   |
| 51  | S1    | 1647 | OMG  | C1'-N9-C8 | -7.39 | 105.74      | 126.73   |
| 7   | L7    | 75   | OMG  | C1'-N9-C8 | -7.33 | 105.89      | 126.73   |
| 1   | L1    | 856  | OMG  | C1'-N9-C4 | 7.30  | 148.04      | 126.49   |
| 52  | S2    | 37   | MIA  | S10-C2-N1 | -7.26 | 90.99       | 116.04   |
| 1   | L1    | 1540 | OMG  | C1'-N9-C8 | -7.25 | 106.13      | 126.73   |
| 1   | L1    | 959  | OMG  | C1'-N9-C4 | 7.23  | 147.85      | 126.49   |
| 51  | S1    | 2151 | OMG  | C1'-N9-C8 | -7.23 | 106.19      | 126.73   |
| 2   | L2    | 71   | OMG  | C1'-N9-C4 | 7.17  | 147.66      | 126.49   |
| 51  | S1    | 2008 | OMG  | C1'-N9-C8 | -7.07 | 106.66      | 126.73   |
| 51  | S1    | 1478 | OMG  | C1'-N9-C8 | -7.06 | 106.67      | 126.73   |
| 1   | L1    | 1626 | OMG  | C1'-N9-C4 | 7.06  | 147.34      | 126.49   |
| 2   | L2    | 1046 | OMG  | C1'-N9-C4 | 6.99  | 147.14      | 126.49   |
| 2   | L2    | 1253 | OMG  | C1'-N9-C4 | 6.97  | 147.09      | 126.49   |
| 2   | L2    | 1360 | OMG  | C1'-N9-C4 | 6.91  | 146.89      | 126.49   |
| 51  | S1    | 1623 | OMG  | C1'-N9-C4 | 6.89  | 146.83      | 126.49   |
| 2   | L2    | 641  | OMG  | C1'-N9-C8 | -6.87 | 107.22      | 126.73   |
| 51  | S1    | 1550 | OMG  | C1'-N9-C4 | 6.84  | 146.70      | 126.49   |
| 2   | L2    | 1231 | OMG  | C1'-N9-C4 | 6.82  | 146.63      | 126.49   |
| 2   | L2    | 1078 | OMG  | C1'-N9-C8 | -6.78 | 107.47      | 126.73   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | L2    | 655  | OMG  | C1'-N9-C4 | 6.78  | 146.50      | 126.49   |
| 51  | S1    | 600  | OMG  | C1'-N9-C4 | 6.76  | 146.45      | 126.49   |
| 52  | S2    | 37   | MIA  | C5-C4-N3  | -6.73 | 120.09      | 127.18   |
| 1   | L1    | 1190 | OMG  | C1'-N9-C8 | -6.69 | 107.72      | 126.73   |
| 2   | L2    | 534  | OMG  | C1'-N9-C4 | 6.65  | 146.13      | 126.49   |
| 51  | S1    | 1829 | OMG  | C1'-N9-C4 | 6.61  | 146.01      | 126.49   |
| 2   | L2    | 1229 | OMG  | C1'-N9-C4 | 6.55  | 145.84      | 126.49   |
| 51  | S1    | 1865 | OMG  | C1'-N9-C4 | 6.53  | 145.76      | 126.49   |
| 2   | L2    | 686  | OMG  | C1'-N9-C4 | 6.44  | 145.50      | 126.49   |
| 4   | L4    | 74   | OMG  | C1'-N9-C4 | 6.37  | 145.29      | 126.49   |
| 1   | L1    | 1540 | OMG  | C1'-N9-C4 | 6.33  | 145.19      | 126.49   |
| 51  | S1    | 1647 | OMG  | C1'-N9-C4 | 6.22  | 144.87      | 126.49   |
| 2   | L2    | 560  | OMU  | C4-N3-C2  | -6.20 | 118.92      | 126.61   |
| 7   | L7    | 75   | OMG  | C1'-N9-C4 | 6.19  | 144.77      | 126.49   |
| 51  | S1    | 2151 | OMG  | C1'-N9-C4 | 6.16  | 144.69      | 126.49   |
| 2   | L2    | 641  | OMG  | C1'-N9-C4 | 5.99  | 144.19      | 126.49   |
| 51  | S1    | 1833 | OMU  | C4-N3-C2  | -5.93 | 119.26      | 126.61   |
| 51  | S1    | 1478 | OMG  | C1'-N9-C4 | 5.88  | 143.85      | 126.49   |
| 1   | L1    | 955  | A2M  | N3-C2-N1  | -5.84 | 119.75      | 128.58   |
| 1   | L1    | 1107 | OMU  | C4-N3-C2  | -5.83 | 119.38      | 126.61   |
| 51  | S1    | 512  | A2M  | N3-C2-N1  | -5.77 | 119.85      | 128.58   |
| 1   | L1    | 678  | A2M  | N3-C2-N1  | -5.77 | 119.85      | 128.58   |
| 2   | L2    | 570  | A2M  | N3-C2-N1  | -5.76 | 119.86      | 128.58   |
| 2   | L2    | 572  | A2M  | N3-C2-N1  | -5.76 | 119.86      | 128.58   |
| 51  | S1    | 2008 | OMG  | C1'-N9-C4 | 5.76  | 143.51      | 126.49   |
| 1   | L1    | 1373 | A2M  | N3-C2-N1  | -5.76 | 119.87      | 128.58   |
| 51  | S1    | 661  | OMU  | C4-N3-C2  | -5.74 | 119.49      | 126.61   |
| 51  | S1    | 8    | OMU  | C4-N3-C2  | -5.73 | 119.49      | 126.61   |
| 2   | L2    | 591  | A2M  | N3-C2-N1  | -5.73 | 119.90      | 128.58   |
| 2   | L2    | 604  | A2M  | N3-C2-N1  | -5.72 | 119.92      | 128.58   |
| 7   | L7    | 162  | A2M  | N3-C2-N1  | -5.72 | 119.92      | 128.58   |
| 1   | L1    | 235  | A2M  | N3-C2-N1  | -5.71 | 119.93      | 128.58   |
| 2   | L2    | 1077 | OMU  | C4-N3-C2  | -5.71 | 119.52      | 126.61   |
| 7   | L7    | 43   | A2M  | N3-C2-N1  | -5.70 | 119.96      | 128.58   |
| 1   | L1    | 697  | A2M  | N3-C2-N1  | -5.68 | 119.98      | 128.58   |
| 2   | L2    | 665  | A2M  | N3-C2-N1  | -5.67 | 120.00      | 128.58   |
| 51  | S1    | 28   | A2M  | N3-C2-N1  | -5.67 | 120.00      | 128.58   |
| 51  | S1    | 897  | A2M  | N3-C2-N1  | -5.67 | 120.00      | 128.58   |
| 2   | L2    | 95   | A2M  | N3-C2-N1  | -5.67 | 120.00      | 128.58   |
| 51  | S1    | 2021 | A2M  | N3-C2-N1  | -5.66 | 120.02      | 128.58   |
| 2   | L2    | 502  | A2M  | N3-C2-N1  | -5.65 | 120.03      | 128.58   |
| 2   | L2    | 628  | A2M  | N3-C2-N1  | -5.65 | 120.03      | 128.58   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | L1    | 1039 | OMU  | C4-N3-C2  | -5.65 | 119.60      | 126.61   |
| 1   | L1    | 305  | A2M  | N3-C2-N1  | -5.63 | 120.06      | 128.58   |
| 2   | L2    | 56   | OMU  | C4-N3-C2  | -5.62 | 119.63      | 126.61   |
| 2   | L2    | 1372 | A2M  | N3-C2-N1  | -5.62 | 120.07      | 128.58   |
| 51  | S1    | 29   | OMU  | C4-N3-C2  | -5.62 | 119.64      | 126.61   |
| 2   | L2    | 1067 | A2M  | N3-C2-N1  | -5.62 | 120.08      | 128.58   |
| 51  | S1    | 479  | A2M  | N3-C2-N1  | -5.62 | 120.08      | 128.58   |
| 1   | L1    | 48   | OMU  | C4-N3-C2  | -5.61 | 119.65      | 126.61   |
| 2   | L2    | 667  | OMU  | C4-N3-C2  | -5.60 | 119.67      | 126.61   |
| 51  | S1    | 1621 | OMU  | C4-N3-C2  | -5.59 | 119.67      | 126.61   |
| 51  | S1    | 98   | A2M  | N3-C2-N1  | -5.59 | 120.12      | 128.58   |
| 51  | S1    | 2185 | MA6  | N1-C2-N3  | -5.57 | 120.15      | 128.58   |
| 51  | S1    | 1979 | OMU  | C4-N3-C2  | -5.55 | 119.73      | 126.61   |
| 3   | L3    | 13   | OMU  | C4-N3-C2  | -5.54 | 119.73      | 126.61   |
| 1   | L1    | 1253 | OMU  | C4-N3-C2  | -5.54 | 119.74      | 126.61   |
| 51  | S1    | 2184 | MA6  | N1-C2-N3  | -5.53 | 120.21      | 128.58   |
| 1   | L1    | 1371 | OMU  | C4-N3-C2  | -5.52 | 119.75      | 126.61   |
| 2   | L2    | 1078 | OMG  | C1'-N9-C4 | 5.52  | 142.78      | 126.49   |
| 51  | S1    | 1777 | OMU  | C4-N3-C2  | -5.52 | 119.77      | 126.61   |
| 1   | L1    | 1659 | OMU  | C4-N3-C2  | -5.51 | 119.77      | 126.61   |
| 51  | S1    | 1662 | OMU  | C4-N3-C2  | -5.51 | 119.77      | 126.61   |
| 51  | S1    | 969  | A2M  | N3-C2-N1  | -5.51 | 120.25      | 128.58   |
| 1   | L1    | 1190 | OMG  | C1'-N9-C4 | 5.50  | 142.73      | 126.49   |
| 7   | L7    | 101  | OMU  | C4-N3-C2  | -5.49 | 119.80      | 126.61   |
| 2   | L2    | 1359 | OMU  | C4-N3-C2  | -5.48 | 119.81      | 126.61   |
| 1   | L1    | 847  | OMU  | C4-N3-C2  | -5.46 | 119.83      | 126.61   |
| 2   | L2    | 1419 | OMU  | C4-N3-C2  | -5.41 | 119.89      | 126.61   |
| 1   | L1    | 845  | OMU  | C4-N3-C2  | -5.41 | 119.90      | 126.61   |
| 2   | L2    | 73   | OMU  | C4-N3-C2  | -5.38 | 119.94      | 126.61   |
| 2   | L2    | 527  | A2M  | N6-C6-N1  | -5.21 | 106.77      | 118.38   |
| 1   | L1    | 69   | A2M  | N6-C6-N1  | -5.21 | 106.78      | 118.38   |
| 1   | L1    | 858  | A2M  | N6-C6-N1  | -5.21 | 106.78      | 118.38   |
| 2   | L2    | 570  | A2M  | C5-C4-N3  | -5.21 | 119.55      | 126.72   |
| 51  | S1    | 1543 | B8N  | C5-C4-N3  | 5.16  | 125.52      | 116.15   |
| 52  | S2    | 37   | MIA  | N6-C6-N1  | 5.15  | 125.23      | 118.33   |
| 1   | L1    | 927  | A2M  | C5-C4-N3  | -5.14 | 119.63      | 126.72   |
| 51  | S1    | 28   | A2M  | C5-C4-N3  | -5.13 | 119.65      | 126.72   |
| 51  | S1    | 479  | A2M  | C5-C4-N3  | -5.13 | 119.66      | 126.72   |
| 51  | S1    | 969  | A2M  | N6-C6-N1  | -5.12 | 106.97      | 118.38   |
| 2   | L2    | 1185 | A2M  | N6-C6-N1  | -5.11 | 107.01      | 118.38   |
| 1   | L1    | 678  | A2M  | C5-C4-N3  | -5.08 | 119.72      | 126.72   |
| 51  | S1    | 2021 | A2M  | C5-C4-N3  | -5.08 | 119.72      | 126.72   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 382  | A2M  | C5-C4-N3 | -5.08 | 119.73      | 126.72   |
| 51  | S1    | 98   | A2M  | C5-C4-N3 | -5.07 | 119.73      | 126.72   |
| 1   | L1    | 305  | A2M  | C5-C4-N3 | -5.06 | 119.74      | 126.72   |
| 1   | L1    | 677  | 1MA  | C5-C4-N3 | -5.05 | 119.83      | 127.27   |
| 51  | S1    | 512  | A2M  | C5-C4-N3 | -5.04 | 119.78      | 126.72   |
| 2   | L2    | 665  | A2M  | C5-C4-N3 | -5.03 | 119.79      | 126.72   |
| 7   | L7    | 43   | A2M  | C5-C4-N3 | -5.03 | 119.79      | 126.72   |
| 2   | L2    | 1067 | A2M  | C5-C4-N3 | -5.03 | 119.79      | 126.72   |
| 2   | L2    | 604  | A2M  | C5-C4-N3 | -5.02 | 119.81      | 126.72   |
| 1   | L1    | 235  | A2M  | C5-C4-N3 | -5.01 | 119.82      | 126.72   |
| 51  | S1    | 2184 | MA6  | C5-C4-N3 | -5.00 | 119.83      | 126.72   |
| 2   | L2    | 71   | OMG  | C5-C4-N3 | -5.00 | 120.44      | 128.39   |
| 2   | L2    | 502  | A2M  | C5-C4-N3 | -5.00 | 119.84      | 126.72   |
| 51  | S1    | 897  | A2M  | C5-C4-N3 | -4.99 | 119.84      | 126.72   |
| 51  | S1    | 1995 | 7MG  | C5-C6-N1 | 4.98  | 119.71      | 110.94   |
| 1   | L1    | 681  | A2M  | N6-C6-N1 | -4.97 | 107.30      | 118.38   |
| 1   | L1    | 955  | A2M  | N6-C6-N1 | -4.96 | 107.32      | 118.38   |
| 51  | S1    | 668  | A2M  | N6-C6-N1 | -4.96 | 107.32      | 118.38   |
| 2   | L2    | 527  | A2M  | N3-C2-N1 | -4.96 | 121.07      | 128.58   |
| 2   | L2    | 572  | A2M  | C5-C4-N3 | -4.95 | 119.90      | 126.72   |
| 1   | L1    | 1373 | A2M  | C5-C4-N3 | -4.94 | 119.91      | 126.72   |
| 1   | L1    | 1539 | A2M  | N6-C6-N1 | -4.94 | 107.38      | 118.38   |
| 2   | L2    | 95   | A2M  | C5-C4-N3 | -4.93 | 119.93      | 126.72   |
| 2   | L2    | 628  | A2M  | C5-C4-N3 | -4.92 | 119.94      | 126.72   |
| 2   | L2    | 1185 | A2M  | C5-C4-N3 | -4.92 | 119.94      | 126.72   |
| 2   | L2    | 1384 | A2M  | C5-C4-N3 | -4.92 | 119.94      | 126.72   |
| 2   | L2    | 570  | A2M  | N6-C6-N1 | -4.90 | 107.46      | 118.38   |
| 51  | S1    | 2185 | MA6  | C5-C4-N3 | -4.90 | 119.97      | 126.72   |
| 51  | S1    | 668  | A2M  | N3-C2-N1 | -4.90 | 121.17      | 128.58   |
| 1   | L1    | 959  | OMG  | C5-C4-N3 | -4.90 | 120.59      | 128.39   |
| 51  | S1    | 512  | A2M  | N6-C6-N1 | -4.89 | 107.49      | 118.38   |
| 1   | L1    | 697  | A2M  | C5-C4-N3 | -4.88 | 119.99      | 126.72   |
| 7   | L7    | 162  | A2M  | C5-C4-N3 | -4.87 | 120.00      | 126.72   |
| 51  | S1    | 1623 | OMG  | C5-C4-N3 | -4.86 | 120.66      | 128.39   |
| 2   | L2    | 628  | A2M  | N6-C6-N1 | -4.85 | 107.56      | 118.38   |
| 2   | L2    | 572  | A2M  | N6-C6-N1 | -4.85 | 107.57      | 118.38   |
| 7   | L7    | 162  | A2M  | N6-C6-N1 | -4.84 | 107.60      | 118.38   |
| 2   | L2    | 1361 | PSU  | C4-N3-C2 | -4.84 | 119.71      | 126.37   |
| 2   | L2    | 665  | A2M  | N6-C6-N1 | -4.84 | 107.60      | 118.38   |
| 2   | L2    | 591  | A2M  | C5-C4-N3 | -4.83 | 120.06      | 126.72   |
| 2   | L2    | 604  | A2M  | N6-C6-N1 | -4.83 | 107.62      | 118.38   |
| 7   | L7    | 74   | PSU  | C4-N3-C2 | -4.83 | 119.72      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 51  | S1    | 479  | A2M  | N6-C6-N1 | -4.82 | 107.63      | 118.38   |
| 7   | L7    | 43   | A2M  | N6-C6-N1 | -4.82 | 107.63      | 118.38   |
| 2   | L2    | 1253 | OMG  | C5-C4-N3 | -4.82 | 120.72      | 128.39   |
| 2   | L2    | 1046 | OMG  | C5-C4-N3 | -4.82 | 120.73      | 128.39   |
| 51  | S1    | 2021 | A2M  | N6-C6-N1 | -4.81 | 107.66      | 118.38   |
| 1   | L1    | 697  | A2M  | N6-C6-N1 | -4.81 | 107.66      | 118.38   |
| 2   | L2    | 1372 | A2M  | C5-C4-N3 | -4.80 | 120.11      | 126.72   |
| 2   | L2    | 502  | A2M  | N6-C6-N1 | -4.80 | 107.69      | 118.38   |
| 51  | S1    | 897  | A2M  | N6-C6-N1 | -4.80 | 107.70      | 118.38   |
| 1   | L1    | 1171 | PSU  | C4-N3-C2 | -4.79 | 119.77      | 126.37   |
| 2   | L2    | 1372 | A2M  | N6-C6-N1 | -4.79 | 107.71      | 118.38   |
| 2   | L2    | 1058 | PSU  | C4-N3-C2 | -4.79 | 119.77      | 126.37   |
| 51  | S1    | 1246 | PSU  | C4-N3-C2 | -4.78 | 119.78      | 126.37   |
| 2   | L2    | 95   | A2M  | N6-C6-N1 | -4.78 | 107.72      | 118.38   |
| 51  | S1    | 28   | A2M  | N6-C6-N1 | -4.78 | 107.73      | 118.38   |
| 1   | L1    | 305  | A2M  | N6-C6-N1 | -4.78 | 107.73      | 118.38   |
| 2   | L2    | 500  | PSU  | C4-N3-C2 | -4.77 | 119.80      | 126.37   |
| 1   | L1    | 1373 | A2M  | N6-C6-N1 | -4.77 | 107.76      | 118.38   |
| 2   | L2    | 1060 | PSU  | C4-N3-C2 | -4.77 | 119.81      | 126.37   |
| 51  | S1    | 2046 | PSU  | C4-N3-C2 | -4.77 | 119.81      | 126.37   |
| 1   | L1    | 235  | A2M  | N6-C6-N1 | -4.76 | 107.77      | 118.38   |
| 1   | L1    | 69   | A2M  | N3-C2-N1 | -4.76 | 121.37      | 128.58   |
| 1   | L1    | 672  | PSU  | N1-C2-N3 | 4.76  | 120.19      | 115.17   |
| 51  | S1    | 1841 | PSU  | C4-N3-C2 | -4.76 | 119.81      | 126.37   |
| 1   | L1    | 774  | PSU  | C4-N3-C2 | -4.76 | 119.81      | 126.37   |
| 1   | L1    | 1181 | PSU  | C4-N3-C2 | -4.76 | 119.81      | 126.37   |
| 1   | L1    | 955  | A2M  | C5-C4-N3 | -4.76 | 120.16      | 126.72   |
| 51  | S1    | 1657 | PSU  | C4-N3-C2 | -4.76 | 119.82      | 126.37   |
| 1   | L1    | 681  | A2M  | C5-C4-N3 | -4.76 | 120.17      | 126.72   |
| 2   | L2    | 1284 | PSU  | C4-N3-C2 | -4.75 | 119.83      | 126.37   |
| 1   | L1    | 927  | A2M  | N3-C2-N1 | -4.75 | 121.39      | 128.58   |
| 2   | L2    | 655  | OMG  | C5-C4-N3 | -4.74 | 120.84      | 128.39   |
| 2   | L2    | 382  | A2M  | N6-C6-N1 | -4.74 | 107.83      | 118.38   |
| 2   | L2    | 597  | PSU  | C4-N3-C2 | -4.73 | 119.85      | 126.37   |
| 1   | L1    | 927  | A2M  | N6-C6-N1 | -4.73 | 107.84      | 118.38   |
| 51  | S1    | 1865 | OMG  | C5-C4-N3 | -4.73 | 120.87      | 128.39   |
| 2   | L2    | 1360 | OMG  | C5-C4-N3 | -4.72 | 120.87      | 128.39   |
| 51  | S1    | 600  | OMG  | C5-C4-N3 | -4.72 | 120.87      | 128.39   |
| 2   | L2    | 626  | PSU  | C4-N3-C2 | -4.72 | 119.88      | 126.37   |
| 2   | L2    | 437  | PSU  | C4-N3-C2 | -4.71 | 119.88      | 126.37   |
| 2   | L2    | 1413 | PSU  | C4-N3-C2 | -4.71 | 119.89      | 126.37   |
| 1   | L1    | 1171 | PSU  | N1-C2-N3 | 4.71  | 120.13      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 1318 | PSU  | C4-N3-C2 | -4.71 | 119.89      | 126.37   |
| 51  | S1    | 104  | PSU  | C4-N3-C2 | -4.70 | 119.89      | 126.37   |
| 2   | L2    | 78   | PSU  | C4-N3-C2 | -4.70 | 119.89      | 126.37   |
| 1   | L1    | 858  | A2M  | N3-C2-N1 | -4.70 | 121.47      | 128.58   |
| 51  | S1    | 12   | PSU  | C4-N3-C2 | -4.70 | 119.90      | 126.37   |
| 2   | L2    | 1213 | PSU  | C4-N3-C2 | -4.70 | 119.90      | 126.37   |
| 2   | L2    | 1067 | A2M  | N6-C6-N1 | -4.70 | 107.92      | 118.38   |
| 2   | L2    | 1382 | PSU  | C4-N3-C2 | -4.70 | 119.90      | 126.37   |
| 2   | L2    | 512  | PSU  | C4-N3-C2 | -4.69 | 119.90      | 126.37   |
| 2   | L2    | 1058 | PSU  | N1-C2-N3 | 4.69  | 120.12      | 115.17   |
| 2   | L2    | 472  | PSU  | C4-N3-C2 | -4.69 | 119.91      | 126.37   |
| 2   | L2    | 1303 | PSU  | C4-N3-C2 | -4.69 | 119.91      | 126.37   |
| 2   | L2    | 1144 | PSU  | C4-N3-C2 | -4.69 | 119.92      | 126.37   |
| 2   | L2    | 1231 | OMG  | C5-C4-N3 | -4.68 | 120.94      | 128.39   |
| 51  | S1    | 1533 | PSU  | C4-N3-C2 | -4.68 | 119.92      | 126.37   |
| 2   | L2    | 1384 | A2M  | N6-C6-N1 | -4.68 | 107.95      | 118.38   |
| 51  | S1    | 2048 | PSU  | C4-N3-C2 | -4.67 | 119.93      | 126.37   |
| 1   | L1    | 678  | A2M  | N6-C6-N1 | -4.67 | 107.97      | 118.38   |
| 51  | S1    | 33   | PSU  | C4-N3-C2 | -4.67 | 119.93      | 126.37   |
| 1   | L1    | 422  | PSU  | C4-N3-C2 | -4.67 | 119.94      | 126.37   |
| 51  | S1    | 98   | A2M  | N6-C6-N1 | -4.67 | 107.98      | 118.38   |
| 51  | S1    | 609  | PSU  | C4-N3-C2 | -4.66 | 119.95      | 126.37   |
| 2   | L2    | 506  | PSU  | C4-N3-C2 | -4.66 | 119.95      | 126.37   |
| 2   | L2    | 662  | PSU  | N1-C2-N3 | 4.65  | 120.07      | 115.17   |
| 1   | L1    | 1539 | A2M  | C5-C4-N3 | -4.65 | 120.32      | 126.72   |
| 2   | L2    | 1194 | PSU  | C4-N3-C2 | -4.64 | 119.97      | 126.37   |
| 51  | S1    | 1156 | PSU  | C4-N3-C2 | -4.64 | 119.98      | 126.37   |
| 2   | L2    | 504  | PSU  | C4-N3-C2 | -4.64 | 119.98      | 126.37   |
| 1   | L1    | 940  | PSU  | C4-N3-C2 | -4.64 | 119.99      | 126.37   |
| 1   | L1    | 672  | PSU  | C4-N3-C2 | -4.63 | 119.99      | 126.37   |
| 1   | L1    | 1093 | PSU  | C4-N3-C2 | -4.63 | 119.99      | 126.37   |
| 1   | L1    | 1017 | PSU  | C4-N3-C2 | -4.63 | 119.99      | 126.37   |
| 2   | L2    | 662  | PSU  | C4-N3-C2 | -4.63 | 120.00      | 126.37   |
| 2   | L2    | 591  | A2M  | N6-C6-N1 | -4.63 | 108.07      | 118.38   |
| 1   | L1    | 239  | PSU  | C4-N3-C2 | -4.63 | 120.00      | 126.37   |
| 2   | L2    | 510  | PSU  | C4-N3-C2 | -4.62 | 120.01      | 126.37   |
| 1   | L1    | 1626 | OMG  | C5-C4-N3 | -4.62 | 121.04      | 128.39   |
| 1   | L1    | 858  | A2M  | C5-C4-N3 | -4.61 | 120.36      | 126.72   |
| 2   | L2    | 534  | OMG  | C5-C4-N3 | -4.61 | 121.05      | 128.39   |
| 1   | L1    | 1533 | PSU  | C4-N3-C2 | -4.61 | 120.03      | 126.37   |
| 2   | L2    | 686  | OMG  | C5-C4-N3 | -4.60 | 121.06      | 128.39   |
| 1   | L1    | 681  | A2M  | N3-C2-N1 | -4.60 | 121.62      | 128.58   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 1413 | PSU  | N1-C2-N3 | 4.60  | 120.02      | 115.17   |
| 2   | L2    | 1361 | PSU  | N1-C2-N3 | 4.60  | 120.02      | 115.17   |
| 1   | L1    | 1528 | PSU  | C4-N3-C2 | -4.59 | 120.05      | 126.37   |
| 2   | L2    | 1382 | PSU  | N1-C2-N3 | 4.58  | 120.00      | 115.17   |
| 51  | S1    | 1995 | 7MG  | C2-N3-C4 | 4.58  | 120.19      | 112.30   |
| 2   | L2    | 593  | PSU  | C4-N3-C2 | -4.58 | 120.06      | 126.37   |
| 51  | S1    | 1566 | PSU  | C4-N3-C2 | -4.58 | 120.07      | 126.37   |
| 51  | S1    | 1647 | OMG  | C5-C4-N3 | -4.57 | 121.11      | 128.39   |
| 51  | S1    | 1539 | PSU  | C4-N3-C2 | -4.57 | 120.07      | 126.37   |
| 1   | L1    | 1524 | OMG  | C5-C4-N3 | -4.57 | 121.11      | 128.39   |
| 1   | L1    | 1664 | PSU  | C4-N3-C2 | -4.57 | 120.08      | 126.37   |
| 51  | S1    | 2202 | PSU  | C4-N3-C2 | -4.56 | 120.09      | 126.37   |
| 51  | S1    | 1539 | PSU  | N1-C2-N3 | 4.56  | 119.97      | 115.17   |
| 1   | L1    | 856  | OMG  | C5-C4-N3 | -4.55 | 121.14      | 128.39   |
| 2   | L2    | 1229 | OMG  | C5-C4-N3 | -4.55 | 121.15      | 128.39   |
| 51  | S1    | 2151 | OMG  | C5-C4-N3 | -4.55 | 121.15      | 128.39   |
| 2   | L2    | 1264 | PSU  | N1-C2-N3 | 4.55  | 119.97      | 115.17   |
| 51  | S1    | 1292 | PSU  | C4-N3-C2 | -4.55 | 120.11      | 126.37   |
| 1   | L1    | 1539 | A2M  | N3-C2-N1 | -4.54 | 121.71      | 128.58   |
| 51  | S1    | 969  | A2M  | C5-C4-N3 | -4.53 | 120.48      | 126.72   |
| 2   | L2    | 1303 | PSU  | N1-C2-N3 | 4.52  | 119.93      | 115.17   |
| 1   | L1    | 1528 | PSU  | N1-C2-N3 | 4.51  | 119.93      | 115.17   |
| 7   | L7    | 69   | PSU  | C4-N3-C2 | -4.51 | 120.16      | 126.37   |
| 2   | L2    | 1144 | PSU  | N1-C2-N3 | 4.51  | 119.92      | 115.17   |
| 2   | L2    | 1185 | A2M  | N3-C2-N1 | -4.51 | 121.76      | 128.58   |
| 2   | L2    | 626  | PSU  | N1-C2-N3 | 4.51  | 119.92      | 115.17   |
| 2   | L2    | 1060 | PSU  | N1-C2-N3 | 4.50  | 119.92      | 115.17   |
| 2   | L2    | 1403 | PSU  | C4-N3-C2 | -4.50 | 120.17      | 126.37   |
| 1   | L1    | 1017 | PSU  | N1-C2-N3 | 4.50  | 119.91      | 115.17   |
| 1   | L1    | 774  | PSU  | N1-C2-N3 | 4.50  | 119.91      | 115.17   |
| 2   | L2    | 597  | PSU  | N1-C2-N3 | 4.49  | 119.91      | 115.17   |
| 2   | L2    | 655  | OMG  | C2-N3-C4 | 4.48  | 120.02      | 112.30   |
| 51  | S1    | 2048 | PSU  | N1-C2-N3 | 4.48  | 119.89      | 115.17   |
| 7   | L7    | 74   | PSU  | N1-C2-N3 | 4.48  | 119.89      | 115.17   |
| 51  | S1    | 12   | PSU  | N1-C2-N3 | 4.47  | 119.89      | 115.17   |
| 51  | S1    | 455  | PSU  | C4-N3-C2 | -4.47 | 120.21      | 126.37   |
| 1   | L1    | 1181 | PSU  | N1-C2-N3 | 4.47  | 119.88      | 115.17   |
| 7   | L7    | 69   | PSU  | N1-C2-N3 | 4.46  | 119.87      | 115.17   |
| 7   | L7    | 75   | OMG  | C5-C4-N3 | -4.46 | 121.30      | 128.39   |
| 1   | L1    | 69   | A2M  | C5-C4-N3 | -4.45 | 120.59      | 126.72   |
| 51  | S1    | 2046 | PSU  | N1-C2-N3 | 4.45  | 119.86      | 115.17   |
| 2   | L2    | 1360 | OMG  | C2-N3-C4 | 4.45  | 119.96      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 1264 | PSU  | C4-N3-C2 | -4.44 | 120.25      | 126.37   |
| 2   | L2    | 504  | PSU  | N1-C2-N3 | 4.44  | 119.85      | 115.17   |
| 51  | S1    | 1623 | OMG  | C2-N3-C4 | 4.44  | 119.95      | 112.30   |
| 51  | S1    | 104  | PSU  | N1-C2-N3 | 4.44  | 119.85      | 115.17   |
| 1   | L1    | 959  | OMG  | C2-N3-C4 | 4.44  | 119.94      | 112.30   |
| 1   | L1    | 1190 | OMG  | C2-N3-C4 | 4.44  | 119.94      | 112.30   |
| 2   | L2    | 1046 | OMG  | C2-N3-C4 | 4.43  | 119.94      | 112.30   |
| 2   | L2    | 500  | PSU  | N1-C2-N3 | 4.43  | 119.84      | 115.17   |
| 51  | S1    | 1647 | OMG  | C2-N3-C4 | 4.43  | 119.93      | 112.30   |
| 2   | L2    | 686  | OMG  | C2-N3-C4 | 4.43  | 119.93      | 112.30   |
| 1   | L1    | 1011 | PSU  | C4-N3-C2 | -4.43 | 120.27      | 126.37   |
| 51  | S1    | 2151 | OMG  | C2-N3-C4 | 4.43  | 119.92      | 112.30   |
| 51  | S1    | 609  | PSU  | N1-C2-N3 | 4.42  | 119.83      | 115.17   |
| 51  | S1    | 1246 | PSU  | N1-C2-N3 | 4.42  | 119.83      | 115.17   |
| 51  | S1    | 1865 | OMG  | C2-N3-C4 | 4.41  | 119.90      | 112.30   |
| 1   | L1    | 422  | PSU  | N1-C2-N3 | 4.41  | 119.82      | 115.17   |
| 2   | L2    | 1213 | PSU  | N1-C2-N3 | 4.41  | 119.82      | 115.17   |
| 51  | S1    | 1657 | PSU  | N1-C2-N3 | 4.41  | 119.81      | 115.17   |
| 4   | L4    | 74   | OMG  | C5-C4-N3 | -4.40 | 121.38      | 128.39   |
| 51  | S1    | 2202 | PSU  | N1-C2-N3 | 4.40  | 119.81      | 115.17   |
| 51  | S1    | 1841 | PSU  | N1-C2-N3 | 4.40  | 119.81      | 115.17   |
| 51  | S1    | 1156 | PSU  | N1-C2-N3 | 4.39  | 119.80      | 115.17   |
| 2   | L2    | 593  | PSU  | N1-C2-N3 | 4.39  | 119.80      | 115.17   |
| 2   | L2    | 1284 | PSU  | N1-C2-N3 | 4.39  | 119.80      | 115.17   |
| 51  | S1    | 600  | OMG  | C2-N3-C4 | 4.39  | 119.86      | 112.30   |
| 51  | S1    | 455  | PSU  | N1-C2-N3 | 4.38  | 119.79      | 115.17   |
| 2   | L2    | 1231 | OMG  | C2-N3-C4 | 4.38  | 119.84      | 112.30   |
| 4   | L4    | 74   | OMG  | C2-N3-C4 | 4.38  | 119.84      | 112.30   |
| 2   | L2    | 1318 | PSU  | N1-C2-N3 | 4.38  | 119.79      | 115.17   |
| 51  | S1    | 33   | PSU  | N1-C2-N3 | 4.38  | 119.78      | 115.17   |
| 51  | S1    | 2008 | OMG  | C2-N3-C4 | 4.37  | 119.83      | 112.30   |
| 1   | L1    | 1093 | PSU  | N1-C2-N3 | 4.37  | 119.77      | 115.17   |
| 1   | L1    | 1533 | PSU  | N1-C2-N3 | 4.36  | 119.76      | 115.17   |
| 51  | S1    | 1550 | OMG  | C5-C4-N3 | -4.36 | 121.46      | 128.39   |
| 2   | L2    | 506  | PSU  | N1-C2-N3 | 4.35  | 119.76      | 115.17   |
| 2   | L2    | 512  | PSU  | N1-C2-N3 | 4.35  | 119.76      | 115.17   |
| 2   | L2    | 534  | OMG  | C2-N3-C4 | 4.35  | 119.79      | 112.30   |
| 2   | L2    | 1194 | PSU  | N1-C2-N3 | 4.35  | 119.75      | 115.17   |
| 2   | L2    | 510  | PSU  | N1-C2-N3 | 4.34  | 119.75      | 115.17   |
| 51  | S1    | 1533 | PSU  | N1-C2-N3 | 4.34  | 119.75      | 115.17   |
| 2   | L2    | 472  | PSU  | N1-C2-N3 | 4.34  | 119.75      | 115.17   |
| 2   | L2    | 437  | PSU  | N1-C2-N3 | 4.34  | 119.74      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 1229 | OMG  | C2-N3-C4 | 4.32  | 119.74      | 112.30   |
| 7   | L7    | 75   | OMG  | C2-N3-C4 | 4.32  | 119.73      | 112.30   |
| 2   | L2    | 1265 | PSU  | N1-C2-N3 | 4.32  | 119.72      | 115.17   |
| 51  | S1    | 2184 | MA6  | C4-C5-C6 | 4.31  | 120.37      | 115.91   |
| 51  | S1    | 1543 | B8N  | C4-N3-C2 | -4.31 | 120.31      | 125.62   |
| 51  | S1    | 668  | A2M  | C5-C4-N3 | -4.31 | 120.78      | 126.72   |
| 51  | S1    | 2184 | MA6  | N9-C8-N7 | -4.30 | 107.83      | 113.94   |
| 51  | S1    | 1829 | OMG  | C5-C4-N3 | -4.30 | 121.55      | 128.39   |
| 1   | L1    | 239  | PSU  | N1-C2-N3 | 4.30  | 119.70      | 115.17   |
| 1   | L1    | 940  | PSU  | N1-C2-N3 | 4.29  | 119.70      | 115.17   |
| 2   | L2    | 1384 | A2M  | N3-C2-N1 | -4.29 | 122.08      | 128.58   |
| 51  | S1    | 1995 | 7MG  | C5-C4-N3 | -4.27 | 120.12      | 128.13   |
| 1   | L1    | 1540 | OMG  | C5-C4-N3 | -4.26 | 121.60      | 128.39   |
| 2   | L2    | 382  | A2M  | N3-C2-N1 | -4.26 | 122.13      | 128.58   |
| 51  | S1    | 1192 | PSU  | C4-N3-C2 | -4.26 | 120.50      | 126.37   |
| 51  | S1    | 1292 | PSU  | N1-C2-N3 | 4.26  | 119.66      | 115.17   |
| 51  | S1    | 1566 | PSU  | N1-C2-N3 | 4.26  | 119.66      | 115.17   |
| 51  | S1    | 2008 | OMG  | C5-C4-N3 | -4.26 | 121.62      | 128.39   |
| 2   | L2    | 78   | PSU  | N1-C2-N3 | 4.24  | 119.64      | 115.17   |
| 51  | S1    | 2185 | MA6  | N9-C8-N7 | -4.24 | 107.92      | 113.94   |
| 1   | L1    | 1664 | PSU  | N1-C2-N3 | 4.24  | 119.64      | 115.17   |
| 51  | S1    | 969  | A2M  | N9-C8-N7 | -4.24 | 107.93      | 113.94   |
| 51  | S1    | 1478 | OMG  | C2-N3-C4 | 4.24  | 119.59      | 112.30   |
| 2   | L2    | 560  | OMU  | N3-C2-N1 | 4.22  | 120.39      | 114.89   |
| 52  | S2    | 37   | MIA  | N9-C8-N7 | -4.22 | 107.95      | 113.94   |
| 2   | L2    | 1403 | PSU  | N1-C2-N3 | 4.21  | 119.61      | 115.17   |
| 2   | L2    | 1078 | OMG  | C2-N3-C4 | 4.20  | 119.53      | 112.30   |
| 2   | L2    | 641  | OMG  | C5-C4-N3 | -4.18 | 121.73      | 128.39   |
| 2   | L2    | 1372 | A2M  | N9-C8-N7 | -4.17 | 108.02      | 113.94   |
| 1   | L1    | 1190 | OMG  | C5-C4-N3 | -4.17 | 121.76      | 128.39   |
| 7   | L7    | 43   | A2M  | N9-C8-N7 | -4.16 | 108.03      | 113.94   |
| 2   | L2    | 1265 | PSU  | C4-N3-C2 | -4.16 | 120.64      | 126.37   |
| 2   | L2    | 95   | A2M  | N9-C8-N7 | -4.16 | 108.04      | 113.94   |
| 1   | L1    | 305  | A2M  | N9-C8-N7 | -4.16 | 108.04      | 113.94   |
| 2   | L2    | 572  | A2M  | N9-C8-N7 | -4.15 | 108.04      | 113.94   |
| 51  | S1    | 2185 | MA6  | C4-C5-C6 | 4.15  | 120.20      | 115.91   |
| 1   | L1    | 955  | A2M  | N9-C8-N7 | -4.14 | 108.06      | 113.94   |
| 51  | S1    | 897  | A2M  | N9-C8-N7 | -4.14 | 108.06      | 113.94   |
| 1   | L1    | 1373 | A2M  | N9-C8-N7 | -4.14 | 108.06      | 113.94   |
| 2   | L2    | 665  | A2M  | N9-C8-N7 | -4.14 | 108.06      | 113.94   |
| 51  | S1    | 512  | A2M  | N9-C8-N7 | -4.14 | 108.06      | 113.94   |
| 2   | L2    | 628  | A2M  | N9-C8-N7 | -4.14 | 108.07      | 113.94   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 502  | A2M  | N9-C8-N7 | -4.13 | 108.07      | 113.94   |
| 51  | S1    | 1478 | OMG  | C5-C4-N3 | -4.12 | 121.83      | 128.39   |
| 51  | S1    | 2021 | A2M  | N9-C8-N7 | -4.12 | 108.10      | 113.94   |
| 1   | L1    | 678  | A2M  | N9-C8-N7 | -4.11 | 108.10      | 113.94   |
| 7   | L7    | 162  | A2M  | N9-C8-N7 | -4.11 | 108.10      | 113.94   |
| 2   | L2    | 604  | A2M  | N9-C8-N7 | -4.10 | 108.12      | 113.94   |
| 51  | S1    | 1192 | PSU  | N1-C2-N3 | 4.10  | 119.49      | 115.17   |
| 2   | L2    | 527  | A2M  | C5-C4-N3 | -4.09 | 121.08      | 126.72   |
| 2   | L2    | 1067 | A2M  | N9-C8-N7 | -4.07 | 108.17      | 113.94   |
| 2   | L2    | 591  | A2M  | N9-C8-N7 | -4.06 | 108.17      | 113.94   |
| 51  | S1    | 1833 | OMU  | C5-C4-N3 | 4.05  | 120.47      | 114.80   |
| 51  | S1    | 98   | A2M  | N9-C8-N7 | -4.03 | 108.22      | 113.94   |
| 2   | L2    | 1308 | 5MC  | C5-C6-N1 | -4.03 | 118.94      | 123.31   |
| 1   | L1    | 235  | A2M  | N9-C8-N7 | -4.02 | 108.23      | 113.94   |
| 51  | S1    | 28   | A2M  | N9-C8-N7 | -4.02 | 108.23      | 113.94   |
| 1   | L1    | 697  | A2M  | N9-C8-N7 | -4.00 | 108.26      | 113.94   |
| 1   | L1    | 858  | A2M  | N9-C8-N7 | -3.97 | 108.31      | 113.94   |
| 51  | S1    | 1833 | OMU  | N3-C2-N1 | 3.96  | 120.05      | 114.89   |
| 51  | S1    | 479  | A2M  | N9-C8-N7 | -3.95 | 108.34      | 113.94   |
| 2   | L2    | 56   | OMU  | N3-C2-N1 | 3.94  | 120.03      | 114.89   |
| 51  | S1    | 969  | A2M  | C5-C6-N6 | 3.93  | 133.03      | 123.29   |
| 51  | S1    | 1995 | 7MG  | C4-C5-N7 | 3.93  | 110.02      | 105.38   |
| 51  | S1    | 8    | OMU  | N3-C2-N1 | 3.92  | 119.99      | 114.89   |
| 2   | L2    | 1078 | OMG  | N9-C8-N7 | -3.91 | 106.14      | 113.40   |
| 52  | S2    | 37   | MIA  | C5-C6-N6 | -3.90 | 114.50      | 122.03   |
| 2   | L2    | 1359 | OMU  | N3-C2-N1 | 3.90  | 119.97      | 114.89   |
| 2   | L2    | 1185 | A2M  | C5-C6-N6 | 3.89  | 132.92      | 123.29   |
| 2   | L2    | 667  | OMU  | N3-C2-N1 | 3.87  | 119.93      | 114.89   |
| 2   | L2    | 1078 | OMG  | C5-C4-N3 | -3.87 | 122.23      | 128.39   |
| 51  | S1    | 2008 | OMG  | N9-C8-N7 | -3.86 | 106.24      | 113.40   |
| 51  | S1    | 1979 | OMU  | N3-C2-N1 | 3.86  | 119.92      | 114.89   |
| 1   | L1    | 1011 | PSU  | N1-C2-N3 | 3.85  | 119.23      | 115.17   |
| 2   | L2    | 1077 | OMU  | C5-C4-N3 | 3.85  | 120.20      | 114.80   |
| 51  | S1    | 1621 | OMU  | N3-C2-N1 | 3.85  | 119.90      | 114.89   |
| 1   | L1    | 845  | OMU  | N3-C2-N1 | 3.84  | 119.89      | 114.89   |
| 1   | L1    | 69   | A2M  | N9-C8-N7 | -3.84 | 108.49      | 113.94   |
| 1   | L1    | 1253 | OMU  | N3-C2-N1 | 3.84  | 119.88      | 114.89   |
| 1   | L1    | 955  | A2M  | C5-C6-N6 | 3.83  | 132.78      | 123.29   |
| 7   | L7    | 101  | OMU  | N3-C2-N1 | 3.83  | 119.88      | 114.89   |
| 2   | L2    | 1264 | PSU  | C6-N1-C2 | -3.83 | 119.14      | 122.69   |
| 2   | L2    | 570  | A2M  | N9-C8-N7 | -3.83 | 108.50      | 113.94   |
| 1   | L1    | 1190 | OMG  | N9-C8-N7 | -3.82 | 106.32      | 113.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | L2    | 1372 | A2M  | C2'-C1'-N9 | -3.81 | 107.48      | 113.75   |
| 1   | L1    | 1107 | OMU  | C5-C4-N3   | 3.81  | 120.14      | 114.80   |
| 1   | L1    | 847  | OMU  | N3-C2-N1   | 3.81  | 119.85      | 114.89   |
| 2   | L2    | 527  | A2M  | N9-C8-N7   | -3.81 | 108.54      | 113.94   |
| 1   | L1    | 1039 | OMU  | C5-C4-N3   | 3.80  | 120.13      | 114.80   |
| 1   | L1    | 1371 | OMU  | N3-C2-N1   | 3.80  | 119.83      | 114.89   |
| 51  | S1    | 661  | OMU  | C5-C4-N3   | 3.79  | 120.11      | 114.80   |
| 1   | L1    | 69   | A2M  | C5-C6-N6   | 3.79  | 132.67      | 123.29   |
| 1   | L1    | 1659 | OMU  | N3-C2-N1   | 3.79  | 119.83      | 114.89   |
| 51  | S1    | 661  | OMU  | N3-C2-N1   | 3.79  | 119.83      | 114.89   |
| 51  | S1    | 29   | OMU  | N3-C2-N1   | 3.79  | 119.82      | 114.89   |
| 51  | S1    | 1662 | OMU  | N3-C2-N1   | 3.79  | 119.82      | 114.89   |
| 51  | S1    | 1543 | B8N  | C1'-C5-C4  | 3.78  | 123.34      | 117.61   |
| 2   | L2    | 560  | OMU  | C5-C4-N3   | 3.78  | 120.09      | 114.80   |
| 52  | S2    | 37   | MIA  | N3-C2-N1   | -3.77 | 120.12      | 127.00   |
| 1   | L1    | 927  | A2M  | N9-C8-N7   | -3.76 | 108.60      | 113.94   |
| 1   | L1    | 1107 | OMU  | N3-C2-N1   | 3.75  | 119.78      | 114.89   |
| 51  | S1    | 1777 | OMU  | N3-C2-N1   | 3.74  | 119.76      | 114.89   |
| 52  | S2    | 37   | MIA  | N3-C4-N9   | 3.74  | 131.74      | 126.99   |
| 51  | S1    | 668  | A2M  | C5-C6-N6   | 3.74  | 132.54      | 123.29   |
| 1   | L1    | 48   | OMU  | N3-C2-N1   | 3.74  | 119.76      | 114.89   |
| 1   | L1    | 681  | A2M  | N9-C8-N7   | -3.74 | 108.64      | 113.94   |
| 2   | L2    | 1419 | OMU  | N3-C2-N1   | 3.73  | 119.75      | 114.89   |
| 51  | S1    | 512  | A2M  | C5-C6-N6   | 3.73  | 132.52      | 123.29   |
| 1   | L1    | 48   | OMU  | C5-C4-N3   | 3.72  | 120.01      | 114.80   |
| 2   | L2    | 628  | A2M  | C5-C6-N6   | 3.72  | 132.50      | 123.29   |
| 1   | L1    | 681  | A2M  | C5-C6-N6   | 3.71  | 132.48      | 123.29   |
| 2   | L2    | 570  | A2M  | C5-C6-N6   | 3.71  | 132.47      | 123.29   |
| 2   | L2    | 1372 | A2M  | C5-C6-N6   | 3.71  | 132.47      | 123.29   |
| 1   | L1    | 1539 | A2M  | C5-C6-N6   | 3.70  | 132.45      | 123.29   |
| 7   | L7    | 162  | A2M  | C5-C6-N6   | 3.70  | 132.45      | 123.29   |
| 2   | L2    | 572  | A2M  | C5-C6-N6   | 3.70  | 132.44      | 123.29   |
| 1   | L1    | 1039 | OMU  | N3-C2-N1   | 3.69  | 119.70      | 114.89   |
| 51  | S1    | 1478 | OMG  | N9-C8-N7   | -3.69 | 106.56      | 113.40   |
| 51  | S1    | 8    | OMU  | C5-C4-N3   | 3.68  | 119.96      | 114.80   |
| 2   | L2    | 665  | A2M  | C5-C6-N6   | 3.68  | 132.39      | 123.29   |
| 3   | L3    | 13   | OMU  | N3-C2-N1   | 3.67  | 119.67      | 114.89   |
| 7   | L7    | 43   | A2M  | C5-C6-N6   | 3.67  | 132.36      | 123.29   |
| 1   | L1    | 858  | A2M  | C5-C6-N6   | 3.66  | 132.36      | 123.29   |
| 1   | L1    | 697  | A2M  | C5-C6-N6   | 3.66  | 132.35      | 123.29   |
| 2   | L2    | 1077 | OMU  | N3-C2-N1   | 3.66  | 119.65      | 114.89   |
| 2   | L2    | 73   | OMU  | N3-C2-N1   | 3.66  | 119.65      | 114.89   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L1    | 1539 | A2M  | N9-C8-N7    | -3.65 | 108.75      | 113.94   |
| 51  | S1    | 668  | A2M  | N9-C8-N7    | -3.65 | 108.75      | 113.94   |
| 51  | S1    | 479  | A2M  | C5-C6-N6    | 3.64  | 132.30      | 123.29   |
| 51  | S1    | 897  | A2M  | C5-C6-N6    | 3.64  | 132.30      | 123.29   |
| 2   | L2    | 502  | A2M  | C5-C6-N6    | 3.64  | 132.29      | 123.29   |
| 3   | L3    | 13   | OMU  | C5-C4-N3    | 3.64  | 119.89      | 114.80   |
| 51  | S1    | 29   | OMU  | C5-C4-N3    | 3.63  | 119.89      | 114.80   |
| 2   | L2    | 73   | OMU  | C5-C4-N3    | 3.63  | 119.89      | 114.80   |
| 2   | L2    | 604  | A2M  | C5-C6-N6    | 3.63  | 132.28      | 123.29   |
| 51  | S1    | 2021 | A2M  | C5-C6-N6    | 3.63  | 132.28      | 123.29   |
| 1   | L1    | 1373 | A2M  | C5-C6-N6    | 3.63  | 132.26      | 123.29   |
| 51  | S1    | 1647 | OMG  | N9-C8-N7    | -3.62 | 106.68      | 113.40   |
| 1   | L1    | 1371 | OMU  | C5-C4-N3    | 3.62  | 119.87      | 114.80   |
| 1   | L1    | 927  | A2M  | N3-C4-N9    | 3.61  | 133.31      | 127.17   |
| 51  | S1    | 28   | A2M  | C5-C6-N6    | 3.61  | 132.21      | 123.29   |
| 1   | L1    | 305  | A2M  | C5-C6-N6    | 3.60  | 132.21      | 123.29   |
| 7   | L7    | 75   | OMG  | N9-C8-N7    | -3.60 | 106.72      | 113.40   |
| 2   | L2    | 527  | A2M  | C5-C6-N6    | 3.60  | 132.21      | 123.29   |
| 2   | L2    | 1382 | PSU  | C6-C5-C4    | 3.60  | 120.60      | 118.17   |
| 2   | L2    | 1067 | A2M  | C5-C6-N6    | 3.60  | 132.20      | 123.29   |
| 2   | L2    | 570  | A2M  | C2-N3-C4    | 3.59  | 120.61      | 111.83   |
| 7   | L7    | 101  | OMU  | C5-C4-N3    | 3.59  | 119.83      | 114.80   |
| 2   | L2    | 1058 | PSU  | C6-C5-C4    | 3.59  | 120.60      | 118.17   |
| 2   | L2    | 95   | A2M  | C5-C6-N6    | 3.59  | 132.18      | 123.29   |
| 4   | L4    | 74   | OMG  | N9-C8-N7    | -3.59 | 106.75      | 113.40   |
| 51  | S1    | 1777 | OMU  | C5-C4-N3    | 3.59  | 119.82      | 114.80   |
| 2   | L2    | 591  | A2M  | C5-C6-N6    | 3.58  | 132.16      | 123.29   |
| 2   | L2    | 1384 | A2M  | N9-C8-N7    | -3.58 | 108.86      | 113.94   |
| 2   | L2    | 1229 | OMG  | N9-C8-N7    | -3.58 | 106.77      | 113.40   |
| 51  | S1    | 1662 | OMU  | C5-C4-N3    | 3.57  | 119.80      | 114.80   |
| 1   | L1    | 235  | A2M  | C5-C6-N6    | 3.57  | 132.12      | 123.29   |
| 2   | L2    | 56   | OMU  | C5-C4-N3    | 3.56  | 119.79      | 114.80   |
| 51  | S1    | 2151 | OMG  | N9-C8-N7    | -3.56 | 106.80      | 113.40   |
| 51  | S1    | 1621 | OMU  | C5-C4-N3    | 3.56  | 119.79      | 114.80   |
| 1   | L1    | 1659 | OMU  | C5-C4-N3    | 3.55  | 119.78      | 114.80   |
| 2   | L2    | 686  | OMG  | N9-C8-N7    | -3.55 | 106.81      | 113.40   |
| 1   | L1    | 1253 | OMU  | C5-C4-N3    | 3.55  | 119.77      | 114.80   |
| 2   | L2    | 667  | OMU  | C5-C4-N3    | 3.55  | 119.77      | 114.80   |
| 2   | L2    | 1419 | OMU  | C5-C4-N3    | 3.54  | 119.77      | 114.80   |
| 52  | S2    | 37   | MIA  | C12-C13-C14 | -3.54 | 120.65      | 127.01   |
| 51  | S1    | 1979 | OMU  | C5-C4-N3    | 3.54  | 119.76      | 114.80   |
| 1   | L1    | 847  | OMU  | C5-C4-N3    | 3.53  | 119.75      | 114.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | L1    | 677  | 1MA  | N1-C2-N3 | -3.52 | 121.81      | 126.00   |
| 2   | L2    | 1185 | A2M  | N9-C8-N7 | -3.52 | 108.95      | 113.94   |
| 51  | S1    | 1192 | PSU  | C6-N1-C2 | -3.51 | 119.43      | 122.69   |
| 51  | S1    | 98   | A2M  | C5-C6-N6 | 3.51  | 131.98      | 123.29   |
| 51  | S1    | 455  | PSU  | C6-N1-C2 | -3.51 | 119.44      | 122.69   |
| 1   | L1    | 678  | A2M  | C5-C6-N6 | 3.50  | 131.96      | 123.29   |
| 2   | L2    | 1253 | OMG  | C2-N3-C4 | 3.50  | 118.33      | 112.30   |
| 2   | L2    | 382  | A2M  | C5-C6-N6 | 3.50  | 131.94      | 123.29   |
| 2   | L2    | 655  | OMG  | N9-C8-N7 | -3.50 | 106.92      | 113.40   |
| 2   | L2    | 534  | OMG  | N9-C8-N7 | -3.48 | 106.94      | 113.40   |
| 1   | L1    | 678  | A2M  | C2-N3-C4 | 3.48  | 120.33      | 111.83   |
| 51  | S1    | 1865 | OMG  | N9-C8-N7 | -3.47 | 106.96      | 113.40   |
| 51  | S1    | 28   | A2M  | C2-N3-C4 | 3.47  | 120.31      | 111.83   |
| 2   | L2    | 604  | A2M  | C2-N3-C4 | 3.47  | 120.30      | 111.83   |
| 1   | L1    | 672  | PSU  | C6-N1-C2 | -3.47 | 119.47      | 122.69   |
| 2   | L2    | 1359 | OMU  | C5-C4-N3 | 3.46  | 119.65      | 114.80   |
| 1   | L1    | 845  | OMU  | C5-C4-N3 | 3.46  | 119.65      | 114.80   |
| 1   | L1    | 927  | A2M  | C5-C6-N6 | 3.46  | 131.86      | 123.29   |
| 51  | S1    | 512  | A2M  | C2-N3-C4 | 3.46  | 120.28      | 111.83   |
| 51  | S1    | 2185 | MA6  | C2-N1-C6 | 3.46  | 120.28      | 111.83   |
| 1   | L1    | 235  | A2M  | C2-N3-C4 | 3.45  | 120.27      | 111.83   |
| 2   | L2    | 1384 | A2M  | C5-C6-N6 | 3.45  | 131.84      | 123.29   |
| 51  | S1    | 2021 | A2M  | C2-N3-C4 | 3.45  | 120.26      | 111.83   |
| 2   | L2    | 662  | PSU  | C6-C5-C4 | 3.45  | 120.50      | 118.17   |
| 2   | L2    | 665  | A2M  | C2-N3-C4 | 3.44  | 120.24      | 111.83   |
| 1   | L1    | 1528 | PSU  | C6-N1-C2 | -3.44 | 119.50      | 122.69   |
| 51  | S1    | 1539 | PSU  | C6-N1-C2 | -3.44 | 119.50      | 122.69   |
| 51  | S1    | 479  | A2M  | C2-N3-C4 | 3.44  | 120.22      | 111.83   |
| 1   | L1    | 305  | A2M  | C2-N3-C4 | 3.43  | 120.22      | 111.83   |
| 7   | L7    | 43   | A2M  | C2-N3-C4 | 3.43  | 120.22      | 111.83   |
| 1   | L1    | 1373 | A2M  | C2-N3-C4 | 3.42  | 120.19      | 111.83   |
| 2   | L2    | 572  | A2M  | C2-N3-C4 | 3.42  | 120.18      | 111.83   |
| 2   | L2    | 1413 | PSU  | C6-C5-C4 | 3.42  | 120.48      | 118.17   |
| 51  | S1    | 600  | OMG  | N9-C8-N7 | -3.42 | 107.07      | 113.40   |
| 2   | L2    | 502  | A2M  | C2-N3-C4 | 3.41  | 120.16      | 111.83   |
| 7   | L7    | 69   | PSU  | C6-C5-C4 | 3.41  | 120.47      | 118.17   |
| 51  | S1    | 897  | A2M  | C2-N3-C4 | 3.41  | 120.15      | 111.83   |
| 51  | S1    | 98   | A2M  | C2-N3-C4 | 3.40  | 120.13      | 111.83   |
| 2   | L2    | 95   | A2M  | C2-N3-C4 | 3.40  | 120.13      | 111.83   |
| 2   | L2    | 1067 | A2M  | C2-N3-C4 | 3.39  | 120.11      | 111.83   |
| 7   | L7    | 162  | A2M  | C2-N3-C4 | 3.39  | 120.10      | 111.83   |
| 2   | L2    | 1361 | PSU  | C6-N1-C2 | -3.38 | 119.55      | 122.69   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | L1    | 955  | A2M  | C2-N3-C4 | 3.38  | 120.09      | 111.83   |
| 1   | L1    | 697  | A2M  | C2-N3-C4 | 3.38  | 120.08      | 111.83   |
| 2   | L2    | 628  | A2M  | C2-N3-C4 | 3.38  | 120.08      | 111.83   |
| 52  | S2    | 37   | MIA  | C4-C5-C6 | 3.38  | 119.59      | 116.78   |
| 51  | S1    | 1623 | OMG  | N9-C8-N7 | -3.37 | 107.14      | 113.40   |
| 51  | S1    | 2184 | MA6  | C2-N1-C6 | 3.37  | 120.07      | 111.83   |
| 2   | L2    | 1360 | OMG  | N9-C8-N7 | -3.37 | 107.14      | 113.40   |
| 2   | L2    | 1046 | OMG  | N9-C8-N7 | -3.37 | 107.15      | 113.40   |
| 2   | L2    | 524  | 5MC  | C5-C6-N1 | -3.36 | 119.66      | 123.31   |
| 2   | L2    | 504  | PSU  | C6-N1-C2 | -3.36 | 119.57      | 122.69   |
| 1   | L1    | 672  | PSU  | C6-C5-C4 | 3.36  | 120.44      | 118.17   |
| 1   | L1    | 1540 | OMG  | N9-C8-N7 | -3.35 | 107.20      | 113.40   |
| 2   | L2    | 641  | OMG  | N9-C8-N7 | -3.34 | 107.21      | 113.40   |
| 51  | S1    | 1543 | B8N  | N3-C2-N1 | 3.34  | 120.80      | 116.72   |
| 2   | L2    | 591  | A2M  | C2-N3-C4 | 3.33  | 119.96      | 111.83   |
| 51  | S1    | 2048 | PSU  | C6-N1-C2 | -3.33 | 119.60      | 122.69   |
| 2   | L2    | 1413 | PSU  | C6-N1-C2 | -3.33 | 119.60      | 122.69   |
| 51  | S1    | 609  | PSU  | C6-N1-C2 | -3.32 | 119.61      | 122.69   |
| 1   | L1    | 1017 | PSU  | C6-N1-C2 | -3.32 | 119.61      | 122.69   |
| 2   | L2    | 662  | PSU  | C6-N1-C2 | -3.32 | 119.61      | 122.69   |
| 7   | L7    | 69   | PSU  | C6-N1-C2 | -3.31 | 119.62      | 122.69   |
| 2   | L2    | 1058 | PSU  | C6-N1-C2 | -3.30 | 119.62      | 122.69   |
| 2   | L2    | 1231 | OMG  | N9-C8-N7 | -3.30 | 107.28      | 113.40   |
| 51  | S1    | 2184 | MA6  | C2-N3-C4 | 3.30  | 119.89      | 111.83   |
| 2   | L2    | 71   | OMG  | C2-N3-C4 | 3.30  | 117.98      | 112.30   |
| 2   | L2    | 1372 | A2M  | C2-N3-C4 | 3.28  | 119.85      | 111.83   |
| 51  | S1    | 2185 | MA6  | C2-N3-C4 | 3.28  | 119.85      | 111.83   |
| 2   | L2    | 626  | PSU  | C6-N1-C2 | -3.28 | 119.64      | 122.69   |
| 51  | S1    | 1539 | PSU  | C6-C5-C4 | 3.27  | 120.38      | 118.17   |
| 51  | S1    | 2202 | PSU  | C6-N1-C2 | -3.27 | 119.66      | 122.69   |
| 1   | L1    | 959  | OMG  | N9-C8-N7 | -3.26 | 107.35      | 113.40   |
| 2   | L2    | 1144 | PSU  | C6-N1-C2 | -3.26 | 119.67      | 122.69   |
| 1   | L1    | 1533 | PSU  | C6-N1-C2 | -3.26 | 119.67      | 122.69   |
| 51  | S1    | 1292 | PSU  | C6-N1-C2 | -3.25 | 119.67      | 122.69   |
| 2   | L2    | 1303 | PSU  | C6-N1-C2 | -3.25 | 119.67      | 122.69   |
| 1   | L1    | 1171 | PSU  | C6-C5-C4 | 3.25  | 120.37      | 118.17   |
| 1   | L1    | 1017 | PSU  | C6-C5-C4 | 3.25  | 120.37      | 118.17   |
| 51  | S1    | 2184 | MA6  | N3-C4-N9 | 3.24  | 132.68      | 127.17   |
| 1   | L1    | 927  | A2M  | C2-N3-C4 | 3.23  | 119.73      | 111.83   |
| 1   | L1    | 678  | A2M  | N3-C4-N9 | 3.23  | 132.67      | 127.17   |
| 2   | L2    | 1213 | PSU  | C6-N1-C2 | -3.23 | 119.69      | 122.69   |
| 51  | S1    | 1829 | OMG  | N9-C8-N7 | -3.23 | 107.41      | 113.40   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 382  | A2M  | N9-C8-N7 | -3.23 | 109.36      | 113.94   |
| 1   | L1    | 774  | PSU  | C6-N1-C2 | -3.22 | 119.70      | 122.69   |
| 51  | S1    | 33   | PSU  | C6-N1-C2 | -3.21 | 119.71      | 122.69   |
| 1   | L1    | 422  | PSU  | C6-N1-C2 | -3.21 | 119.71      | 122.69   |
| 51  | S1    | 969  | A2M  | C2-N3-C4 | 3.21  | 119.67      | 111.83   |
| 1   | L1    | 1093 | PSU  | C6-N1-C2 | -3.21 | 119.71      | 122.69   |
| 51  | S1    | 1566 | PSU  | C6-N1-C2 | -3.20 | 119.72      | 122.69   |
| 2   | L2    | 1265 | PSU  | C6-N1-C2 | -3.20 | 119.72      | 122.69   |
| 2   | L2    | 1194 | PSU  | C6-N1-C2 | -3.20 | 119.72      | 122.69   |
| 2   | L2    | 593  | PSU  | C6-N1-C2 | -3.20 | 119.72      | 122.69   |
| 1   | L1    | 1540 | OMG  | C2-N3-C4 | 3.20  | 117.80      | 112.30   |
| 51  | S1    | 1156 | PSU  | C6-N1-C2 | -3.19 | 119.73      | 122.69   |
| 51  | S1    | 12   | PSU  | C6-N1-C2 | -3.19 | 119.73      | 122.69   |
| 1   | L1    | 858  | A2M  | C2-N3-C4 | 3.19  | 119.62      | 111.83   |
| 2   | L2    | 1382 | PSU  | C6-N1-C2 | -3.18 | 119.74      | 122.69   |
| 51  | S1    | 104  | PSU  | C6-N1-C2 | -3.18 | 119.74      | 122.69   |
| 2   | L2    | 1403 | PSU  | C6-C5-C4 | 3.18  | 120.32      | 118.17   |
| 2   | L2    | 512  | PSU  | C6-N1-C2 | -3.17 | 119.75      | 122.69   |
| 2   | L2    | 641  | OMG  | C2-N3-C4 | 3.17  | 117.75      | 112.30   |
| 2   | L2    | 1284 | PSU  | C6-N1-C2 | -3.16 | 119.76      | 122.69   |
| 1   | L1    | 856  | OMG  | C2-N3-C4 | 3.16  | 117.74      | 112.30   |
| 1   | L1    | 1626 | OMG  | C2-N3-C4 | 3.16  | 117.73      | 112.30   |
| 51  | S1    | 1657 | PSU  | C6-N1-C2 | -3.15 | 119.76      | 122.69   |
| 2   | L2    | 510  | PSU  | C6-N1-C2 | -3.15 | 119.77      | 122.69   |
| 2   | L2    | 1384 | A2M  | N3-C4-N9 | 3.15  | 132.52      | 127.17   |
| 51  | S1    | 2046 | PSU  | C6-N1-C2 | -3.15 | 119.77      | 122.69   |
| 2   | L2    | 597  | PSU  | C6-N1-C2 | -3.15 | 119.77      | 122.69   |
| 2   | L2    | 506  | PSU  | C6-N1-C2 | -3.15 | 119.77      | 122.69   |
| 1   | L1    | 1171 | PSU  | C6-N1-C2 | -3.13 | 119.78      | 122.69   |
| 7   | L7    | 74   | PSU  | C6-N1-C2 | -3.13 | 119.78      | 122.69   |
| 51  | S1    | 1550 | OMG  | N9-C8-N7 | -3.13 | 107.60      | 113.40   |
| 2   | L2    | 500  | PSU  | C6-N1-C2 | -3.12 | 119.80      | 122.69   |
| 51  | S1    | 1829 | OMG  | C2-N3-C4 | 3.11  | 117.66      | 112.30   |
| 2   | L2    | 1060 | PSU  | C6-N1-C2 | -3.11 | 119.80      | 122.69   |
| 51  | S1    | 1841 | PSU  | C6-N1-C2 | -3.11 | 119.80      | 122.69   |
| 1   | L1    | 940  | PSU  | C6-N1-C2 | -3.11 | 119.81      | 122.69   |
| 51  | S1    | 1995 | 7MG  | C5-C4-N9 | 3.11  | 110.31      | 106.33   |
| 51  | S1    | 1841 | PSU  | C6-C5-C4 | 3.10  | 120.27      | 118.17   |
| 1   | L1    | 1107 | OMU  | O4-C4-C5 | -3.10 | 119.82      | 125.16   |
| 1   | L1    | 69   | A2M  | C2-N3-C4 | 3.09  | 119.39      | 111.83   |
| 1   | L1    | 1524 | OMG  | C2-N3-C4 | 3.08  | 117.61      | 112.30   |
| 51  | S1    | 2185 | MA6  | N3-C4-N9 | 3.08  | 132.41      | 127.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | L1    | 1181 | PSU  | C6-N1-C2 | -3.08 | 119.83      | 122.69   |
| 51  | S1    | 98   | A2M  | N3-C4-N9 | 3.08  | 132.41      | 127.17   |
| 51  | S1    | 1544 | 5MC  | C5-C6-N1 | -3.08 | 119.97      | 123.31   |
| 1   | L1    | 1664 | PSU  | C6-N1-C2 | -3.08 | 119.84      | 122.69   |
| 51  | S1    | 1533 | PSU  | C6-N1-C2 | -3.07 | 119.84      | 122.69   |
| 1   | L1    | 305  | A2M  | N3-C4-N9 | 3.07  | 132.40      | 127.17   |
| 51  | S1    | 512  | A2M  | N3-C4-N9 | 3.07  | 132.40      | 127.17   |
| 1   | L1    | 681  | A2M  | C2-N3-C4 | 3.07  | 119.33      | 111.83   |
| 2   | L2    | 472  | PSU  | C6-N1-C2 | -3.07 | 119.84      | 122.69   |
| 1   | L1    | 239  | PSU  | C6-N1-C2 | -3.06 | 119.85      | 122.69   |
| 51  | S1    | 28   | A2M  | N3-C4-N9 | 3.06  | 132.38      | 127.17   |
| 2   | L2    | 1185 | A2M  | C2-N3-C4 | 3.06  | 119.30      | 111.83   |
| 51  | S1    | 479  | A2M  | N3-C4-N9 | 3.06  | 132.36      | 127.17   |
| 2   | L2    | 1361 | PSU  | C6-C5-C4 | 3.05  | 120.23      | 118.17   |
| 2   | L2    | 527  | A2M  | C2-N3-C4 | 3.05  | 119.28      | 111.83   |
| 2   | L2    | 604  | A2M  | N3-C4-N9 | 3.05  | 132.35      | 127.17   |
| 1   | L1    | 959  | OMG  | N9-C4-N3 | 3.05  | 132.04      | 125.95   |
| 2   | L2    | 1403 | PSU  | C6-N1-C2 | -3.05 | 119.86      | 122.69   |
| 51  | S1    | 1246 | PSU  | C6-N1-C2 | -3.05 | 119.86      | 122.69   |
| 7   | L7    | 43   | A2M  | N3-C4-N9 | 3.04  | 132.34      | 127.17   |
| 1   | L1    | 1539 | A2M  | C2-N3-C4 | 3.04  | 119.26      | 111.83   |
| 2   | L2    | 1318 | PSU  | C6-N1-C2 | -3.04 | 119.87      | 122.69   |
| 2   | L2    | 1067 | A2M  | N3-C4-N9 | 3.04  | 132.33      | 127.17   |
| 51  | S1    | 1550 | OMG  | C2-N3-C4 | 3.03  | 117.52      | 112.30   |
| 2   | L2    | 665  | A2M  | N3-C4-N9 | 3.03  | 132.32      | 127.17   |
| 2   | L2    | 1303 | PSU  | C6-C5-C4 | 3.03  | 120.22      | 118.17   |
| 2   | L2    | 1265 | PSU  | O2-C2-N1 | -3.03 | 119.67      | 122.79   |
| 2   | L2    | 382  | A2M  | N3-C4-N9 | 3.03  | 132.31      | 127.17   |
| 1   | L1    | 677  | 1MA  | C2-N3-C4 | 3.02  | 118.46      | 112.53   |
| 51  | S1    | 2021 | A2M  | N3-C4-N9 | 3.02  | 132.30      | 127.17   |
| 51  | S1    | 668  | A2M  | C2-N3-C4 | 3.01  | 119.19      | 111.83   |
| 2   | L2    | 1253 | OMG  | N9-C8-N7 | -3.01 | 107.82      | 113.40   |
| 1   | L1    | 1181 | PSU  | C6-C5-C4 | 3.01  | 120.20      | 118.17   |
| 2   | L2    | 500  | PSU  | C6-C5-C4 | 3.01  | 120.20      | 118.17   |
| 2   | L2    | 437  | PSU  | C6-N1-C2 | -3.01 | 119.90      | 122.69   |
| 2   | L2    | 382  | A2M  | C2-N3-C4 | 3.00  | 119.17      | 111.83   |
| 51  | S1    | 1777 | OMU  | O4-C4-C5 | -2.99 | 120.00      | 125.16   |
| 1   | L1    | 856  | OMG  | N9-C8-N7 | -2.99 | 107.85      | 113.40   |
| 2   | L2    | 1046 | OMG  | N9-C4-N3 | 2.99  | 131.93      | 125.95   |
| 51  | S1    | 1657 | PSU  | C6-C5-C4 | 2.98  | 120.19      | 118.17   |
| 2   | L2    | 71   | OMG  | N9-C4-N3 | 2.97  | 131.89      | 125.95   |
| 2   | L2    | 1384 | A2M  | C2-N3-C4 | 2.97  | 119.08      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | L1    | 1011 | PSU  | C6-N1-C2   | -2.97 | 119.94      | 122.69   |
| 51  | S1    | 897  | A2M  | N3-C4-N9   | 2.97  | 132.21      | 127.17   |
| 2   | L2    | 502  | A2M  | N3-C4-N9   | 2.96  | 132.20      | 127.17   |
| 2   | L2    | 597  | PSU  | C6-C5-C4   | 2.96  | 120.17      | 118.17   |
| 3   | L3    | 13   | OMU  | O4-C4-C5   | -2.95 | 120.07      | 125.16   |
| 1   | L1    | 1626 | OMG  | N9-C8-N7   | -2.95 | 107.92      | 113.40   |
| 1   | L1    | 235  | A2M  | N3-C4-N9   | 2.95  | 132.19      | 127.17   |
| 51  | S1    | 2184 | MA6  | C5-N7-C8   | 2.95  | 108.09      | 103.45   |
| 2   | L2    | 1060 | PSU  | C6-C5-C4   | 2.95  | 120.16      | 118.17   |
| 2   | L2    | 572  | A2M  | N3-C4-N9   | 2.95  | 132.18      | 127.17   |
| 52  | S2    | 37   | MIA  | C5-N7-C8   | 2.95  | 108.08      | 103.45   |
| 51  | S1    | 29   | OMU  | O4-C4-C5   | -2.94 | 120.08      | 125.16   |
| 52  | S2    | 37   | MIA  | C2-N3-C4   | 2.94  | 120.00      | 112.29   |
| 2   | L2    | 1265 | PSU  | C6-C5-C4   | 2.94  | 120.16      | 118.17   |
| 2   | L2    | 95   | A2M  | N3-C4-N9   | 2.93  | 132.16      | 127.17   |
| 2   | L2    | 628  | A2M  | N3-C4-N9   | 2.93  | 132.15      | 127.17   |
| 1   | L1    | 69   | A2M  | C2'-C1'-N9 | -2.93 | 108.94      | 113.75   |
| 51  | S1    | 1246 | PSU  | C6-C5-C4   | 2.93  | 120.15      | 118.17   |
| 2   | L2    | 78   | PSU  | C6-N1-C2   | -2.92 | 119.98      | 122.69   |
| 51  | S1    | 2021 | A2M  | C5-N7-C8   | 2.92  | 108.04      | 103.45   |
| 2   | L2    | 1419 | OMU  | O4-C4-C5   | -2.92 | 120.13      | 125.16   |
| 2   | L2    | 1213 | PSU  | C6-C5-C4   | 2.92  | 120.14      | 118.17   |
| 7   | L7    | 43   | A2M  | C5-N7-C8   | 2.92  | 108.04      | 103.45   |
| 2   | L2    | 665  | A2M  | C5-N7-C8   | 2.92  | 108.03      | 103.45   |
| 51  | S1    | 1623 | OMG  | C2-N1-C6   | -2.92 | 119.82      | 125.11   |
| 1   | L1    | 774  | PSU  | C6-C5-C4   | 2.91  | 120.14      | 118.17   |
| 1   | L1    | 305  | A2M  | C5-N7-C8   | 2.91  | 108.03      | 103.45   |
| 2   | L2    | 591  | A2M  | N3-C4-N9   | 2.91  | 132.12      | 127.17   |
| 1   | L1    | 1253 | OMU  | O4-C4-C5   | -2.91 | 120.14      | 125.16   |
| 7   | L7    | 74   | PSU  | C6-C5-C4   | 2.91  | 120.14      | 118.17   |
| 51  | S1    | 2046 | PSU  | C6-C5-C4   | 2.91  | 120.14      | 118.17   |
| 2   | L2    | 572  | A2M  | C5-N7-C8   | 2.91  | 108.02      | 103.45   |
| 2   | L2    | 56   | OMU  | O4-C4-C5   | -2.91 | 120.15      | 125.16   |
| 2   | L2    | 1144 | PSU  | C6-C5-C4   | 2.91  | 120.14      | 118.17   |
| 51  | S1    | 512  | A2M  | C5-N7-C8   | 2.91  | 108.02      | 103.45   |
| 51  | S1    | 1995 | 7MG  | C2-N1-C6   | -2.90 | 119.84      | 125.11   |
| 1   | L1    | 1373 | A2M  | C5-N7-C8   | 2.90  | 108.01      | 103.45   |
| 2   | L2    | 628  | A2M  | C5-N7-C8   | 2.90  | 108.01      | 103.45   |
| 2   | L2    | 1067 | A2M  | C5-N7-C8   | 2.90  | 108.01      | 103.45   |
| 2   | L2    | 1231 | OMG  | C2-N1-C6   | -2.90 | 119.86      | 125.11   |
| 2   | L2    | 1372 | A2M  | N3-C4-N9   | 2.89  | 132.09      | 127.17   |
| 2   | L2    | 604  | A2M  | C5-N7-C8   | 2.89  | 107.99      | 103.45   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | S1    | 897  | A2M  | C5-N7-C8   | 2.89  | 107.99      | 103.45   |
| 51  | S1    | 2185 | MA6  | C5-N7-C8   | 2.89  | 107.99      | 103.45   |
| 1   | L1    | 856  | OMG  | N9-C4-N3   | 2.89  | 131.73      | 125.95   |
| 1   | L1    | 1373 | A2M  | N3-C4-N9   | 2.89  | 132.08      | 127.17   |
| 51  | S1    | 1621 | OMU  | O4-C4-C5   | -2.89 | 120.18      | 125.16   |
| 1   | L1    | 845  | OMU  | O4-C4-C5   | -2.89 | 120.18      | 125.16   |
| 51  | S1    | 600  | OMG  | C2-N1-C6   | -2.89 | 119.88      | 125.11   |
| 51  | S1    | 1979 | OMU  | O4-C4-C5   | -2.89 | 120.18      | 125.16   |
| 7   | L7    | 162  | A2M  | N3-C4-N9   | 2.89  | 132.07      | 127.17   |
| 51  | S1    | 1662 | OMU  | O4-C4-C5   | -2.88 | 120.19      | 125.16   |
| 2   | L2    | 626  | PSU  | C6-C5-C4   | 2.88  | 120.12      | 118.17   |
| 2   | L2    | 686  | OMG  | C2-N1-C6   | -2.88 | 119.89      | 125.11   |
| 1   | L1    | 239  | PSU  | C6-C5-C4   | 2.88  | 120.11      | 118.17   |
| 2   | L2    | 570  | A2M  | N3-C4-N9   | 2.88  | 132.06      | 127.17   |
| 2   | L2    | 1372 | A2M  | C5-N7-C8   | 2.87  | 107.97      | 103.45   |
| 2   | L2    | 472  | PSU  | C6-C5-C4   | 2.87  | 120.11      | 118.17   |
| 51  | S1    | 28   | A2M  | C5-N7-C8   | 2.87  | 107.97      | 103.45   |
| 51  | S1    | 1623 | OMG  | N9-C4-N3   | 2.87  | 131.70      | 125.95   |
| 2   | L2    | 534  | OMG  | C2-N1-C6   | -2.87 | 119.90      | 125.11   |
| 2   | L2    | 502  | A2M  | C5-N7-C8   | 2.87  | 107.96      | 103.45   |
| 1   | L1    | 847  | OMU  | O4-C4-C5   | -2.87 | 120.21      | 125.16   |
| 2   | L2    | 593  | PSU  | C6-C5-C4   | 2.87  | 120.11      | 118.17   |
| 2   | L2    | 71   | OMG  | N9-C8-N7   | -2.87 | 108.08      | 113.40   |
| 1   | L1    | 1659 | OMU  | O4-C4-C5   | -2.87 | 120.22      | 125.16   |
| 7   | L7    | 162  | A2M  | C5-N7-C8   | 2.87  | 107.95      | 103.45   |
| 2   | L2    | 95   | A2M  | C5-N7-C8   | 2.86  | 107.95      | 103.45   |
| 1   | L1    | 959  | OMG  | C2-N1-C6   | -2.86 | 119.92      | 125.11   |
| 2   | L2    | 667  | OMU  | O4-C4-C5   | -2.86 | 120.23      | 125.16   |
| 2   | L2    | 527  | A2M  | O4'-C1'-N9 | 2.86  | 113.58      | 108.09   |
| 2   | L2    | 1046 | OMG  | C2-N1-C6   | -2.86 | 119.92      | 125.11   |
| 1   | L1    | 1528 | PSU  | C6-C5-C4   | 2.86  | 120.10      | 118.17   |
| 2   | L2    | 1185 | A2M  | N3-C4-N9   | 2.86  | 132.03      | 127.17   |
| 51  | S1    | 8    | OMU  | O4-C4-C5   | -2.86 | 120.24      | 125.16   |
| 1   | L1    | 955  | A2M  | C5-N7-C8   | 2.85  | 107.94      | 103.45   |
| 1   | L1    | 1171 | PSU  | O2-C2-N1   | -2.85 | 119.85      | 122.79   |
| 51  | S1    | 98   | A2M  | C5-N7-C8   | 2.85  | 107.93      | 103.45   |
| 51  | S1    | 479  | A2M  | C5-N7-C8   | 2.85  | 107.92      | 103.45   |
| 1   | L1    | 678  | A2M  | C5-N7-C8   | 2.85  | 107.92      | 103.45   |
| 1   | L1    | 697  | A2M  | N3-C4-N9   | 2.85  | 132.01      | 127.17   |
| 2   | L2    | 1360 | OMG  | N9-C4-N3   | 2.83  | 131.62      | 125.95   |
| 2   | L2    | 570  | A2M  | C5-N7-C8   | 2.83  | 107.91      | 103.45   |
| 2   | L2    | 1359 | OMU  | O4-C4-C5   | -2.83 | 120.28      | 125.16   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | L2    | 1361 | PSU  | O2-C2-N1   | -2.83 | 119.87      | 122.79   |
| 1   | L1    | 1371 | OMU  | O4-C4-C5   | -2.83 | 120.28      | 125.16   |
| 51  | S1    | 1543 | B8N  | O4-C4-N3   | -2.83 | 115.39      | 119.99   |
| 1   | L1    | 955  | A2M  | N3-C4-N9   | 2.83  | 131.97      | 127.17   |
| 51  | S1    | 2151 | OMG  | C2-N1-C6   | -2.82 | 119.99      | 125.11   |
| 51  | S1    | 969  | A2M  | C5-N7-C8   | 2.82  | 107.88      | 103.45   |
| 1   | L1    | 48   | OMU  | O4-C4-C5   | -2.82 | 120.30      | 125.16   |
| 1   | L1    | 681  | A2M  | N3-C4-N9   | 2.82  | 131.96      | 127.17   |
| 51  | S1    | 1647 | OMG  | C2-N1-C6   | -2.81 | 120.01      | 125.11   |
| 2   | L2    | 1078 | OMG  | C2-N1-C6   | -2.81 | 120.01      | 125.11   |
| 1   | L1    | 235  | A2M  | C5-N7-C8   | 2.81  | 107.87      | 103.45   |
| 1   | L1    | 1190 | OMG  | C2-N1-C6   | -2.81 | 120.01      | 125.11   |
| 51  | S1    | 1865 | OMG  | C2-N1-C6   | -2.81 | 120.01      | 125.11   |
| 2   | L2    | 73   | OMU  | O4-C4-C5   | -2.81 | 120.32      | 125.16   |
| 51  | S1    | 1156 | PSU  | C6-C5-C4   | 2.81  | 120.07      | 118.17   |
| 2   | L2    | 1318 | PSU  | C6-C5-C4   | 2.81  | 120.07      | 118.17   |
| 51  | S1    | 1995 | 7MG  | N9-C4-N3   | 2.80  | 129.56      | 125.46   |
| 51  | S1    | 1478 | OMG  | C2-N1-C6   | -2.80 | 120.04      | 125.11   |
| 2   | L2    | 1253 | OMG  | N9-C4-N3   | 2.80  | 131.54      | 125.95   |
| 2   | L2    | 591  | A2M  | C5-N7-C8   | 2.79  | 107.84      | 103.45   |
| 51  | S1    | 1865 | OMG  | N9-C4-N3   | 2.79  | 131.54      | 125.95   |
| 4   | L4    | 74   | OMG  | C2-N1-C6   | -2.79 | 120.05      | 125.11   |
| 2   | L2    | 655  | OMG  | C2-N1-C6   | -2.79 | 120.05      | 125.11   |
| 51  | S1    | 2061 | 5MC  | C5-C6-N1   | -2.78 | 120.29      | 123.31   |
| 1   | L1    | 1093 | PSU  | C6-C5-C4   | 2.78  | 120.05      | 118.17   |
| 51  | S1    | 661  | OMU  | O4-C4-C5   | -2.77 | 120.38      | 125.16   |
| 1   | L1    | 697  | A2M  | C5-N7-C8   | 2.77  | 107.80      | 103.45   |
| 2   | L2    | 1185 | A2M  | C5-N7-C8   | 2.77  | 107.80      | 103.45   |
| 51  | S1    | 33   | PSU  | C6-C5-C4   | 2.76  | 120.04      | 118.17   |
| 51  | S1    | 1995 | 7MG  | O6-C6-C5   | -2.76 | 120.84      | 127.62   |
| 1   | L1    | 681  | A2M  | C5-N7-C8   | 2.76  | 107.78      | 103.45   |
| 51  | S1    | 600  | OMG  | N9-C4-N3   | 2.76  | 131.46      | 125.95   |
| 1   | L1    | 858  | A2M  | C5-N7-C8   | 2.76  | 107.78      | 103.45   |
| 51  | S1    | 2008 | OMG  | C2-N1-C6   | -2.75 | 120.12      | 125.11   |
| 2   | L2    | 506  | PSU  | C6-C5-C4   | 2.75  | 120.03      | 118.17   |
| 7   | L7    | 101  | OMU  | O4-C4-C5   | -2.75 | 120.42      | 125.16   |
| 2   | L2    | 504  | PSU  | O2-C2-N1   | -2.75 | 119.95      | 122.79   |
| 2   | L2    | 1360 | OMG  | C2-N1-C6   | -2.75 | 120.12      | 125.11   |
| 1   | L1    | 422  | PSU  | C6-C5-C4   | 2.75  | 120.03      | 118.17   |
| 51  | S1    | 897  | A2M  | C2'-C1'-N9 | -2.74 | 109.23      | 113.75   |
| 51  | S1    | 609  | PSU  | O2-C2-N1   | -2.74 | 119.96      | 122.79   |
| 2   | L2    | 655  | OMG  | N9-C4-N3   | 2.74  | 131.43      | 125.95   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | S1    | 104  | PSU  | C6-C5-C4    | 2.74  | 120.02      | 118.17   |
| 51  | S1    | 1533 | PSU  | C6-C5-C4    | 2.73  | 120.02      | 118.17   |
| 2   | L2    | 597  | PSU  | O2-C2-N1    | -2.73 | 119.97      | 122.79   |
| 7   | L7    | 69   | PSU  | O2-C2-N1    | -2.73 | 119.97      | 122.79   |
| 2   | L2    | 1229 | OMG  | N9-C4-N3    | 2.73  | 131.42      | 125.95   |
| 2   | L2    | 560  | OMU  | O4-C4-C5    | -2.73 | 120.46      | 125.16   |
| 7   | L7    | 75   | OMG  | C2-N1-C6    | -2.73 | 120.17      | 125.11   |
| 1   | L1    | 927  | A2M  | C5-N7-C8    | 2.73  | 107.74      | 103.45   |
| 51  | S1    | 609  | PSU  | C6-C5-C4    | 2.73  | 120.01      | 118.17   |
| 2   | L2    | 504  | PSU  | C6-C5-C4    | 2.73  | 120.01      | 118.17   |
| 1   | L1    | 858  | A2M  | N3-C4-N9    | 2.72  | 131.80      | 127.17   |
| 2   | L2    | 1231 | OMG  | N9-C4-N3    | 2.72  | 131.40      | 125.95   |
| 51  | S1    | 455  | PSU  | O2-C2-N1    | -2.72 | 119.98      | 122.79   |
| 7   | L7    | 43   | A2M  | C2'-C1'-N9  | -2.71 | 109.29      | 113.75   |
| 51  | S1    | 12   | PSU  | C6-C5-C4    | 2.71  | 120.00      | 118.17   |
| 1   | L1    | 1039 | OMU  | O4-C4-C5    | -2.71 | 120.49      | 125.16   |
| 2   | L2    | 1229 | OMG  | C2-N1-C6    | -2.71 | 120.19      | 125.11   |
| 1   | L1    | 1626 | OMG  | N9-C4-N3    | 2.71  | 131.37      | 125.95   |
| 2   | L2    | 500  | PSU  | O2-C2-N1    | -2.70 | 120.00      | 122.79   |
| 2   | L2    | 1384 | A2M  | C5-N7-C8    | 2.70  | 107.69      | 103.45   |
| 51  | S1    | 2048 | PSU  | C6-C5-C4    | 2.70  | 119.99      | 118.17   |
| 1   | L1    | 940  | PSU  | C6-C5-C4    | 2.70  | 119.99      | 118.17   |
| 1   | L1    | 1539 | A2M  | C5-N7-C8    | 2.69  | 107.68      | 103.45   |
| 2   | L2    | 1382 | PSU  | O2-C2-N1    | -2.69 | 120.01      | 122.79   |
| 2   | L2    | 1308 | 5MC  | C4'-O4'-C1' | -2.69 | 103.52      | 109.47   |
| 1   | L1    | 1528 | PSU  | O2-C2-N1    | -2.69 | 120.01      | 122.79   |
| 2   | L2    | 1058 | PSU  | O2-C2-N1    | -2.69 | 120.02      | 122.79   |
| 1   | L1    | 69   | A2M  | C5-N7-C8    | 2.68  | 107.67      | 103.45   |
| 1   | L1    | 69   | A2M  | N3-C4-N9    | 2.68  | 131.73      | 127.17   |
| 2   | L2    | 510  | PSU  | C6-C5-C4    | 2.68  | 119.98      | 118.17   |
| 2   | L2    | 512  | PSU  | C6-C5-C4    | 2.67  | 119.98      | 118.17   |
| 2   | L2    | 662  | PSU  | O2-C2-N1    | -2.67 | 120.03      | 122.79   |
| 1   | L1    | 1524 | OMG  | N9-C4-N3    | 2.67  | 131.30      | 125.95   |
| 51  | S1    | 2008 | OMG  | C5-C6-N1    | 2.67  | 120.04      | 113.25   |
| 2   | L2    | 527  | A2M  | C2'-C1'-N9  | -2.66 | 109.38      | 113.75   |
| 2   | L2    | 534  | OMG  | N9-C4-N3    | 2.66  | 131.26      | 125.95   |
| 2   | L2    | 1185 | A2M  | C4-C5-N7    | -2.65 | 107.55      | 110.58   |
| 51  | S1    | 2202 | PSU  | C6-C5-C4    | 2.65  | 119.96      | 118.17   |
| 51  | S1    | 104  | PSU  | O2-C2-N1    | -2.65 | 120.06      | 122.79   |
| 51  | S1    | 1543 | B8N  | C32-C31-N3  | -2.65 | 107.53      | 112.16   |
| 51  | S1    | 1292 | PSU  | C6-C5-C4    | 2.65  | 119.96      | 118.17   |
| 1   | L1    | 1533 | PSU  | O2-C2-N1    | -2.64 | 120.06      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | L2    | 1264 | PSU  | O2-C2-N1    | -2.64 | 120.06      | 122.79   |
| 2   | L2    | 626  | PSU  | O2-C2-N1    | -2.64 | 120.06      | 122.79   |
| 1   | L1    | 1190 | OMG  | C5-C6-N1    | 2.64  | 119.96      | 113.25   |
| 2   | L2    | 686  | OMG  | N9-C4-N3    | 2.63  | 131.22      | 125.95   |
| 51  | S1    | 1647 | OMG  | C5-C6-N1    | 2.63  | 119.95      | 113.25   |
| 51  | S1    | 1246 | PSU  | O2-C2-N1    | -2.63 | 120.08      | 122.79   |
| 2   | L2    | 686  | OMG  | C5-C6-N1    | 2.63  | 119.95      | 113.25   |
| 51  | S1    | 1623 | OMG  | C5-C6-N1    | 2.63  | 119.95      | 113.25   |
| 1   | L1    | 1017 | PSU  | O2-C2-N1    | -2.63 | 120.08      | 122.79   |
| 1   | L1    | 1533 | PSU  | C6-C5-C4    | 2.63  | 119.95      | 118.17   |
| 51  | S1    | 668  | A2M  | C5-N7-C8    | 2.63  | 107.58      | 103.45   |
| 2   | L2    | 1078 | OMG  | N2-C2-N1    | 2.63  | 122.30      | 116.76   |
| 51  | S1    | 2048 | PSU  | O2-C2-N1    | -2.62 | 120.08      | 122.79   |
| 51  | S1    | 1647 | OMG  | N9-C4-N3    | 2.62  | 131.19      | 125.95   |
| 2   | L2    | 527  | A2M  | C4'-O4'-C1' | -2.62 | 103.68      | 109.47   |
| 51  | S1    | 1865 | OMG  | C5-C6-N1    | 2.62  | 119.92      | 113.25   |
| 2   | L2    | 655  | OMG  | C5-C6-N1    | 2.61  | 119.91      | 113.25   |
| 2   | L2    | 1194 | PSU  | C6-C5-C4    | 2.61  | 119.94      | 118.17   |
| 2   | L2    | 1303 | PSU  | O2-C2-N1    | -2.61 | 120.09      | 122.79   |
| 51  | S1    | 1478 | OMG  | C5-C6-N1    | 2.61  | 119.90      | 113.25   |
| 2   | L2    | 1413 | PSU  | O2-C2-N1    | -2.61 | 120.10      | 122.79   |
| 51  | S1    | 2151 | OMG  | C5-C6-N1    | 2.61  | 119.89      | 113.25   |
| 2   | L2    | 78   | PSU  | C6-C5-C4    | 2.61  | 119.93      | 118.17   |
| 2   | L2    | 512  | PSU  | O2-C2-N1    | -2.61 | 120.10      | 122.79   |
| 1   | L1    | 1524 | OMG  | N9-C8-N7    | -2.60 | 108.57      | 113.40   |
| 4   | L4    | 74   | OMG  | C5-C6-N1    | 2.60  | 119.88      | 113.25   |
| 51  | S1    | 12   | PSU  | O2-C2-N1    | -2.60 | 120.11      | 122.79   |
| 2   | L2    | 1046 | OMG  | C5-C6-N1    | 2.60  | 119.87      | 113.25   |
| 7   | L7    | 74   | PSU  | O2-C2-N1    | -2.60 | 120.11      | 122.79   |
| 1   | L1    | 959  | OMG  | C5-C6-N1    | 2.60  | 119.87      | 113.25   |
| 2   | L2    | 1360 | OMG  | C5-C6-N1    | 2.60  | 119.86      | 113.25   |
| 2   | L2    | 437  | PSU  | C6-C5-C4    | 2.59  | 119.92      | 118.17   |
| 51  | S1    | 1192 | PSU  | O2-C2-N1    | -2.59 | 120.12      | 122.79   |
| 1   | L1    | 1539 | A2M  | C4-C5-N7    | -2.59 | 107.62      | 110.58   |
| 51  | S1    | 600  | OMG  | C5-C6-N1    | 2.59  | 119.84      | 113.25   |
| 51  | S1    | 2046 | PSU  | O2-C2-N1    | -2.59 | 120.12      | 122.79   |
| 2   | L2    | 1284 | PSU  | C6-C5-C4    | 2.59  | 119.92      | 118.17   |
| 2   | L2    | 1194 | PSU  | O2-C2-N1    | -2.58 | 120.13      | 122.79   |
| 2   | L2    | 1077 | OMU  | O4-C4-C5    | -2.58 | 120.72      | 125.16   |
| 2   | L2    | 1231 | OMG  | C5-C6-N1    | 2.58  | 119.81      | 113.25   |
| 51  | S1    | 1533 | PSU  | O2-C2-N1    | -2.58 | 120.13      | 122.79   |
| 1   | L1    | 697  | A2M  | C2'-C1'-N9  | -2.57 | 109.52      | 113.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | L2    | 527  | A2M  | C5-N7-C8 | 2.57  | 107.49      | 103.45   |
| 2   | L2    | 534  | OMG  | C5-C6-N1 | 2.57  | 119.80      | 113.25   |
| 2   | L2    | 71   | OMG  | C2-N1-C6 | -2.57 | 120.45      | 125.11   |
| 1   | L1    | 677  | 1MA  | N9-C4-N3 | 2.57  | 132.76      | 126.90   |
| 2   | L2    | 382  | A2M  | C5-N7-C8 | 2.57  | 107.49      | 103.45   |
| 2   | L2    | 472  | PSU  | O2-C2-N1 | -2.56 | 120.14      | 122.79   |
| 2   | L2    | 1229 | OMG  | C5-C6-N1 | 2.56  | 119.78      | 113.25   |
| 51  | S1    | 1550 | OMG  | N9-C4-N3 | 2.56  | 131.07      | 125.95   |
| 7   | L7    | 75   | OMG  | C5-C6-N1 | 2.56  | 119.77      | 113.25   |
| 51  | S1    | 2202 | PSU  | O2-C2-N1 | -2.56 | 120.15      | 122.79   |
| 51  | S1    | 1657 | PSU  | O2-C2-N1 | -2.56 | 120.15      | 122.79   |
| 51  | S1    | 33   | PSU  | O2-C2-N1 | -2.55 | 120.15      | 122.79   |
| 51  | S1    | 1841 | PSU  | O2-C2-N1 | -2.55 | 120.16      | 122.79   |
| 2   | L2    | 593  | PSU  | O2-C2-N1 | -2.55 | 120.16      | 122.79   |
| 1   | L1    | 239  | PSU  | O2-C2-N1 | -2.55 | 120.16      | 122.79   |
| 51  | S1    | 1566 | PSU  | C6-C5-C4 | 2.55  | 119.89      | 118.17   |
| 1   | L1    | 774  | PSU  | O2-C2-N1 | -2.54 | 120.17      | 122.79   |
| 2   | L2    | 1078 | OMG  | C5-C6-N1 | 2.54  | 119.72      | 113.25   |
| 1   | L1    | 1539 | A2M  | N3-C4-N9 | 2.54  | 131.48      | 127.17   |
| 1   | L1    | 1181 | PSU  | O2-C2-N1 | -2.53 | 120.17      | 122.79   |
| 2   | L2    | 1284 | PSU  | O2-C2-N1 | -2.53 | 120.18      | 122.79   |
| 51  | S1    | 2184 | MA6  | C4-N9-C8 | 2.53  | 108.39      | 105.74   |
| 2   | L2    | 1060 | PSU  | O2-C2-N1 | -2.52 | 120.19      | 122.79   |
| 2   | L2    | 527  | A2M  | C4-N9-C8 | 2.52  | 108.38      | 105.74   |
| 1   | L1    | 681  | A2M  | C4-C5-N7 | -2.51 | 107.71      | 110.58   |
| 51  | S1    | 1833 | OMU  | O4-C4-C5 | -2.51 | 120.83      | 125.16   |
| 1   | L1    | 1190 | OMG  | C8-N7-C5 | 2.51  | 108.74      | 104.26   |
| 7   | L7    | 75   | OMG  | N9-C4-N3 | 2.51  | 130.97      | 125.95   |
| 1   | L1    | 1011 | PSU  | O2-C2-N1 | -2.51 | 120.20      | 122.79   |
| 51  | S1    | 1292 | PSU  | O2-C2-N1 | -2.51 | 120.20      | 122.79   |
| 51  | S1    | 2008 | OMG  | C8-N7-C5 | 2.50  | 108.71      | 104.26   |
| 2   | L2    | 527  | A2M  | N3-C4-N9 | 2.50  | 131.41      | 127.17   |
| 1   | L1    | 677  | 1MA  | N9-C8-N7 | -2.49 | 108.78      | 113.40   |
| 2   | L2    | 437  | PSU  | O2-C2-N1 | -2.49 | 120.22      | 122.79   |
| 1   | L1    | 1093 | PSU  | O2-C2-N1 | -2.49 | 120.22      | 122.79   |
| 2   | L2    | 1403 | PSU  | O2-C2-N1 | -2.49 | 120.22      | 122.79   |
| 51  | S1    | 668  | A2M  | C4-C5-N7 | -2.48 | 107.74      | 110.58   |
| 2   | L2    | 1078 | OMG  | C8-N7-C5 | 2.48  | 108.69      | 104.26   |
| 1   | L1    | 927  | A2M  | C4-N9-C8 | 2.48  | 108.34      | 105.74   |
| 1   | L1    | 422  | PSU  | O2-C2-N1 | -2.48 | 120.23      | 122.79   |
| 51  | S1    | 969  | A2M  | N3-C4-N9 | 2.47  | 131.37      | 127.17   |
| 51  | S1    | 1995 | 7MG  | N9-C8-N7 | 2.46  | 106.86      | 103.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | L4    | 74   | OMG  | N9-C4-N3    | 2.46  | 130.88      | 125.95   |
| 2   | L2    | 506  | PSU  | O2-C2-N1    | -2.46 | 120.25      | 122.79   |
| 51  | S1    | 1539 | PSU  | O2-C2-N1    | -2.46 | 120.25      | 122.79   |
| 2   | L2    | 1067 | A2M  | C2'-C1'-N9  | -2.46 | 109.71      | 113.75   |
| 51  | S1    | 1566 | PSU  | O2-C2-N1    | -2.46 | 120.25      | 122.79   |
| 1   | L1    | 940  | PSU  | O2-C2-N1    | -2.46 | 120.26      | 122.79   |
| 2   | L2    | 1384 | A2M  | C2'-C1'-N9  | -2.45 | 109.71      | 113.75   |
| 51  | S1    | 2151 | OMG  | C8-N7-C5    | 2.45  | 108.63      | 104.26   |
| 2   | L2    | 1046 | OMG  | O6-C6-C5    | -2.45 | 120.06      | 126.53   |
| 51  | S1    | 668  | A2M  | N3-C4-N9    | 2.45  | 131.33      | 127.17   |
| 51  | S1    | 1647 | OMG  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 1   | L1    | 858  | A2M  | C4-C5-N7    | -2.44 | 107.79      | 110.58   |
| 2   | L2    | 1231 | OMG  | O6-C6-C5    | -2.43 | 120.11      | 126.53   |
| 51  | S1    | 2151 | OMG  | N9-C4-N3    | 2.43  | 130.81      | 125.95   |
| 51  | S1    | 668  | A2M  | C3'-C2'-C1' | 2.43  | 107.45      | 102.81   |
| 2   | L2    | 1253 | OMG  | C2-N1-C6    | -2.42 | 120.72      | 125.11   |
| 1   | L1    | 858  | A2M  | C4-N9-C8    | 2.42  | 108.28      | 105.74   |
| 52  | S2    | 37   | MIA  | C4-C5-N7    | -2.42 | 107.81      | 110.58   |
| 7   | L7    | 75   | OMG  | C8-N7-C5    | 2.42  | 108.58      | 104.26   |
| 1   | L1    | 1190 | OMG  | N2-C2-N1    | 2.42  | 121.87      | 116.76   |
| 2   | L2    | 1213 | PSU  | O2-C2-N1    | -2.42 | 120.29      | 122.79   |
| 1   | L1    | 1626 | OMG  | C2-N1-C6    | -2.42 | 120.72      | 125.11   |
| 1   | L1    | 69   | A2M  | C4-N9-C8    | 2.42  | 108.27      | 105.74   |
| 51  | S1    | 2185 | MA6  | C4-N9-C8    | 2.41  | 108.27      | 105.74   |
| 2   | L2    | 1144 | PSU  | O2-C2-N1    | -2.41 | 120.30      | 122.79   |
| 1   | L1    | 856  | OMG  | C2-N1-C6    | -2.41 | 120.74      | 125.11   |
| 51  | S1    | 98   | A2M  | C2'-C1'-N9  | -2.41 | 109.79      | 113.75   |
| 2   | L2    | 641  | OMG  | C2-N1-C6    | -2.41 | 120.75      | 125.11   |
| 1   | L1    | 959  | OMG  | O6-C6-C5    | -2.40 | 120.18      | 126.53   |
| 2   | L2    | 382  | A2M  | C4-C5-N7    | -2.40 | 107.84      | 110.58   |
| 51  | S1    | 1478 | OMG  | O6-C6-C5    | -2.40 | 120.20      | 126.53   |
| 2   | L2    | 1078 | OMG  | O6-C6-C5    | -2.40 | 120.21      | 126.53   |
| 2   | L2    | 655  | OMG  | C8-N7-C5    | 2.39  | 108.53      | 104.26   |
| 2   | L2    | 1229 | OMG  | O6-C6-C5    | -2.39 | 120.22      | 126.53   |
| 2   | L2    | 686  | OMG  | C8-N7-C5    | 2.39  | 108.52      | 104.26   |
| 51  | S1    | 1829 | OMG  | C8-N7-C5    | 2.39  | 108.52      | 104.26   |
| 1   | L1    | 1373 | A2M  | C2'-C1'-N9  | -2.39 | 109.82      | 113.75   |
| 1   | L1    | 1190 | OMG  | O6-C6-C5    | -2.39 | 120.23      | 126.53   |
| 7   | L7    | 101  | OMU  | O3'-C3'-C2' | 2.39  | 117.86      | 111.19   |
| 51  | S1    | 600  | OMG  | O6-C6-C5    | -2.39 | 120.24      | 126.53   |
| 4   | L4    | 74   | OMG  | O6-C6-C5    | -2.38 | 120.24      | 126.53   |
| 1   | L1    | 1664 | PSU  | O2-C2-N1    | -2.38 | 120.33      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | S1    | 1647 | OMG  | O6-C6-C5    | -2.38 | 120.24      | 126.53   |
| 2   | L2    | 686  | OMG  | O6-C6-C5    | -2.38 | 120.25      | 126.53   |
| 51  | S1    | 1623 | OMG  | O6-C6-C5    | -2.38 | 120.25      | 126.53   |
| 2   | L2    | 570  | A2M  | C4-C5-N7    | -2.38 | 107.86      | 110.58   |
| 1   | L1    | 1664 | PSU  | C6-C5-C4    | 2.37  | 119.78      | 118.17   |
| 2   | L2    | 1360 | OMG  | O6-C6-C5    | -2.37 | 120.27      | 126.53   |
| 2   | L2    | 1229 | OMG  | C8-N7-C5    | 2.37  | 108.48      | 104.26   |
| 2   | L2    | 570  | A2M  | C5-C4-N9    | 2.37  | 108.39      | 105.81   |
| 1   | L1    | 69   | A2M  | C4-C5-N7    | -2.36 | 107.88      | 110.58   |
| 2   | L2    | 1318 | PSU  | O2-C2-N1    | -2.36 | 120.36      | 122.79   |
| 2   | L2    | 641  | OMG  | C8-N7-C5    | 2.36  | 108.46      | 104.26   |
| 51  | S1    | 1865 | OMG  | C8-N7-C5    | 2.36  | 108.46      | 104.26   |
| 2   | L2    | 534  | OMG  | O6-C6-C5    | -2.35 | 120.32      | 126.53   |
| 51  | S1    | 1865 | OMG  | O6-C6-C5    | -2.35 | 120.32      | 126.53   |
| 1   | L1    | 1540 | OMG  | N9-C4-N3    | 2.35  | 130.65      | 125.95   |
| 1   | L1    | 1540 | OMG  | C2-N1-C6    | -2.35 | 120.85      | 125.11   |
| 51  | S1    | 1829 | OMG  | C2-N1-C6    | -2.35 | 120.85      | 125.11   |
| 4   | L4    | 74   | OMG  | C8-N7-C5    | 2.35  | 108.44      | 104.26   |
| 51  | S1    | 2008 | OMG  | N9-C4-N3    | 2.34  | 130.64      | 125.95   |
| 51  | S1    | 1478 | OMG  | C8-N7-C5    | 2.34  | 108.44      | 104.26   |
| 51  | S1    | 969  | A2M  | C4-C5-N7    | -2.34 | 107.91      | 110.58   |
| 1   | L1    | 1540 | OMG  | C8-N7-C5    | 2.34  | 108.43      | 104.26   |
| 51  | S1    | 1550 | OMG  | C2-N1-C6    | -2.34 | 120.88      | 125.11   |
| 2   | L2    | 572  | A2M  | C2'-C1'-N9  | -2.33 | 109.91      | 113.75   |
| 51  | S1    | 600  | OMG  | C8-N7-C5    | 2.32  | 108.40      | 104.26   |
| 2   | L2    | 510  | PSU  | O2-C2-N1    | -2.32 | 120.39      | 122.79   |
| 2   | L2    | 1384 | A2M  | C4-C5-N7    | -2.32 | 107.93      | 110.58   |
| 2   | L2    | 1308 | 5MC  | C5-C4-N3    | -2.32 | 119.38      | 121.75   |
| 51  | S1    | 1623 | OMG  | C8-N7-C5    | 2.32  | 108.39      | 104.26   |
| 2   | L2    | 534  | OMG  | C8-N7-C5    | 2.31  | 108.38      | 104.26   |
| 7   | L7    | 75   | OMG  | O6-C6-C5    | -2.31 | 120.44      | 126.53   |
| 51  | S1    | 2021 | A2M  | O2'-C2'-C1' | 2.30  | 113.36      | 108.99   |
| 51  | S1    | 2021 | A2M  | C4-C5-N7    | -2.30 | 107.95      | 110.58   |
| 51  | S1    | 969  | A2M  | C4-N9-C8    | 2.29  | 108.14      | 105.74   |
| 51  | S1    | 2008 | OMG  | O6-C6-C5    | -2.29 | 120.50      | 126.53   |
| 2   | L2    | 655  | OMG  | O6-C6-C5    | -2.28 | 120.50      | 126.53   |
| 52  | S2    | 37   | MIA  | C16-C14-C15 | 2.28  | 119.84      | 114.59   |
| 2   | L2    | 1046 | OMG  | C8-N7-C5    | 2.28  | 108.32      | 104.26   |
| 1   | L1    | 678  | A2M  | C4-N9-C8    | 2.28  | 108.13      | 105.74   |
| 1   | L1    | 1373 | A2M  | C4-C5-N7    | -2.27 | 107.98      | 110.58   |
| 2   | L2    | 1372 | A2M  | C4-N9-C8    | 2.27  | 108.12      | 105.74   |
| 1   | L1    | 1527 | OMC  | O2-C2-N3    | -2.27 | 118.75      | 122.33   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51  | S1    | 2151 | OMG  | O6-C6-C5   | -2.26 | 120.56      | 126.53   |
| 2   | L2    | 1360 | OMG  | C8-N7-C5   | 2.26  | 108.29      | 104.26   |
| 51  | S1    | 28   | A2M  | C4-C5-N7   | -2.26 | 108.00      | 110.58   |
| 51  | S1    | 1478 | OMG  | N2-C2-N1   | 2.25  | 121.52      | 116.76   |
| 2   | L2    | 502  | A2M  | C4-C5-N7   | -2.25 | 108.01      | 110.58   |
| 1   | L1    | 1190 | OMG  | C2'-C1'-N9 | -2.25 | 109.97      | 114.24   |
| 2   | L2    | 628  | A2M  | C4-C5-N7   | -2.25 | 108.01      | 110.58   |
| 2   | L2    | 78   | PSU  | O2-C2-N1   | -2.25 | 120.47      | 122.79   |
| 3   | L3    | 13   | OMU  | O2-C2-N1   | -2.25 | 119.87      | 122.80   |
| 1   | L1    | 1524 | OMG  | C2-N1-C6   | -2.25 | 121.04      | 125.11   |
| 2   | L2    | 665  | A2M  | C4-C5-N7   | -2.25 | 108.01      | 110.58   |
| 2   | L2    | 382  | A2M  | C6-C5-C4   | 2.24  | 120.24      | 117.18   |
| 51  | S1    | 8    | OMU  | O2-C2-N1   | -2.24 | 119.88      | 122.80   |
| 1   | L1    | 955  | A2M  | C4-N9-C8   | 2.24  | 108.09      | 105.74   |
| 7   | L7    | 43   | A2M  | C4-C5-N7   | -2.24 | 108.02      | 110.58   |
| 51  | S1    | 479  | A2M  | C4-C5-N7   | -2.24 | 108.02      | 110.58   |
| 7   | L7    | 101  | OMU  | C2'-C1'-N1 | -2.24 | 110.00      | 114.24   |
| 7   | L7    | 162  | A2M  | C4-C5-N7   | -2.23 | 108.03      | 110.58   |
| 2   | L2    | 1231 | OMG  | C8-N7-C5   | 2.23  | 108.23      | 104.26   |
| 1   | L1    | 305  | A2M  | C4-C5-N7   | -2.23 | 108.04      | 110.58   |
| 51  | S1    | 1156 | PSU  | O2-C2-N1   | -2.23 | 120.49      | 122.79   |
| 51  | S1    | 897  | A2M  | C4-C5-N7   | -2.22 | 108.04      | 110.58   |
| 2   | L2    | 71   | OMG  | C8-N7-C5   | 2.22  | 108.22      | 104.26   |
| 2   | L2    | 1067 | A2M  | C4-C5-N7   | -2.22 | 108.05      | 110.58   |
| 2   | L2    | 1359 | OMU  | O2-C2-N1   | -2.22 | 119.91      | 122.80   |
| 1   | L1    | 955  | A2M  | C4-C5-N7   | -2.21 | 108.05      | 110.58   |
| 2   | L2    | 95   | A2M  | C4-C5-N7   | -2.21 | 108.05      | 110.58   |
| 1   | L1    | 959  | OMG  | C8-N7-C5   | 2.21  | 108.20      | 104.26   |
| 51  | S1    | 29   | OMU  | O2-C2-N1   | -2.21 | 119.93      | 122.80   |
| 2   | L2    | 95   | A2M  | C4-N9-C8   | 2.20  | 108.04      | 105.74   |
| 7   | L7    | 43   | A2M  | C4-N9-C8   | 2.20  | 108.04      | 105.74   |
| 51  | S1    | 512  | A2M  | C4-C5-N7   | -2.19 | 108.07      | 110.58   |
| 1   | L1    | 1539 | A2M  | C5-C4-N9   | 2.19  | 108.20      | 105.81   |
| 51  | S1    | 668  | A2M  | C4-N9-C8   | 2.19  | 108.03      | 105.74   |
| 2   | L2    | 527  | A2M  | C4-C5-N7   | -2.19 | 108.08      | 110.58   |
| 1   | L1    | 305  | A2M  | C4-N9-C8   | 2.18  | 108.03      | 105.74   |
| 2   | L2    | 572  | A2M  | C4-C5-N7   | -2.18 | 108.09      | 110.58   |
| 2   | L2    | 1372 | A2M  | C4-C5-N7   | -2.18 | 108.09      | 110.58   |
| 2   | L2    | 1384 | A2M  | C6-C5-C4   | 2.18  | 120.16      | 117.18   |
| 1   | L1    | 235  | A2M  | C4-C5-N7   | -2.18 | 108.09      | 110.58   |
| 2   | L2    | 1253 | OMG  | C8-N7-C5   | 2.17  | 108.13      | 104.26   |
| 51  | S1    | 512  | A2M  | C4-N9-C8   | 2.17  | 108.02      | 105.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 52  | S2    | 37   | MIA  | C5-C4-N9    | 2.17  | 108.17      | 105.81   |
| 2   | L2    | 604  | A2M  | C4-C5-N7    | -2.17 | 108.10      | 110.58   |
| 2   | L2    | 1303 | PSU  | O4'-C1'-C2' | 2.17  | 108.15      | 105.15   |
| 1   | L1    | 856  | OMG  | O6-C6-C5    | -2.17 | 120.81      | 126.53   |
| 51  | S1    | 1829 | OMG  | N9-C4-N3    | 2.17  | 130.28      | 125.95   |
| 2   | L2    | 56   | OMU  | O2-C2-N1    | -2.16 | 119.98      | 122.80   |
| 2   | L2    | 1078 | OMG  | C4-C5-N7    | -2.16 | 107.24      | 110.67   |
| 51  | S1    | 98   | A2M  | C4-C5-N7    | -2.16 | 108.11      | 110.58   |
| 7   | L7    | 69   | PSU  | O4'-C1'-C2' | 2.16  | 108.14      | 105.15   |
| 2   | L2    | 591  | A2M  | C4-N9-C8    | 2.16  | 108.00      | 105.74   |
| 1   | L1    | 697  | A2M  | C4-C5-N7    | -2.15 | 108.12      | 110.58   |
| 1   | L1    | 681  | A2M  | C4-N9-C8    | 2.15  | 108.00      | 105.74   |
| 2   | L2    | 628  | A2M  | C4-N9-C8    | 2.15  | 108.00      | 105.74   |
| 2   | L2    | 665  | A2M  | C4-N9-C8    | 2.15  | 108.00      | 105.74   |
| 2   | L2    | 502  | A2M  | C4-N9-C8    | 2.15  | 107.99      | 105.74   |
| 7   | L7    | 162  | A2M  | C4-N9-C8    | 2.15  | 107.99      | 105.74   |
| 2   | L2    | 1384 | A2M  | C4-N9-C8    | 2.14  | 107.99      | 105.74   |
| 1   | L1    | 1190 | OMG  | C4-C5-N7    | -2.14 | 107.27      | 110.67   |
| 51  | S1    | 969  | A2M  | C5-C4-N9    | 2.14  | 108.14      | 105.81   |
| 2   | L2    | 1067 | A2M  | C6-C5-C4    | 2.14  | 120.10      | 117.18   |
| 52  | S2    | 37   | MIA  | C4-N9-C8    | 2.14  | 107.98      | 105.74   |
| 2   | L2    | 95   | A2M  | C2'-C1'-N9  | -2.12 | 110.25      | 113.75   |
| 51  | S1    | 455  | PSU  | C6-C5-C4    | 2.12  | 119.61      | 118.17   |
| 1   | L1    | 927  | A2M  | C6-C5-C4    | 2.12  | 120.08      | 117.18   |
| 51  | S1    | 897  | A2M  | C4-N9-C8    | 2.12  | 107.96      | 105.74   |
| 51  | S1    | 1550 | OMG  | O6-C6-C5    | -2.12 | 120.94      | 126.53   |
| 51  | S1    | 1478 | OMG  | N9-C4-N3    | 2.12  | 130.19      | 125.95   |
| 51  | S1    | 1621 | OMU  | O2-C2-N1    | -2.12 | 120.04      | 122.80   |
| 1   | L1    | 1626 | OMG  | C8-N7-C5    | 2.12  | 108.03      | 104.26   |
| 2   | L2    | 1382 | PSU  | O4'-C1'-C2' | 2.11  | 108.08      | 105.15   |
| 2   | L2    | 591  | A2M  | C4-C5-N7    | -2.11 | 108.17      | 110.58   |
| 51  | S1    | 98   | A2M  | C6-C5-C4    | 2.11  | 120.06      | 117.18   |
| 51  | S1    | 1550 | OMG  | C8-N7-C5    | 2.11  | 108.02      | 104.26   |
| 1   | L1    | 672  | PSU  | O2-C2-N1    | -2.11 | 120.61      | 122.79   |
| 2   | L2    | 1403 | PSU  | O4'-C1'-C2' | 2.11  | 108.07      | 105.15   |
| 51  | S1    | 2008 | OMG  | C2'-C1'-N9  | -2.11 | 110.24      | 114.24   |
| 2   | L2    | 641  | OMG  | N9-C4-N3    | 2.11  | 130.17      | 125.95   |
| 1   | L1    | 1107 | OMU  | O2-C2-N1    | -2.10 | 120.06      | 122.80   |
| 2   | L2    | 604  | A2M  | C4-N9-C8    | 2.10  | 107.94      | 105.74   |
| 2   | L2    | 1078 | OMG  | C6-C5-N7    | 2.10  | 134.10      | 130.29   |
| 51  | S1    | 2185 | MA6  | C4-C5-N7    | -2.09 | 108.19      | 110.58   |
| 1   | L1    | 1373 | A2M  | C4-N9-C8    | 2.09  | 107.94      | 105.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | S1    | 479  | A2M  | C6-C5-C4    | 2.09  | 120.03      | 117.18   |
| 1   | L1    | 1524 | OMG  | O6-C6-C5    | -2.09 | 121.02      | 126.53   |
| 2   | L2    | 572  | A2M  | C4-N9-C8    | 2.09  | 107.93      | 105.74   |
| 1   | L1    | 1626 | OMG  | O6-C6-C5    | -2.08 | 121.03      | 126.53   |
| 51  | S1    | 2021 | A2M  | C4-N9-C8    | 2.08  | 107.93      | 105.74   |
| 51  | S1    | 2184 | MA6  | C4-C5-N7    | -2.08 | 108.20      | 110.58   |
| 2   | L2    | 71   | OMG  | O6-C6-C5    | -2.08 | 121.03      | 126.53   |
| 51  | S1    | 28   | A2M  | C6-C5-C4    | 2.08  | 120.02      | 117.18   |
| 2   | L2    | 604  | A2M  | C2'-C1'-N9  | -2.07 | 110.34      | 113.75   |
| 1   | L1    | 1659 | OMU  | O2-C2-N1    | -2.07 | 120.10      | 122.80   |
| 1   | L1    | 48   | OMU  | O2-C2-N1    | -2.07 | 120.10      | 122.80   |
| 1   | L1    | 1253 | OMU  | O2-C2-N1    | -2.06 | 120.11      | 122.80   |
| 2   | L2    | 1067 | A2M  | C4-N9-C8    | 2.06  | 107.90      | 105.74   |
| 1   | L1    | 856  | OMG  | C8-N7-C5    | 2.06  | 107.93      | 104.26   |
| 51  | S1    | 2008 | OMG  | N1-C2-N3    | -2.06 | 119.55      | 123.32   |
| 1   | L1    | 1190 | OMG  | N1-C2-N3    | -2.06 | 119.55      | 123.32   |
| 1   | L1    | 678  | A2M  | C4-C5-N7    | -2.06 | 108.23      | 110.58   |
| 1   | L1    | 1010 | OMC  | O2-C2-N3    | -2.05 | 119.09      | 122.33   |
| 1   | L1    | 305  | A2M  | C6-C5-C4    | 2.05  | 119.98      | 117.18   |
| 1   | L1    | 1190 | OMG  | N9-C4-N3    | 2.05  | 130.06      | 125.95   |
| 1   | L1    | 955  | A2M  | C2'-C1'-N9  | -2.05 | 110.38      | 113.75   |
| 51  | S1    | 2151 | OMG  | C4-C5-N7    | -2.05 | 107.42      | 110.67   |
| 51  | S1    | 1979 | OMU  | O2-C2-N1    | -2.05 | 120.13      | 122.80   |
| 4   | L4    | 74   | OMG  | N2-C2-N1    | 2.04  | 121.07      | 116.76   |
| 51  | S1    | 2021 | A2M  | C6-C5-C4    | 2.04  | 119.97      | 117.18   |
| 51  | S1    | 98   | A2M  | C4-N9-C8    | 2.04  | 107.88      | 105.74   |
| 2   | L2    | 504  | PSU  | O4'-C1'-C2' | 2.04  | 107.97      | 105.15   |
| 2   | L2    | 1231 | OMG  | N2-C2-N1    | 2.04  | 121.06      | 116.76   |
| 2   | L2    | 1185 | A2M  | C5-C4-N9    | 2.04  | 108.03      | 105.81   |
| 51  | S1    | 512  | A2M  | C2'-C1'-N9  | -2.04 | 110.40      | 113.75   |
| 2   | L2    | 502  | A2M  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 2   | L2    | 570  | A2M  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 1   | L1    | 927  | A2M  | C4-C5-N7    | -2.03 | 108.26      | 110.58   |
| 1   | L1    | 845  | OMU  | O2-C2-N1    | -2.03 | 120.15      | 122.80   |
| 51  | S1    | 897  | A2M  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 7   | L7    | 43   | A2M  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 51  | S1    | 1543 | B8N  | O4-C4-C5    | -2.02 | 119.09      | 122.58   |
| 1   | L1    | 1373 | A2M  | C5-C4-N9    | 2.02  | 108.01      | 105.81   |
| 2   | L2    | 667  | OMU  | O2-C2-N1    | -2.02 | 120.17      | 122.80   |
| 1   | L1    | 1190 | OMG  | C6-C5-N7    | 2.02  | 133.96      | 130.29   |
| 2   | L2    | 1372 | A2M  | C6-C5-C4    | 2.02  | 119.93      | 117.18   |
| 2   | L2    | 591  | A2M  | C6-C5-C4    | 2.01  | 119.92      | 117.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L1    | 678  | A2M  | C6-C5-C4    | 2.01  | 119.92      | 117.18   |
| 51  | S1    | 1777 | OMU  | O2-C2-N1    | -2.01 | 120.18      | 122.80   |
| 1   | L1    | 697  | A2M  | C5-C4-N9    | 2.01  | 108.00      | 105.81   |
| 51  | S1    | 969  | A2M  | C3'-C2'-C1' | 2.01  | 106.65      | 102.81   |
| 51  | S1    | 2008 | OMG  | C8-N9-C4    | 2.01  | 109.79      | 106.03   |
| 51  | S1    | 1829 | OMG  | C4-C5-N7    | -2.00 | 107.50      | 110.67   |
| 2   | L2    | 1253 | OMG  | O6-C6-C5    | -2.00 | 121.25      | 126.53   |
| 2   | L2    | 1264 | PSU  | C6-C5-C4    | 2.00  | 119.52      | 118.17   |
| 1   | L1    | 235  | A2M  | C5-C4-N9    | 2.00  | 107.99      | 105.81   |

There are no chirality outliers.

All (111) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | L1    | 681  | A2M  | O4'-C4'-C5'-O5' |
| 1   | L1    | 955  | A2M  | C1'-C2'-O2'-CM' |
| 1   | L1    | 1010 | OMC  | C1'-C2'-O2'-CM2 |
| 1   | L1    | 1011 | PSU  | C2'-C1'-C5-C4   |
| 1   | L1    | 1011 | PSU  | C2'-C1'-C5-C6   |
| 1   | L1    | 1039 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | L1    | 1171 | PSU  | C3'-C4'-C5'-O5' |
| 1   | L1    | 1171 | PSU  | O4'-C4'-C5'-O5' |
| 1   | L1    | 1371 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | L1    | 1540 | OMG  | O4'-C4'-C5'-O5' |
| 1   | L1    | 1552 | OMC  | C1'-C2'-O2'-CM2 |
| 2   | L2    | 534  | OMG  | O4'-C4'-C5'-O5' |
| 2   | L2    | 591  | A2M  | C1'-C2'-O2'-CM' |
| 2   | L2    | 604  | A2M  | C1'-C2'-O2'-CM' |
| 2   | L2    | 665  | A2M  | C1'-C2'-O2'-CM' |
| 2   | L2    | 1046 | OMG  | O4'-C4'-C5'-O5' |
| 2   | L2    | 1185 | A2M  | C1'-C2'-O2'-CM' |
| 2   | L2    | 1229 | OMG  | O4'-C4'-C5'-O5' |
| 2   | L2    | 1248 | OMC  | C1'-C2'-O2'-CM2 |
| 2   | L2    | 1308 | 5MC  | C2'-C1'-N1-C6   |
| 7   | L7    | 162  | A2M  | C1'-C2'-O2'-CM' |
| 51  | S1    | 29   | OMU  | C1'-C2'-O2'-CM2 |
| 51  | S1    | 98   | A2M  | C1'-C2'-O2'-CM' |
| 51  | S1    | 668  | A2M  | C1'-C2'-O2'-CM' |
| 51  | S1    | 1543 | B8N  | O4'-C4'-C5'-O5' |
| 51  | S1    | 1662 | OMU  | C1'-C2'-O2'-CM2 |
| 51  | S1    | 2021 | A2M  | C1'-C2'-O2'-CM' |
| 51  | S1    | 2202 | PSU  | O4'-C1'-C5-C6   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 52  | S2    | 37   | MIA  | N1-C2-S10-C11   |
| 52  | S2    | 37   | MIA  | N3-C2-S10-C11   |
| 2   | L2    | 1308 | 5MC  | C2'-C1'-N1-C2   |
| 1   | L1    | 681  | A2M  | C3'-C4'-C5'-O5' |
| 1   | L1    | 1371 | OMU  | C3'-C4'-C5'-O5' |
| 1   | L1    | 1540 | OMG  | C3'-C4'-C5'-O5' |
| 2   | L2    | 534  | OMG  | C3'-C4'-C5'-O5' |
| 2   | L2    | 1229 | OMG  | C3'-C4'-C5'-O5' |
| 2   | L2    | 1264 | PSU  | C3'-C4'-C5'-O5' |
| 2   | L2    | 1361 | PSU  | C3'-C4'-C5'-O5' |
| 2   | L2    | 1361 | PSU  | O4'-C4'-C5'-O5' |
| 51  | S1    | 455  | PSU  | C3'-C4'-C5'-O5' |
| 51  | S1    | 600  | OMG  | O4'-C4'-C5'-O5' |
| 51  | S1    | 1543 | B8N  | C3'-C4'-C5'-O5' |
| 2   | L2    | 665  | A2M  | O4'-C4'-C5'-O5' |
| 2   | L2    | 665  | A2M  | C3'-C4'-C5'-O5' |
| 51  | S1    | 455  | PSU  | O4'-C4'-C5'-O5' |
| 2   | L2    | 443  | OMC  | C2'-C1'-N1-C6   |
| 2   | L2    | 1046 | OMG  | C3'-C4'-C5'-O5' |
| 51  | S1    | 1543 | B8N  | N34-C33-C34-O36 |
| 1   | L1    | 1371 | OMU  | O4'-C4'-C5'-O5' |
| 2   | L2    | 1264 | PSU  | O4'-C4'-C5'-O5' |
| 51  | S1    | 668  | A2M  | O4'-C4'-C5'-O5' |
| 1   | L1    | 1524 | OMG  | O4'-C4'-C5'-O5' |
| 51  | S1    | 512  | A2M  | C3'-C4'-C5'-O5' |
| 51  | S1    | 668  | A2M  | C3'-C4'-C5'-O5' |
| 51  | S1    | 1995 | 7MG  | O4'-C4'-C5'-O5' |
| 51  | S1    | 1995 | 7MG  | C3'-C4'-C5'-O5' |
| 1   | L1    | 1010 | OMC  | O4'-C4'-C5'-O5' |
| 1   | L1    | 1524 | OMG  | C3'-C4'-C5'-O5' |
| 2   | L2    | 443  | OMC  | C2'-C1'-N1-C2   |
| 51  | S1    | 600  | OMG  | C3'-C4'-C5'-O5' |
| 2   | L2    | 570  | A2M  | O4'-C4'-C5'-O5' |
| 2   | L2    | 570  | A2M  | C3'-C4'-C5'-O5' |
| 51  | S1    | 8    | OMU  | C2'-C1'-N1-C6   |
| 2   | L2    | 570  | A2M  | C2'-C1'-N9-C8   |
| 51  | S1    | 969  | A2M  | C2'-C1'-N9-C8   |
| 4   | L4    | 74   | OMG  | C3'-C4'-C5'-O5' |
| 52  | S2    | 37   | MIA  | C5-C6-N6-C12    |
| 51  | S1    | 668  | A2M  | C2'-C1'-N9-C8   |
| 2   | L2    | 443  | OMC  | O4'-C1'-N1-C6   |
| 51  | S1    | 98   | A2M  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 51  | S1    | 512  | A2M  | O4'-C4'-C5'-O5' |
| 51  | S1    | 1544 | 5MC  | O4'-C4'-C5'-O5' |
| 2   | L2    | 1308 | 5MC  | O4'-C1'-N1-C6   |
| 51  | S1    | 8    | OMU  | O4'-C1'-N1-C6   |
| 2   | L2    | 560  | OMU  | C4'-C5'-O5'-P   |
| 1   | L1    | 677  | 1MA  | C2'-C1'-N9-C8   |
| 1   | L1    | 681  | A2M  | C4'-C5'-O5'-P   |
| 51  | S1    | 2185 | MA6  | C4'-C5'-O5'-P   |
| 1   | L1    | 1011 | PSU  | O4'-C1'-C5-C4   |
| 2   | L2    | 1382 | PSU  | O4'-C1'-C5-C4   |
| 51  | S1    | 1657 | PSU  | O4'-C1'-C5-C4   |
| 2   | L2    | 570  | A2M  | C2'-C1'-N9-C4   |
| 51  | S1    | 969  | A2M  | C2'-C1'-N9-C4   |
| 2   | L2    | 443  | OMC  | O4'-C1'-N1-C2   |
| 2   | L2    | 1308 | 5MC  | O4'-C1'-N1-C2   |
| 52  | S2    | 37   | MIA  | N1-C6-N6-C12    |
| 51  | S1    | 668  | A2M  | C2'-C1'-N9-C4   |
| 1   | L1    | 1524 | OMG  | C3'-C2'-O2'-CM2 |
| 2   | L2    | 1248 | OMC  | C4'-C5'-O5'-P   |
| 51  | S1    | 1829 | OMG  | O4'-C4'-C5'-O5' |
| 51  | S1    | 2059 | OMC  | O4'-C4'-C5'-O5' |
| 51  | S1    | 668  | A2M  | O4'-C1'-N9-C8   |
| 1   | L1    | 677  | 1MA  | C2'-C1'-N9-C4   |
| 2   | L2    | 1361 | PSU  | C4'-C5'-O5'-P   |
| 51  | S1    | 1478 | OMG  | C4'-C5'-O5'-P   |
| 2   | L2    | 1046 | OMG  | C1'-C2'-O2'-CM2 |
| 2   | L2    | 1384 | A2M  | C1'-C2'-O2'-CM' |
| 51  | S1    | 1829 | OMG  | C4'-C5'-O5'-P   |
| 1   | L1    | 1011 | PSU  | O4'-C1'-C5-C6   |
| 2   | L2    | 570  | A2M  | O4'-C1'-N9-C8   |
| 51  | S1    | 969  | A2M  | O4'-C1'-N9-C8   |
| 2   | L2    | 502  | A2M  | C3'-C2'-O2'-CM' |
| 51  | S1    | 1623 | OMG  | O4'-C4'-C5'-O5' |
| 51  | S1    | 8    | OMU  | O4'-C1'-N1-C2   |
| 51  | S1    | 1833 | OMU  | O4'-C4'-C5'-O5' |
| 2   | L2    | 1185 | A2M  | C4'-C5'-O5'-P   |
| 51  | S1    | 969  | A2M  | C3'-C2'-O2'-CM' |
| 2   | L2    | 1185 | A2M  | C3'-C4'-C5'-O5' |
| 1   | L1    | 1010 | OMC  | C3'-C4'-C5'-O5' |
| 51  | S1    | 8    | OMU  | C2'-C1'-N1-C2   |
| 51  | S1    | 1543 | B8N  | N34-C33-C34-O35 |

There are no ring outliers.

63 monomers are involved in 85 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | L2    | 570  | A2M  | 1       | 0            |
| 1   | L1    | 959  | OMG  | 1       | 0            |
| 1   | L1    | 681  | A2M  | 1       | 0            |
| 1   | L1    | 1626 | OMG  | 2       | 0            |
| 1   | L1    | 1190 | OMG  | 2       | 0            |
| 2   | L2    | 1078 | OMG  | 1       | 0            |
| 2   | L2    | 512  | PSU  | 1       | 0            |
| 1   | L1    | 1371 | OMU  | 1       | 0            |
| 1   | L1    | 1010 | OMC  | 1       | 0            |
| 51  | S1    | 1829 | OMG  | 1       | 0            |
| 2   | L2    | 1253 | OMG  | 1       | 0            |
| 51  | S1    | 2008 | OMG  | 3       | 0            |
| 1   | L1    | 1524 | OMG  | 2       | 0            |
| 2   | L2    | 1185 | A2M  | 1       | 0            |
| 2   | L2    | 1308 | 5MC  | 2       | 0            |
| 1   | L1    | 1659 | OMU  | 1       | 0            |
| 51  | S1    | 29   | OMU  | 4       | 0            |
| 2   | L2    | 1264 | PSU  | 1       | 0            |
| 51  | S1    | 2019 | OMC  | 1       | 0            |
| 2   | L2    | 1284 | PSU  | 1       | 0            |
| 1   | L1    | 1017 | PSU  | 1       | 0            |
| 2   | L2    | 560  | OMU  | 1       | 0            |
| 51  | S1    | 1550 | OMG  | 2       | 0            |
| 51  | S1    | 479  | A2M  | 1       | 0            |
| 51  | S1    | 668  | A2M  | 1       | 0            |
| 51  | S1    | 2140 | OMC  | 1       | 0            |
| 2   | L2    | 56   | OMU  | 1       | 0            |
| 1   | L1    | 1528 | PSU  | 1       | 0            |
| 2   | L2    | 382  | A2M  | 3       | 0            |
| 1   | L1    | 678  | A2M  | 3       | 0            |
| 51  | S1    | 2059 | OMC  | 1       | 0            |
| 2   | L2    | 1318 | PSU  | 1       | 0            |
| 1   | L1    | 235  | A2M  | 1       | 0            |
| 1   | L1    | 955  | A2M  | 1       | 0            |
| 52  | S2    | 37   | MIA  | 1       | 0            |
| 2   | L2    | 1360 | OMG  | 2       | 0            |
| 51  | S1    | 38   | OMC  | 1       | 0            |
| 1   | L1    | 1039 | OMU  | 1       | 0            |
| 51  | S1    | 1543 | B8N  | 1       | 0            |
| 2   | L2    | 443  | OMC  | 1       | 0            |
| 1   | L1    | 927  | A2M  | 1       | 0            |
| 51  | S1    | 969  | A2M  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | L1    | 1527 | OMC  | 2       | 0            |
| 51  | S1    | 1539 | PSU  | 2       | 0            |
| 2   | L2    | 1248 | OMC  | 2       | 0            |
| 1   | L1    | 1253 | OMU  | 1       | 0            |
| 7   | L7    | 69   | PSU  | 1       | 0            |
| 1   | L1    | 1373 | A2M  | 1       | 0            |
| 1   | L1    | 1552 | OMC  | 1       | 0            |
| 7   | L7    | 43   | A2M  | 1       | 0            |
| 51  | S1    | 1662 | OMU  | 1       | 0            |
| 51  | S1    | 98   | A2M  | 2       | 0            |
| 2   | L2    | 591  | A2M  | 3       | 0            |
| 51  | S1    | 28   | A2M  | 1       | 0            |
| 2   | L2    | 14   | OMC  | 2       | 0            |
| 1   | L1    | 845  | OMU  | 1       | 0            |
| 7   | L7    | 162  | A2M  | 2       | 0            |
| 51  | S1    | 18   | OMC  | 1       | 0            |
| 1   | L1    | 669  | OMC  | 1       | 0            |
| 2   | L2    | 1397 | OMC  | 1       | 0            |
| 1   | L1    | 305  | A2M  | 1       | 0            |
| 2   | L2    | 95   | A2M  | 1       | 0            |
| 51  | S1    | 1566 | PSU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 535 ligands modelled in this entry, 492 are monoatomic - leaving 43 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 93  | PUT  | S1    | 2443 | -    | 5,5,5        | 0.24 | 0           | 4,4,4       | 0.13 | 0           |
| 93  | PUT  | L4    | 218  | -    | 5,5,5        | 0.24 | 0           | 4,4,4       | 0.12 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 89  | SPD  | L1    | 1811 | -    | 9,9,9        | 0.42 | 0        | 8,8,8       | 0.40 | 0        |
| 94  | PAR  | S1    | 2446 | -    | 44,45,45     | 3.61 | 10 (22%) | 63,67,67    | 1.16 | 6 (9%)   |
| 89  | SPD  | L1    | 1812 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.22 | 0        |
| 89  | SPD  | L1    | 1806 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.38 | 0        |
| 89  | SPD  | L2    | 1601 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.17 | 0        |
| 93  | PUT  | L1    | 1971 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.14 | 0        |
| 94  | PAR  | S1    | 2445 | 92   | 44,45,45     | 3.64 | 10 (22%) | 63,67,67    | 1.04 | 4 (6%)   |
| 93  | PUT  | L1    | 1973 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.12 | 0        |
| 93  | PUT  | L1    | 1977 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.13 | 0        |
| 93  | PUT  | L1    | 1974 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.14 | 0        |
| 94  | PAR  | L1    | 1978 | -    | 44,45,45     | 3.63 | 10 (22%) | 63,67,67    | 1.14 | 3 (4%)   |
| 89  | SPD  | L1    | 1808 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.35 | 0        |
| 93  | PUT  | L1    | 1975 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.14 | 0        |
| 89  | SPD  | S1    | 2301 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.26 | 0        |
| 93  | PUT  | L2    | 1724 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.15 | 0        |
| 89  | SPD  | L1    | 1815 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.24 | 0        |
| 89  | SPD  | L1    | 1813 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.18 | 0        |
| 89  | SPD  | L1    | 1801 | -    | 9,9,9        | 0.42 | 0        | 8,8,8       | 0.43 | 0        |
| 89  | SPD  | S1    | 2447 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.31 | 0        |
| 93  | PUT  | L2    | 1725 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.13 | 0        |
| 89  | SPD  | L1    | 1804 | -    | 9,9,9        | 0.42 | 0        | 8,8,8       | 0.33 | 0        |
| 89  | SPD  | L1    | 1814 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.22 | 0        |
| 89  | SPD  | LM    | 301  | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.15 | 0        |
| 94  | PAR  | L7    | 208  | -    | 44,45,45     | 3.52 | 10 (22%) | 63,67,67    | 1.34 | 10 (15%) |
| 94  | PAR  | L2    | 1728 | -    | 44,45,45     | 3.59 | 10 (22%) | 63,67,67    | 1.23 | 5 (7%)   |
| 93  | PUT  | L2    | 1727 | -    | 5,5,5        | 0.23 | 0        | 4,4,4       | 0.19 | 0        |
| 93  | PUT  | S1    | 2444 | -    | 5,5,5        | 0.25 | 0        | 4,4,4       | 0.13 | 0        |
| 94  | PAR  | L2    | 1729 | -    | 44,45,45     | 3.57 | 9 (20%)  | 63,67,67    | 1.37 | 11 (17%) |
| 89  | SPD  | L2    | 1602 | 2    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.20 | 0        |
| 89  | SPD  | L1    | 1805 | -    | 9,9,9        | 0.46 | 0        | 8,8,8       | 0.23 | 0        |
| 89  | SPD  | L1    | 1809 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.27 | 0        |
| 89  | SPD  | L1    | 1803 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.24 | 0        |
| 93  | PUT  | L1    | 1976 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.15 | 0        |
| 93  | PUT  | L2    | 1723 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.14 | 0        |
| 93  | PUT  | L5    | 207  | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.15 | 0        |
| 89  | SPD  | S1    | 2302 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.34 | 0        |
| 89  | SPD  | L1    | 1810 | -    | 9,9,9        | 0.42 | 0        | 8,8,8       | 0.30 | 0        |
| 93  | PUT  | L1    | 1972 | 1    | 5,5,5        | 0.25 | 0        | 4,4,4       | 0.10 | 0        |
| 93  | PUT  | L2    | 1726 | -    | 5,5,5        | 0.24 | 0        | 4,4,4       | 0.12 | 0        |
| 89  | SPD  | L1    | 1807 | -    | 9,9,9        | 0.42 | 0        | 8,8,8       | 0.36 | 0        |
| 89  | SPD  | L1    | 1802 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.20 | 0        |

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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 93  | PUT  | S1    | 2443 | -    | -       | 1/3/3/3     | -       |
| 93  | PUT  | L4    | 218  | -    | -       | 0/3/3/3     | -       |
| 89  | SPD  | L1    | 1811 | -    | -       | 2/7/7/7     | -       |
| 94  | PAR  | S1    | 2446 | -    | -       | 10/18/94/94 | 0/4/4/4 |
| 89  | SPD  | L1    | 1812 | -    | -       | 0/7/7/7     | -       |
| 89  | SPD  | L1    | 1806 | -    | -       | 1/7/7/7     | -       |
| 89  | SPD  | L2    | 1601 | -    | -       | 1/7/7/7     | -       |
| 93  | PUT  | L1    | 1971 | -    | -       | 0/3/3/3     | -       |
| 94  | PAR  | S1    | 2445 | 92   | -       | 7/18/94/94  | 0/4/4/4 |
| 93  | PUT  | L1    | 1973 | -    | -       | 0/3/3/3     | -       |
| 93  | PUT  | L1    | 1977 | -    | -       | 0/3/3/3     | -       |
| 93  | PUT  | L1    | 1974 | -    | -       | 0/3/3/3     | -       |
| 94  | PAR  | L1    | 1978 | -    | -       | 8/18/94/94  | 0/4/4/4 |
| 89  | SPD  | L1    | 1808 | -    | -       | 0/7/7/7     | -       |
| 93  | PUT  | L1    | 1975 | -    | -       | 1/3/3/3     | -       |
| 89  | SPD  | S1    | 2301 | -    | -       | 2/7/7/7     | -       |
| 93  | PUT  | L2    | 1724 | -    | -       | 1/3/3/3     | -       |
| 89  | SPD  | L1    | 1815 | -    | -       | 0/7/7/7     | -       |
| 89  | SPD  | L1    | 1813 | -    | -       | 1/7/7/7     | -       |
| 89  | SPD  | L1    | 1801 | -    | -       | 3/7/7/7     | -       |
| 89  | SPD  | S1    | 2447 | -    | -       | 2/7/7/7     | -       |
| 93  | PUT  | L2    | 1725 | -    | -       | 0/3/3/3     | -       |
| 89  | SPD  | L1    | 1804 | -    | -       | 2/7/7/7     | -       |
| 89  | SPD  | L1    | 1814 | -    | -       | 0/7/7/7     | -       |
| 89  | SPD  | LM    | 301  | -    | -       | 0/7/7/7     | -       |
| 94  | PAR  | L7    | 208  | -    | -       | 9/18/94/94  | 0/4/4/4 |
| 94  | PAR  | L2    | 1728 | -    | -       | 5/18/94/94  | 0/4/4/4 |
| 93  | PUT  | L2    | 1727 | -    | -       | 0/3/3/3     | -       |
| 93  | PUT  | S1    | 2444 | -    | -       | 1/3/3/3     | -       |
| 94  | PAR  | L2    | 1729 | -    | -       | 12/18/94/94 | 0/4/4/4 |
| 89  | SPD  | L2    | 1602 | 2    | -       | 1/7/7/7     | -       |
| 89  | SPD  | L1    | 1805 | -    | -       | 2/7/7/7     | -       |
| 89  | SPD  | L1    | 1809 | -    | -       | 2/7/7/7     | -       |
| 89  | SPD  | L1    | 1803 | -    | -       | 0/7/7/7     | -       |
| 93  | PUT  | L1    | 1976 | -    | -       | 0/3/3/3     | -       |
| 93  | PUT  | L2    | 1723 | -    | -       | 1/3/3/3     | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 93  | PUT  | L5    | 207  | -    | -       | 0/3/3/3  | -     |
| 89  | SPD  | S1    | 2302 | -    | -       | 0/7/7/7  | -     |
| 89  | SPD  | L1    | 1810 | -    | -       | 0/7/7/7  | -     |
| 93  | PUT  | L1    | 1972 | 1    | -       | 0/3/3/3  | -     |
| 93  | PUT  | L2    | 1726 | -    | -       | 0/3/3/3  | -     |
| 89  | SPD  | L1    | 1807 | -    | -       | 1/7/7/7  | -     |
| 89  | SPD  | L1    | 1802 | -    | -       | 1/7/7/7  | -     |

All (59) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 94  | S1    | 2445 | PAR  | C13-C23 | -15.78 | 1.32        | 1.52     |
| 94  | L1    | 1978 | PAR  | C13-C23 | -15.71 | 1.32        | 1.52     |
| 94  | S1    | 2446 | PAR  | C13-C23 | -15.55 | 1.33        | 1.52     |
| 94  | L2    | 1728 | PAR  | C13-C23 | -15.26 | 1.33        | 1.52     |
| 94  | L7    | 208  | PAR  | C13-C23 | -15.08 | 1.33        | 1.52     |
| 94  | L2    | 1729 | PAR  | C13-C23 | -14.92 | 1.33        | 1.52     |
| 94  | L2    | 1729 | PAR  | O43-C13 | 13.63  | 1.65        | 1.41     |
| 94  | L2    | 1728 | PAR  | O43-C13 | 13.59  | 1.65        | 1.41     |
| 94  | S1    | 2445 | PAR  | O43-C13 | 13.51  | 1.65        | 1.41     |
| 94  | L1    | 1978 | PAR  | O43-C13 | 13.40  | 1.65        | 1.41     |
| 94  | S1    | 2446 | PAR  | O43-C13 | 13.38  | 1.65        | 1.41     |
| 94  | L7    | 208  | PAR  | O43-C13 | 13.28  | 1.65        | 1.41     |
| 94  | L7    | 208  | PAR  | O43-C43 | -6.33  | 1.30        | 1.45     |
| 94  | L2    | 1729 | PAR  | O43-C43 | -6.18  | 1.31        | 1.45     |
| 94  | S1    | 2446 | PAR  | O43-C43 | -6.10  | 1.31        | 1.45     |
| 94  | L2    | 1728 | PAR  | O43-C43 | -6.09  | 1.31        | 1.45     |
| 94  | L1    | 1978 | PAR  | O43-C43 | -5.91  | 1.31        | 1.45     |
| 94  | S1    | 2445 | PAR  | O43-C43 | -5.86  | 1.32        | 1.45     |
| 94  | L1    | 1978 | PAR  | C34-C24 | -4.73  | 1.47        | 1.53     |
| 94  | L1    | 1978 | PAR  | O54-C14 | 4.36   | 1.53        | 1.41     |
| 94  | S1    | 2445 | PAR  | O54-C14 | 4.36   | 1.53        | 1.41     |
| 94  | S1    | 2446 | PAR  | C34-C24 | -4.35  | 1.48        | 1.53     |
| 94  | L2    | 1728 | PAR  | O54-C14 | 4.34   | 1.53        | 1.41     |
| 94  | L2    | 1729 | PAR  | O54-C14 | 4.34   | 1.53        | 1.41     |
| 94  | S1    | 2446 | PAR  | O54-C14 | 4.30   | 1.52        | 1.41     |
| 94  | S1    | 2445 | PAR  | C34-C24 | -4.30  | 1.48        | 1.53     |
| 94  | L2    | 1728 | PAR  | C34-C24 | -4.27  | 1.48        | 1.53     |
| 94  | L2    | 1729 | PAR  | C34-C24 | -4.27  | 1.48        | 1.53     |
| 94  | L7    | 208  | PAR  | O54-C14 | 4.18   | 1.52        | 1.41     |
| 94  | S1    | 2445 | PAR  | O33-C33 | -3.84  | 1.34        | 1.43     |
| 94  | L2    | 1729 | PAR  | O33-C33 | -3.83  | 1.34        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 94  | L2    | 1729 | PAR  | O51-C11 | 3.80  | 1.51        | 1.41     |
| 94  | L1    | 1978 | PAR  | O33-C33 | -3.79 | 1.34        | 1.43     |
| 94  | L2    | 1728 | PAR  | O33-C33 | -3.78 | 1.34        | 1.43     |
| 94  | S1    | 2445 | PAR  | O51-C11 | 3.73  | 1.51        | 1.41     |
| 94  | L7    | 208  | PAR  | O33-C33 | -3.73 | 1.34        | 1.43     |
| 94  | L1    | 1978 | PAR  | O51-C11 | 3.73  | 1.51        | 1.41     |
| 94  | L2    | 1728 | PAR  | O51-C11 | 3.70  | 1.51        | 1.41     |
| 94  | S1    | 2446 | PAR  | O51-C11 | 3.65  | 1.51        | 1.41     |
| 94  | L7    | 208  | PAR  | O51-C11 | 3.64  | 1.51        | 1.41     |
| 94  | S1    | 2446 | PAR  | O33-C33 | -3.62 | 1.34        | 1.43     |
| 94  | S1    | 2445 | PAR  | C31-C21 | -3.48 | 1.49        | 1.53     |
| 94  | L7    | 208  | PAR  | C24-N24 | 3.41  | 1.52        | 1.47     |
| 94  | S1    | 2446 | PAR  | C31-C21 | -3.36 | 1.49        | 1.53     |
| 94  | S1    | 2445 | PAR  | C24-N24 | 3.31  | 1.52        | 1.47     |
| 94  | S1    | 2446 | PAR  | C24-N24 | 3.30  | 1.52        | 1.47     |
| 94  | L2    | 1728 | PAR  | C24-N24 | 3.27  | 1.52        | 1.47     |
| 94  | L2    | 1729 | PAR  | C24-N24 | 3.21  | 1.52        | 1.47     |
| 94  | L2    | 1729 | PAR  | C31-C21 | -3.21 | 1.49        | 1.53     |
| 94  | L2    | 1728 | PAR  | C31-C21 | -3.20 | 1.49        | 1.53     |
| 94  | L1    | 1978 | PAR  | C24-N24 | 3.19  | 1.52        | 1.47     |
| 94  | L7    | 208  | PAR  | C34-C24 | -3.14 | 1.49        | 1.53     |
| 94  | L1    | 1978 | PAR  | C31-C21 | -3.05 | 1.49        | 1.53     |
| 94  | L7    | 208  | PAR  | C31-C21 | -2.89 | 1.49        | 1.53     |
| 94  | S1    | 2446 | PAR  | C33-C43 | 2.28  | 1.58        | 1.52     |
| 94  | L1    | 1978 | PAR  | C33-C43 | 2.25  | 1.58        | 1.52     |
| 94  | S1    | 2445 | PAR  | C33-C43 | 2.21  | 1.58        | 1.52     |
| 94  | L7    | 208  | PAR  | C33-C43 | 2.19  | 1.58        | 1.52     |
| 94  | L2    | 1728 | PAR  | C33-C43 | 2.04  | 1.58        | 1.52     |

All (39) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 94  | L1    | 1978 | PAR  | C14-O33-C33 | -4.21 | 107.99      | 117.98   |
| 94  | L7    | 208  | PAR  | C44-C34-C24 | 3.95  | 117.55      | 110.99   |
| 94  | L2    | 1728 | PAR  | C14-O33-C33 | -3.74 | 109.12      | 117.98   |
| 94  | L7    | 208  | PAR  | C11-O11-C42 | -3.24 | 110.29      | 117.98   |
| 94  | L2    | 1728 | PAR  | C13-O52-C52 | -3.18 | 110.44      | 117.98   |
| 94  | L2    | 1728 | PAR  | C11-O11-C42 | -3.09 | 110.66      | 117.98   |
| 94  | L2    | 1729 | PAR  | C34-C44-C54 | 3.08  | 115.81      | 110.23   |
| 94  | L1    | 1978 | PAR  | C11-O11-C42 | -3.05 | 110.75      | 117.98   |
| 94  | L2    | 1728 | PAR  | C13-C23-C33 | 3.04  | 105.76      | 102.10   |
| 94  | S1    | 2445 | PAR  | C13-O52-C52 | -3.02 | 110.81      | 117.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 94  | L2    | 1729 | PAR  | C13-C23-C33 | 2.98  | 105.68      | 102.10   |
| 94  | L2    | 1729 | PAR  | O52-C13-O43 | -2.94 | 108.37      | 111.37   |
| 94  | L2    | 1729 | PAR  | C14-O33-C33 | -2.93 | 111.02      | 117.98   |
| 94  | S1    | 2446 | PAR  | C14-O33-C33 | -2.93 | 111.03      | 117.98   |
| 94  | L7    | 208  | PAR  | C14-C24-C34 | 2.92  | 117.61      | 110.29   |
| 94  | L2    | 1729 | PAR  | C11-O11-C42 | -2.92 | 111.07      | 117.98   |
| 94  | S1    | 2445 | PAR  | C14-O33-C33 | -2.90 | 111.10      | 117.98   |
| 94  | L2    | 1729 | PAR  | O52-C52-C62 | 2.87  | 114.53      | 107.23   |
| 94  | S1    | 2446 | PAR  | C13-C23-C33 | 2.87  | 105.55      | 102.10   |
| 94  | L7    | 208  | PAR  | C14-O33-C33 | -2.86 | 111.21      | 117.98   |
| 94  | L7    | 208  | PAR  | O52-C13-O43 | 2.82  | 114.25      | 111.37   |
| 94  | S1    | 2446 | PAR  | C13-O52-C52 | -2.79 | 111.37      | 117.98   |
| 94  | L1    | 1978 | PAR  | C13-O52-C52 | -2.54 | 111.96      | 117.98   |
| 94  | L2    | 1729 | PAR  | C22-C12-C62 | 2.51  | 113.84      | 110.08   |
| 94  | S1    | 2446 | PAR  | O51-C51-C41 | 2.51  | 114.22      | 109.70   |
| 94  | L2    | 1728 | PAR  | O43-C13-C23 | 2.50  | 108.16      | 104.98   |
| 94  | L7    | 208  | PAR  | C13-C23-C33 | 2.42  | 105.02      | 102.10   |
| 94  | S1    | 2445 | PAR  | C11-O11-C42 | -2.41 | 112.25      | 117.98   |
| 94  | L2    | 1729 | PAR  | O54-C54-C44 | 2.36  | 113.94      | 109.70   |
| 94  | S1    | 2445 | PAR  | O51-C51-C41 | 2.23  | 113.72      | 109.70   |
| 94  | L7    | 208  | PAR  | C52-C42-C32 | 2.18  | 115.34      | 111.31   |
| 94  | L2    | 1729 | PAR  | C44-C34-C24 | 2.11  | 114.49      | 110.99   |
| 94  | L7    | 208  | PAR  | C22-C32-C42 | 2.08  | 114.59      | 109.50   |
| 94  | L7    | 208  | PAR  | O54-C54-C64 | 2.07  | 110.05      | 106.07   |
| 94  | S1    | 2446 | PAR  | O11-C42-C32 | -2.07 | 104.25      | 109.18   |
| 94  | L2    | 1729 | PAR  | O51-C11-C21 | 2.06  | 114.64      | 110.08   |
| 94  | L7    | 208  | PAR  | C34-C44-C54 | 2.06  | 113.96      | 110.23   |
| 94  | S1    | 2446 | PAR  | C22-C32-C42 | 2.06  | 114.54      | 109.50   |
| 94  | L2    | 1729 | PAR  | C61-C51-C41 | -2.05 | 107.98      | 113.02   |

There are no chirality outliers.

All (77) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 94  | L1    | 1978 | PAR  | C23-C13-O52-C52 |
| 94  | L1    | 1978 | PAR  | O43-C43-C53-O53 |
| 94  | L1    | 1978 | PAR  | C44-C54-C64-N64 |
| 94  | L1    | 1978 | PAR  | O54-C54-C64-N64 |
| 94  | L2    | 1729 | PAR  | C23-C13-O52-C52 |
| 94  | L2    | 1729 | PAR  | O43-C13-O52-C52 |
| 94  | L2    | 1729 | PAR  | C24-C14-O33-C33 |
| 94  | L2    | 1729 | PAR  | C44-C54-C64-N64 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 94  | L2    | 1729 | PAR  | O54-C54-C64-N64 |
| 94  | L7    | 208  | PAR  | C23-C13-O52-C52 |
| 94  | L7    | 208  | PAR  | O43-C13-O52-C52 |
| 94  | L7    | 208  | PAR  | O54-C54-C64-N64 |
| 94  | S1    | 2445 | PAR  | O43-C43-C53-O53 |
| 94  | S1    | 2446 | PAR  | C24-C14-O33-C33 |
| 94  | S1    | 2446 | PAR  | O54-C14-O33-C33 |
| 94  | L2    | 1729 | PAR  | C62-C52-O52-C13 |
| 94  | L2    | 1729 | PAR  | O54-C14-O33-C33 |
| 94  | S1    | 2445 | PAR  | O54-C14-O33-C33 |
| 94  | L1    | 1978 | PAR  | C33-C43-C53-O53 |
| 94  | S1    | 2445 | PAR  | C33-C43-C53-O53 |
| 89  | L1    | 1801 | SPD  | N6-C7-C8-C9     |
| 89  | L1    | 1809 | SPD  | N6-C7-C8-C9     |
| 94  | L7    | 208  | PAR  | O43-C43-C53-O53 |
| 94  | L7    | 208  | PAR  | C33-C43-C53-O53 |
| 94  | L1    | 1978 | PAR  | O51-C51-C61-O61 |
| 94  | L2    | 1728 | PAR  | O51-C51-C61-O61 |
| 94  | L2    | 1728 | PAR  | C41-C51-C61-O61 |
| 94  | S1    | 2446 | PAR  | O51-C51-C61-O61 |
| 94  | L1    | 1978 | PAR  | C41-C51-C61-O61 |
| 94  | L2    | 1728 | PAR  | O54-C14-O33-C33 |
| 94  | S1    | 2446 | PAR  | C33-C43-C53-O53 |
| 89  | L1    | 1811 | SPD  | C2-C3-C4-C5     |
| 89  | S1    | 2301 | SPD  | C8-C7-N6-C5     |
| 94  | S1    | 2446 | PAR  | C41-C51-C61-O61 |
| 94  | L1    | 1978 | PAR  | O43-C13-O52-C52 |
| 94  | S1    | 2446 | PAR  | O51-C11-O11-C42 |
| 94  | S1    | 2446 | PAR  | O43-C43-C53-O53 |
| 89  | L1    | 1811 | SPD  | C8-C7-N6-C5     |
| 94  | L7    | 208  | PAR  | O51-C51-C61-O61 |
| 94  | S1    | 2446 | PAR  | C44-C54-C64-N64 |
| 94  | L2    | 1729 | PAR  | C33-C43-C53-O53 |
| 94  | L7    | 208  | PAR  | O54-C14-O33-C33 |
| 94  | S1    | 2446 | PAR  | C52-C42-O11-C11 |
| 94  | L2    | 1728 | PAR  | O51-C11-O11-C42 |
| 94  | S1    | 2446 | PAR  | O54-C54-C64-N64 |
| 89  | L1    | 1806 | SPD  | N1-C2-C3-C4     |
| 89  | L1    | 1802 | SPD  | C4-C5-N6-C7     |
| 89  | L1    | 1804 | SPD  | N1-C2-C3-C4     |
| 89  | L1    | 1801 | SPD  | C4-C5-N6-C7     |
| 94  | S1    | 2445 | PAR  | C43-C33-O33-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 94  | L2    | 1729 | PAR  | O51-C11-O11-C42 |
| 93  | L2    | 1724 | PUT  | C1-C2-C3-C4     |
| 89  | L2    | 1602 | SPD  | C2-C3-C4-C5     |
| 94  | L2    | 1729 | PAR  | C41-C51-C61-O61 |
| 94  | L2    | 1729 | PAR  | O43-C43-C53-O53 |
| 89  | S1    | 2301 | SPD  | C2-C3-C4-C5     |
| 94  | L7    | 208  | PAR  | C62-C52-O52-C13 |
| 89  | L1    | 1801 | SPD  | C8-C7-N6-C5     |
| 89  | L1    | 1807 | SPD  | C4-C5-N6-C7     |
| 94  | L7    | 208  | PAR  | C42-C52-O52-C13 |
| 89  | L1    | 1804 | SPD  | C8-C7-N6-C5     |
| 89  | L2    | 1601 | SPD  | C8-C7-N6-C5     |
| 93  | L2    | 1723 | PUT  | C1-C2-C3-C4     |
| 93  | S1    | 2444 | PUT  | C1-C2-C3-C4     |
| 93  | L1    | 1975 | PUT  | C1-C2-C3-C4     |
| 89  | L1    | 1805 | SPD  | C4-C5-N6-C7     |
| 89  | L1    | 1809 | SPD  | C8-C7-N6-C5     |
| 94  | S1    | 2445 | PAR  | O51-C11-O11-C42 |
| 89  | S1    | 2447 | SPD  | N1-C2-C3-C4     |
| 89  | L1    | 1813 | SPD  | C2-C3-C4-C5     |
| 93  | S1    | 2443 | PUT  | C1-C2-C3-C4     |
| 89  | L1    | 1805 | SPD  | C7-C8-C9-N10    |
| 94  | L2    | 1728 | PAR  | C43-C33-O33-C14 |
| 94  | S1    | 2445 | PAR  | C23-C33-O33-C14 |
| 94  | L2    | 1729 | PAR  | O51-C51-C61-O61 |
| 89  | S1    | 2447 | SPD  | C8-C7-N6-C5     |
| 94  | S1    | 2445 | PAR  | C52-C42-O11-C11 |

There are no ring outliers.

20 monomers are involved in 43 short contacts:

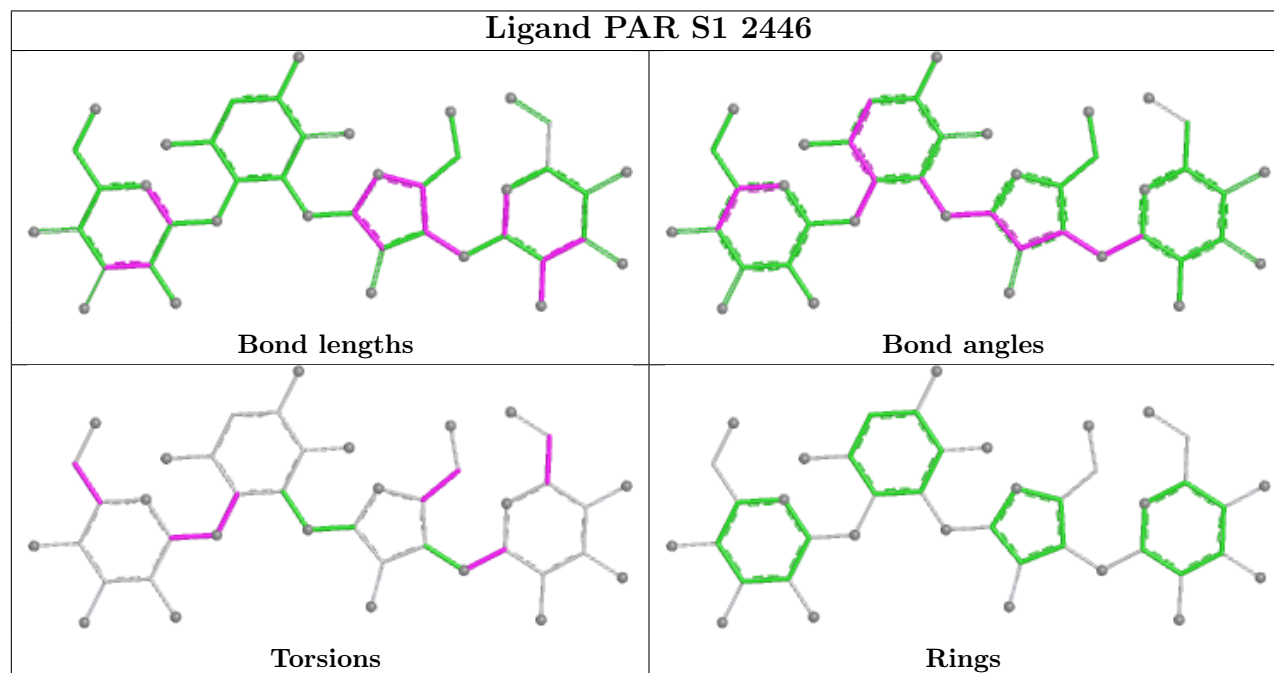
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 89  | L1    | 1811 | SPD  | 3       | 0            |
| 94  | S1    | 2446 | PAR  | 3       | 0            |
| 89  | L1    | 1806 | SPD  | 2       | 0            |
| 94  | S1    | 2445 | PAR  | 2       | 0            |
| 93  | L1    | 1977 | PUT  | 1       | 0            |
| 94  | L1    | 1978 | PAR  | 3       | 0            |
| 89  | L1    | 1808 | SPD  | 1       | 0            |
| 89  | S1    | 2301 | SPD  | 1       | 0            |
| 89  | L1    | 1815 | SPD  | 1       | 0            |
| 89  | L1    | 1813 | SPD  | 4       | 0            |

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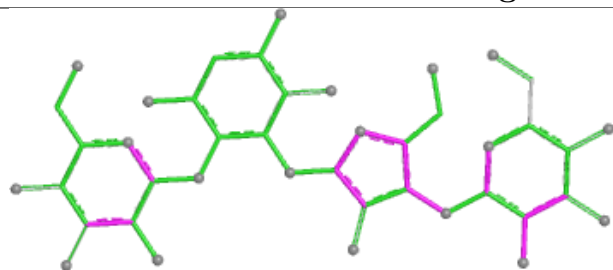
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 89  | S1    | 2447 | SPD  | 2       | 0            |
| 89  | L1    | 1814 | SPD  | 1       | 0            |
| 89  | LM    | 301  | SPD  | 3       | 0            |
| 94  | L7    | 208  | PAR  | 4       | 0            |
| 94  | L2    | 1728 | PAR  | 1       | 0            |
| 93  | L2    | 1727 | PUT  | 1       | 0            |
| 94  | L2    | 1729 | PAR  | 5       | 0            |
| 89  | L2    | 1602 | SPD  | 1       | 0            |
| 89  | S1    | 2302 | SPD  | 2       | 0            |
| 89  | L1    | 1802 | SPD  | 2       | 0            |

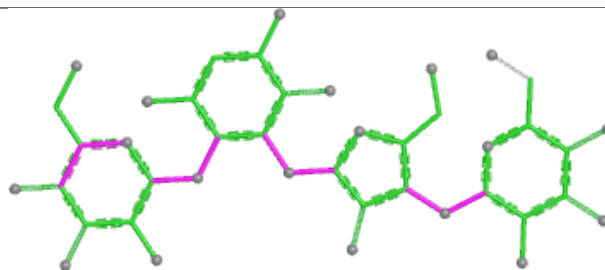
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



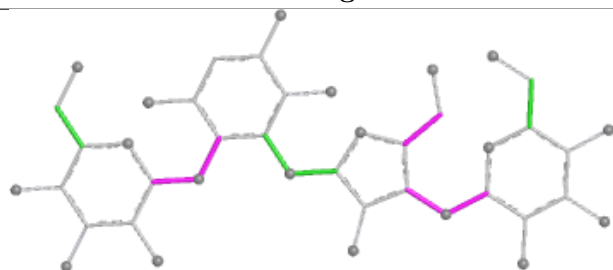
## Ligand PAR S1 2445



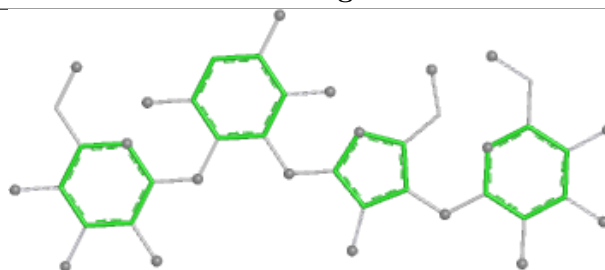
Bond lengths



Bond angles

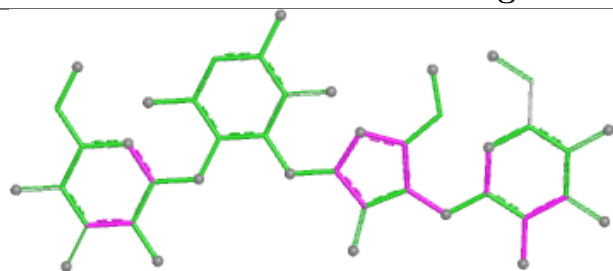


Torsions

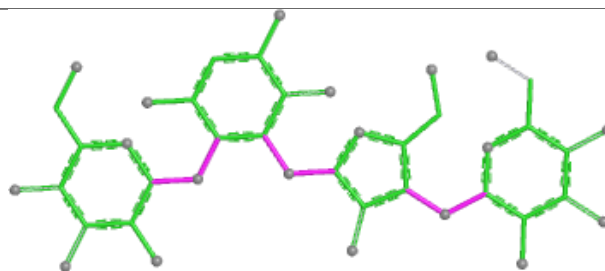


Rings

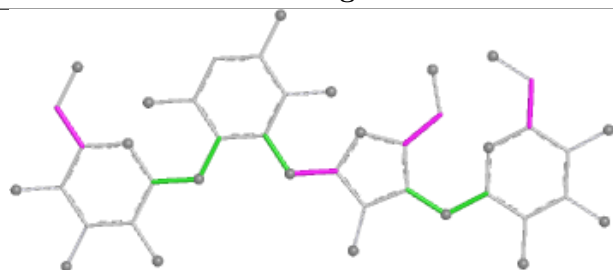
## Ligand PAR L1 1978



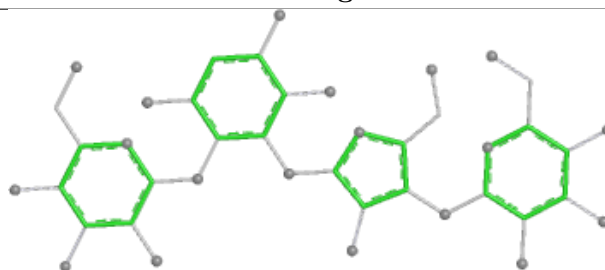
Bond lengths



Bond angles

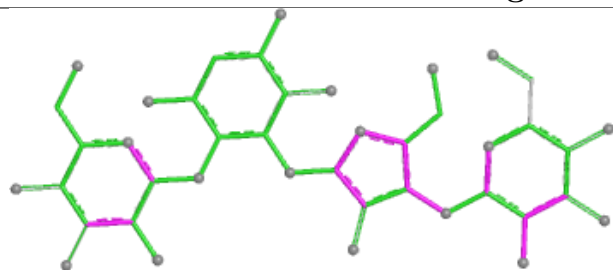


Torsions

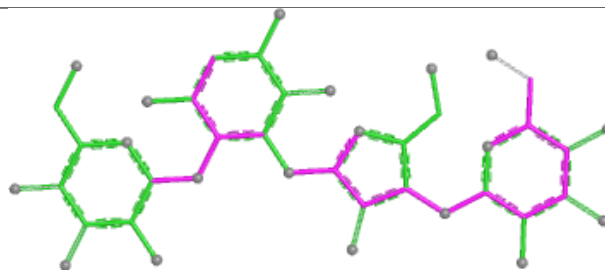


Rings

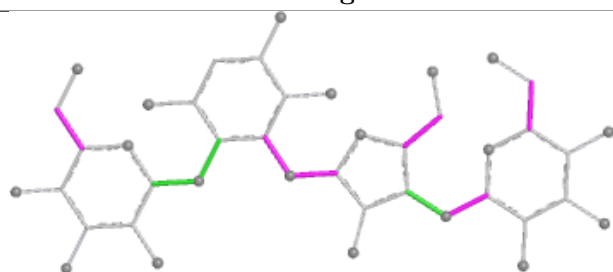
## Ligand PAR L7 208



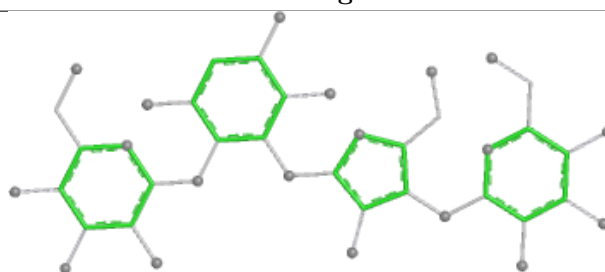
Bond lengths



Bond angles

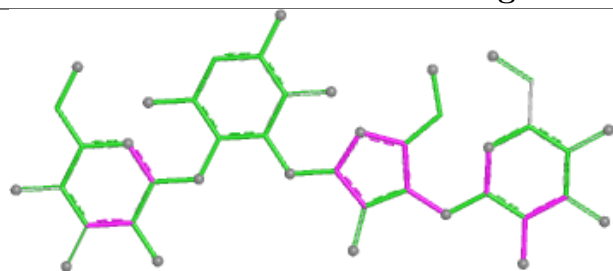


Torsions

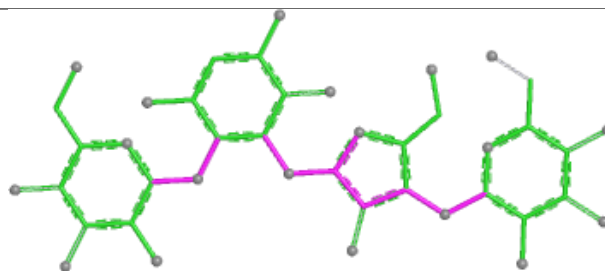


Rings

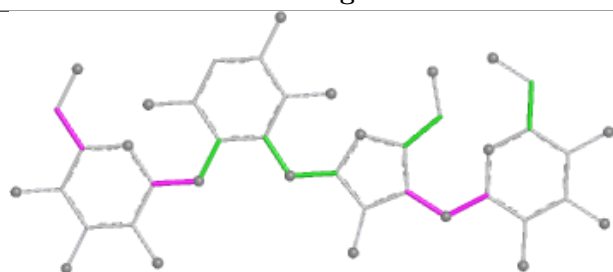
## Ligand PAR L2 1728



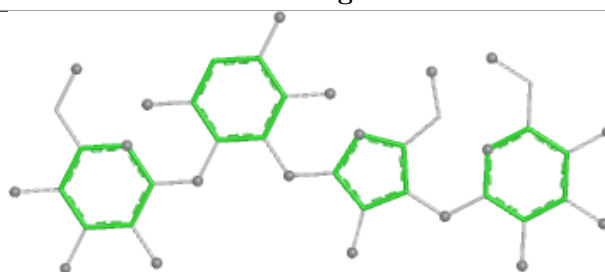
Bond lengths



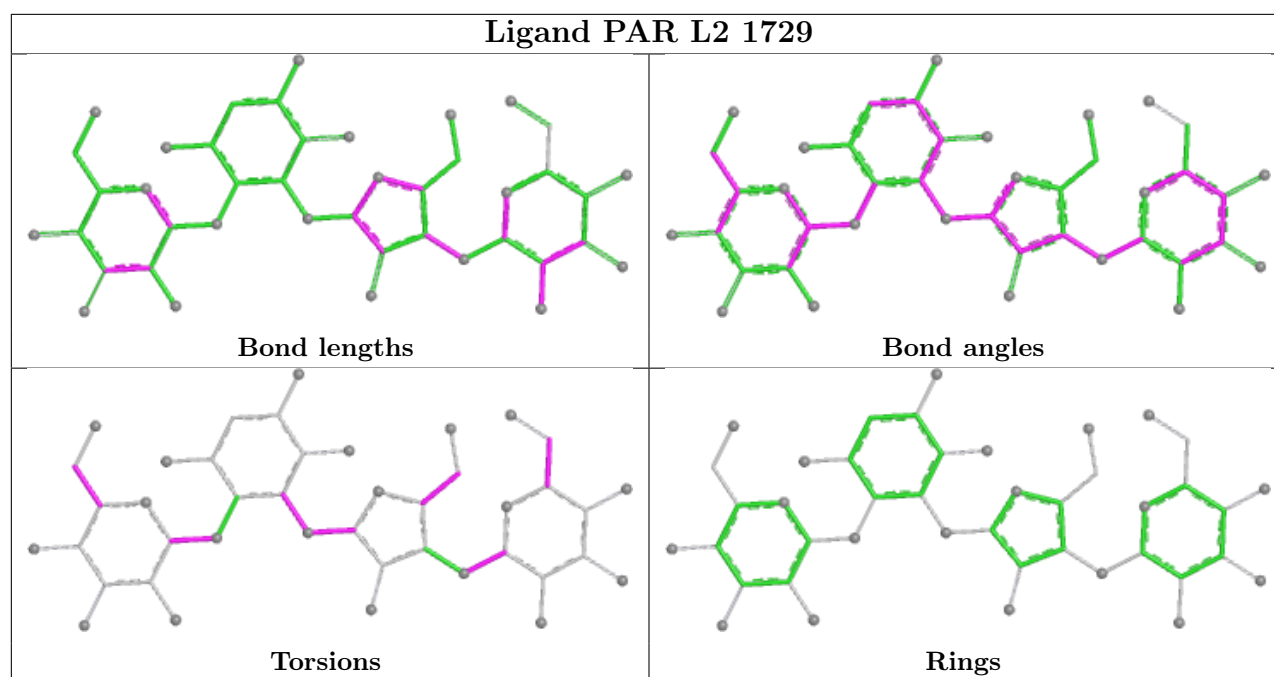
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 51  | S1    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | S1    | 1543:B8N  | O3'    | 1544:5MC  | P      | 4.02         |

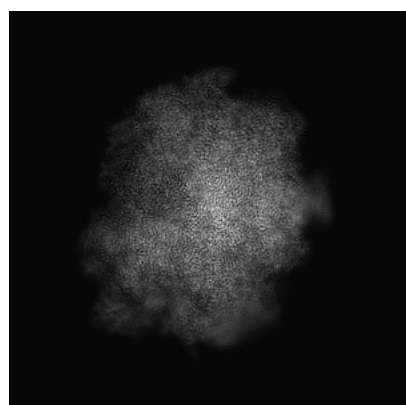
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50852. These allow visual inspection of the internal detail of the map and identification of artifacts.

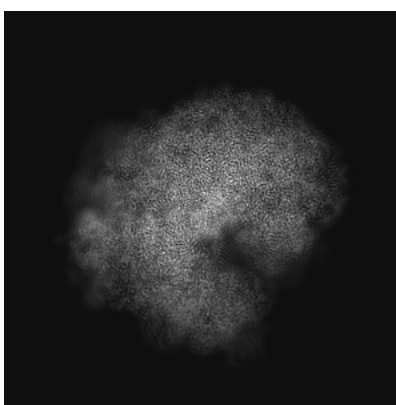
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

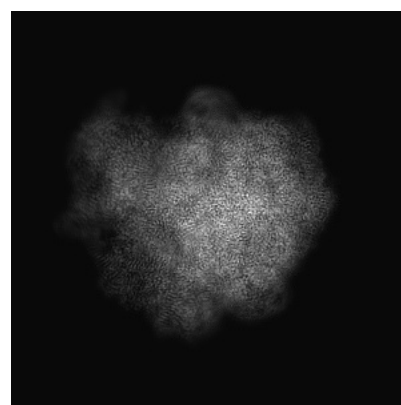
#### 6.1.1 Primary map



X



Y

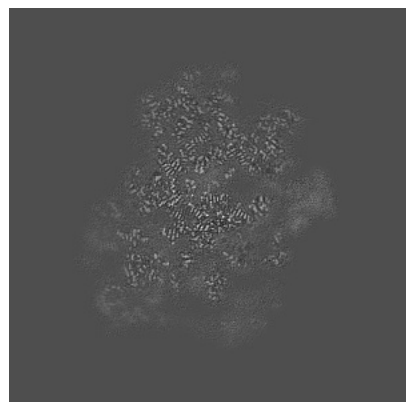


Z

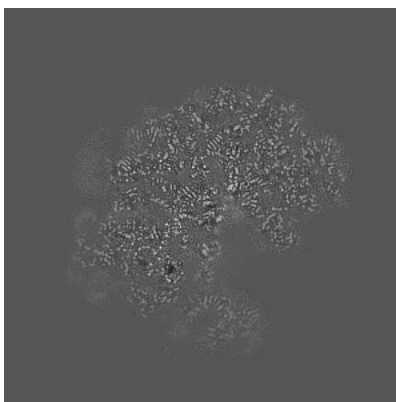
The images above show the map projected in three orthogonal directions.

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

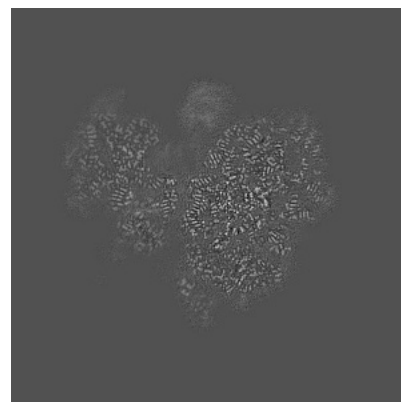
#### 6.2.1 Primary map



X Index: 240



Y Index: 240



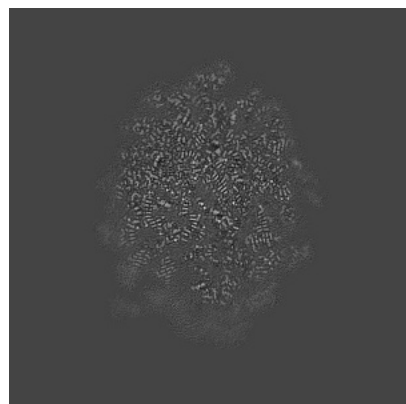
Z Index: 240



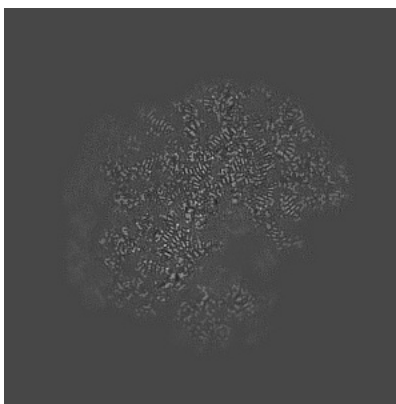
The images above show central slices of the map in three orthogonal directions.

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

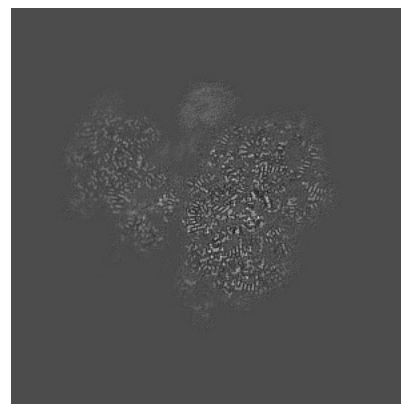
### 6.3.1 Primary map



X Index: 271



Y Index: 253

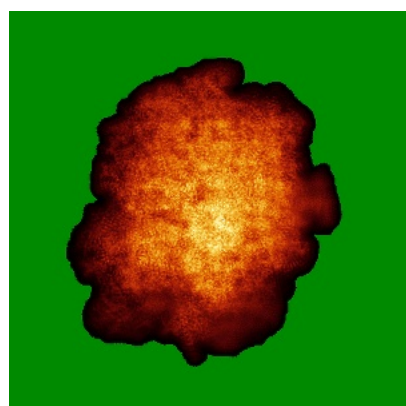


Z Index: 243

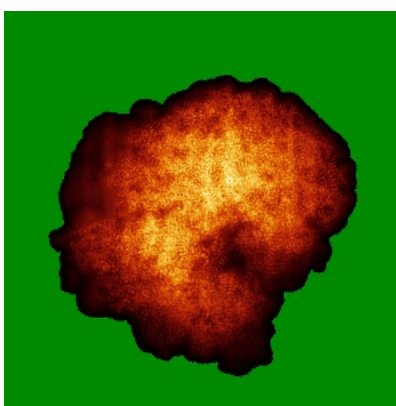
The images above show the largest variance slices of the map in three orthogonal directions.

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

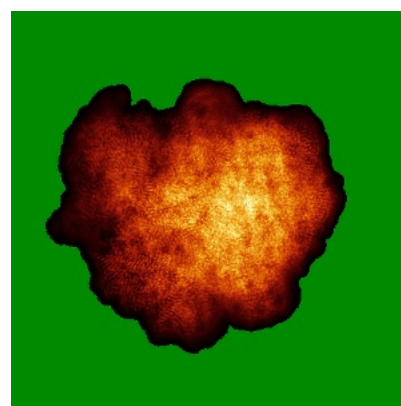
### 6.4.1 Primary map



X



Y

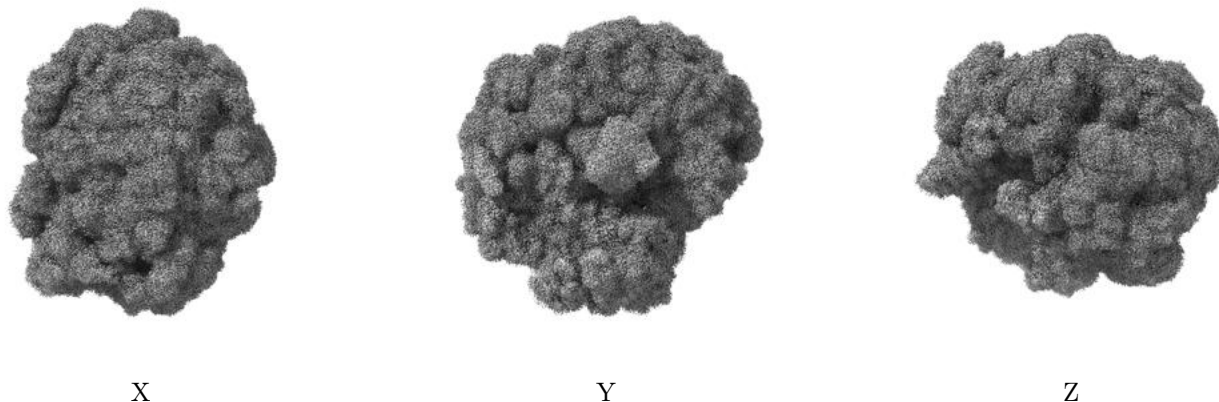


Z

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 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

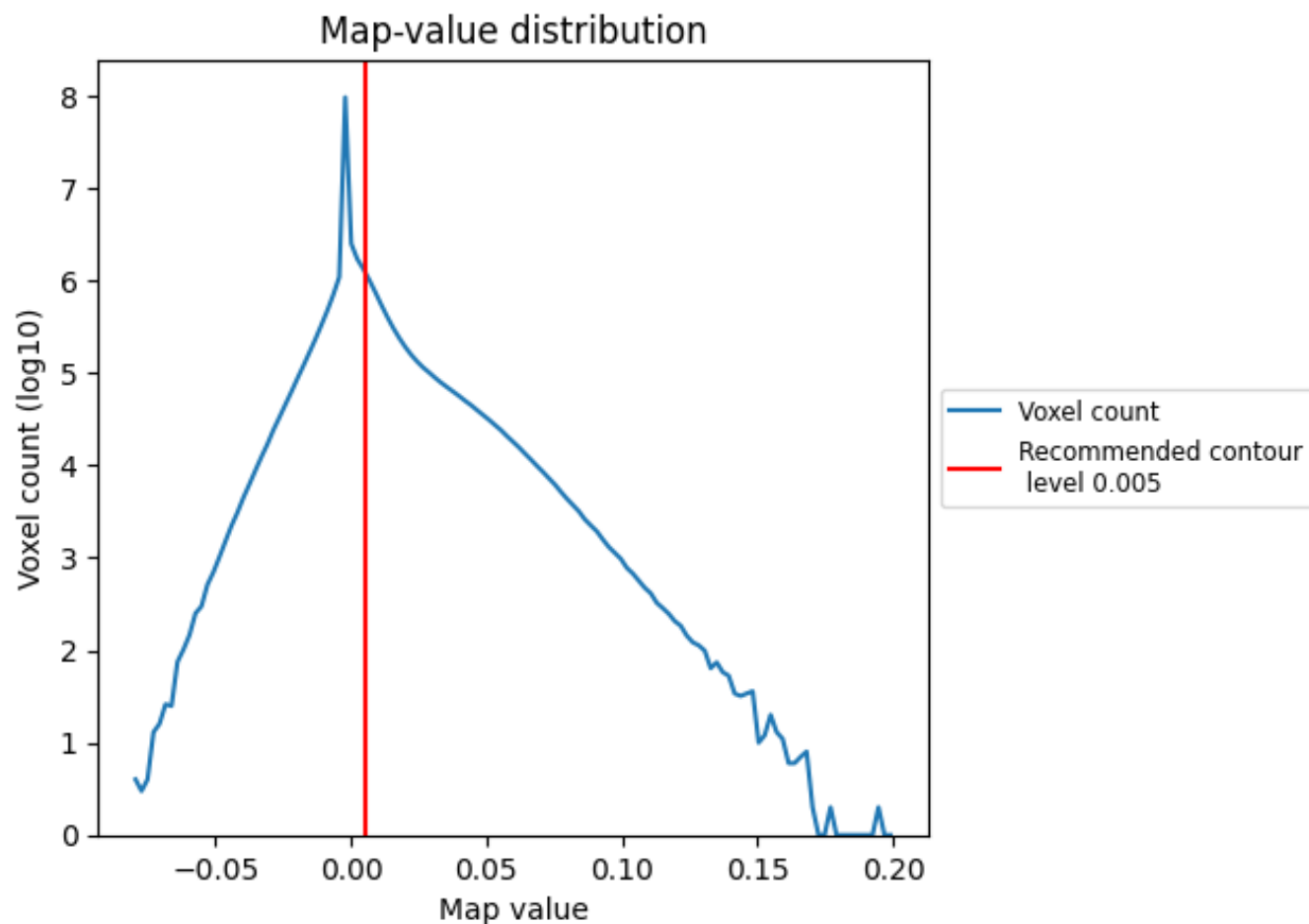
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

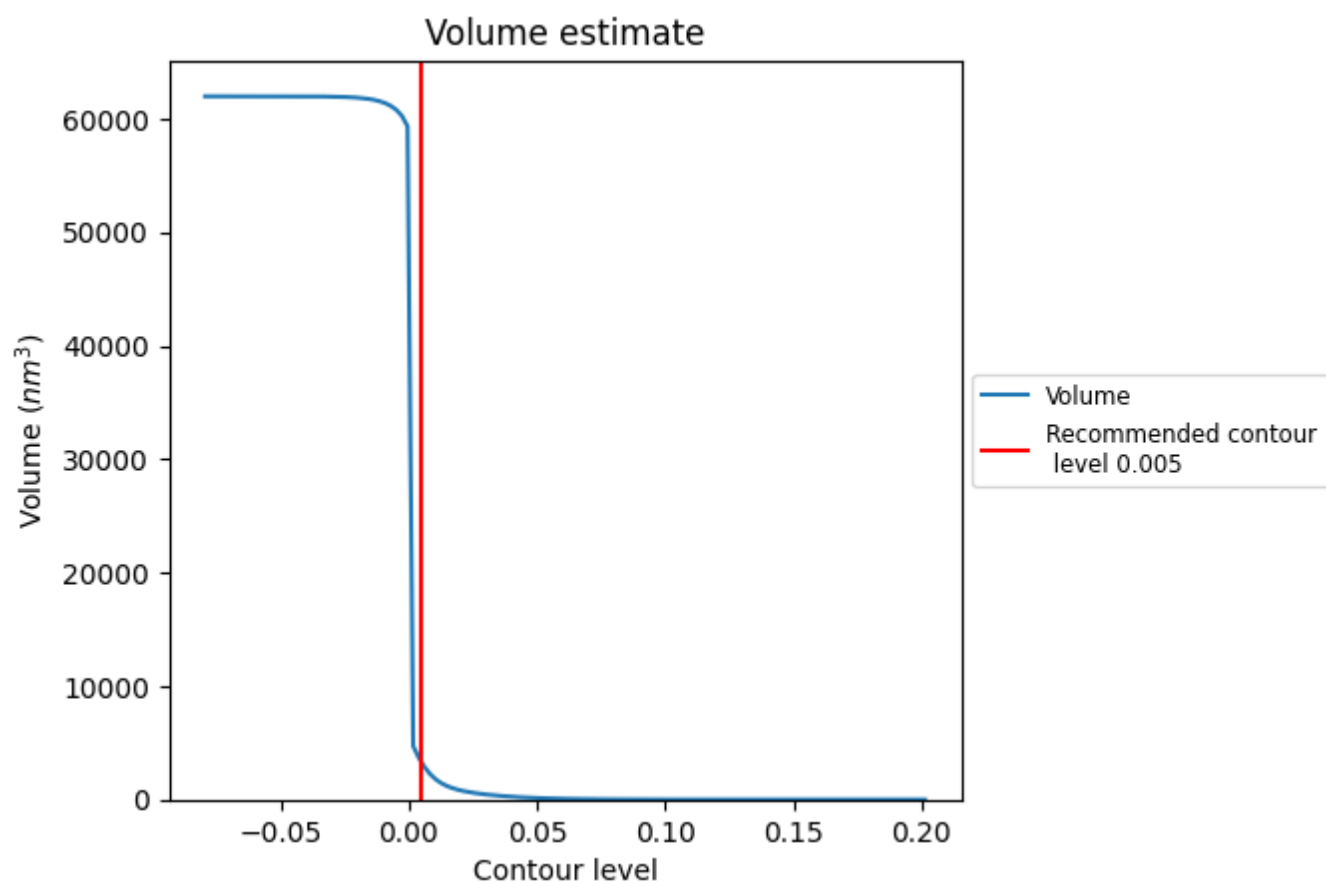
This section contains the results of statistical analysis of the map.

### 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.

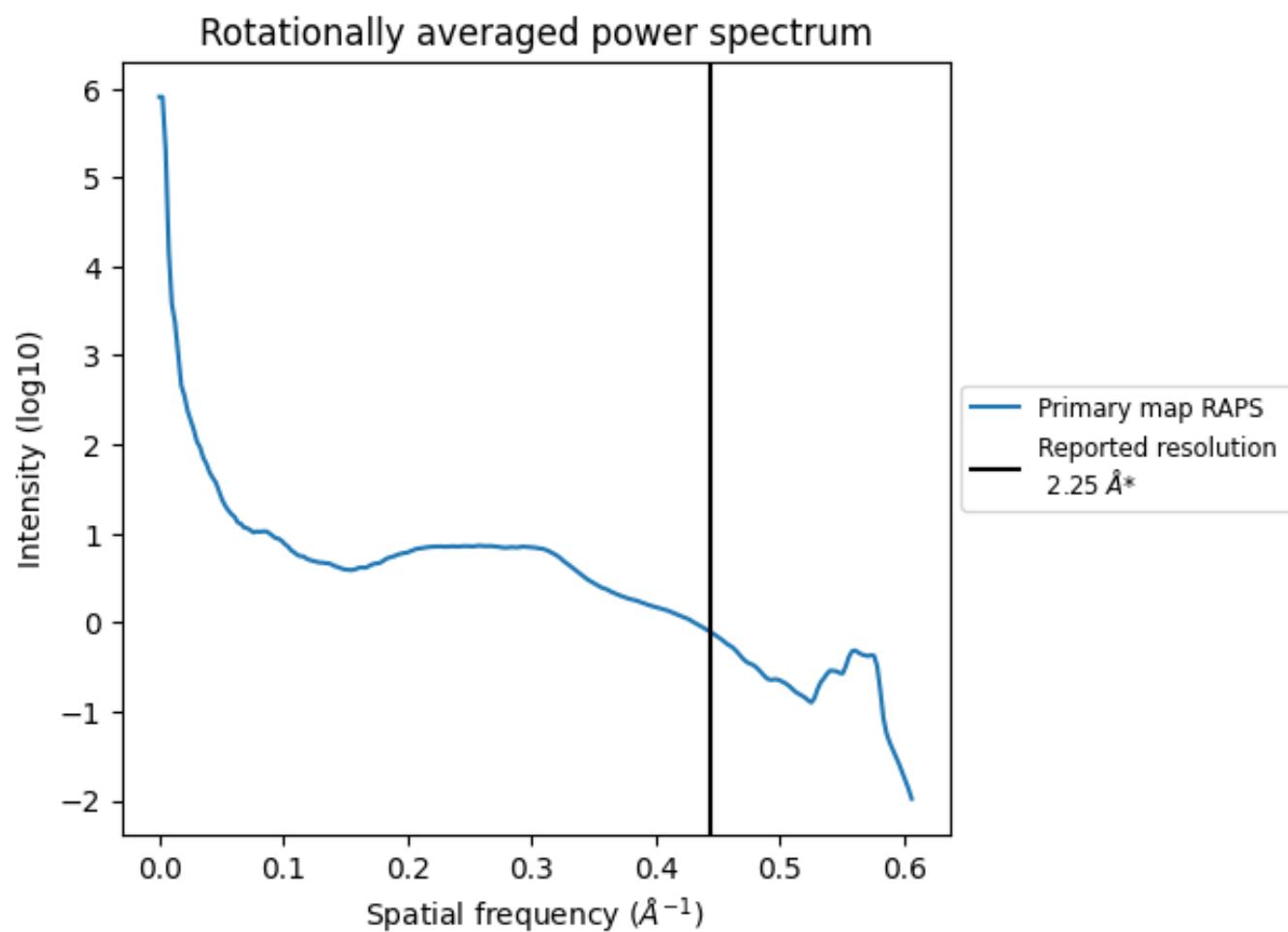
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $3258 \text{ nm}^3$ ; this corresponds to an approximate mass of 2943 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 ⓘ

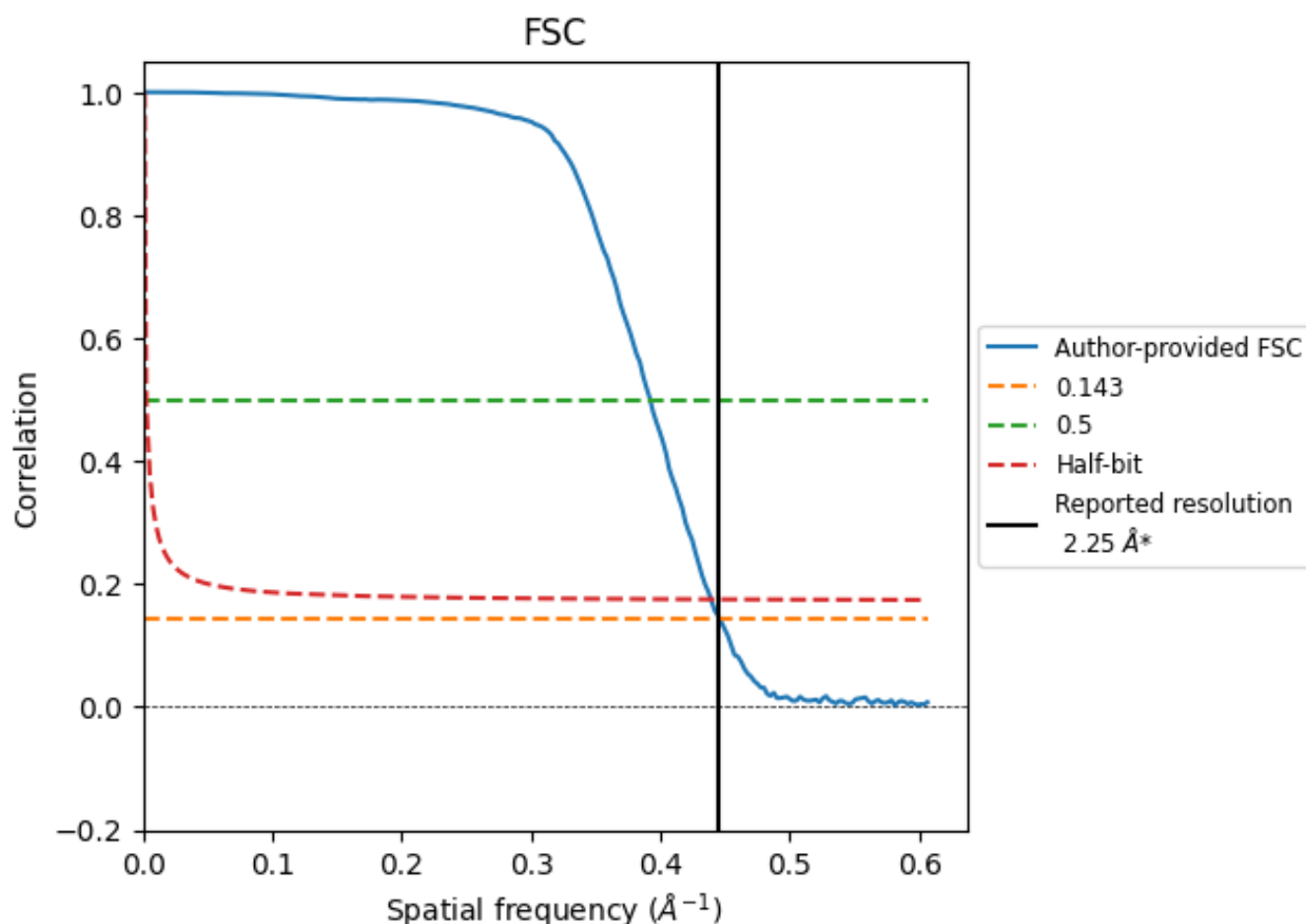


\*Reported resolution corresponds to spatial frequency of 0.444 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.444 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

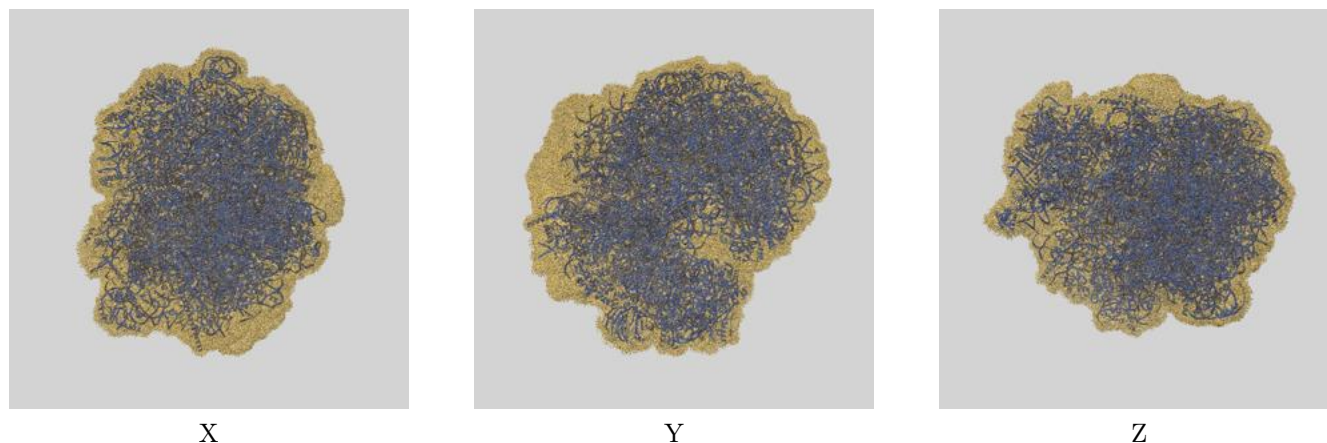
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.25                               | -    | -        |
| Author-provided FSC curve | 2.24                               | 2.55 | 2.28     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-50852 and PDB model 9FXO. Per-residue inclusion information can be found in section 3 on page 29.

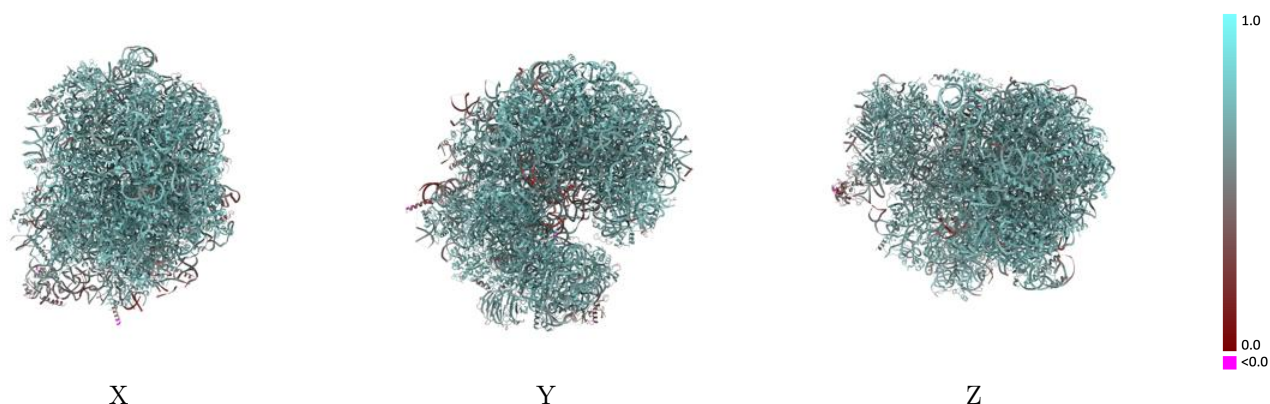
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

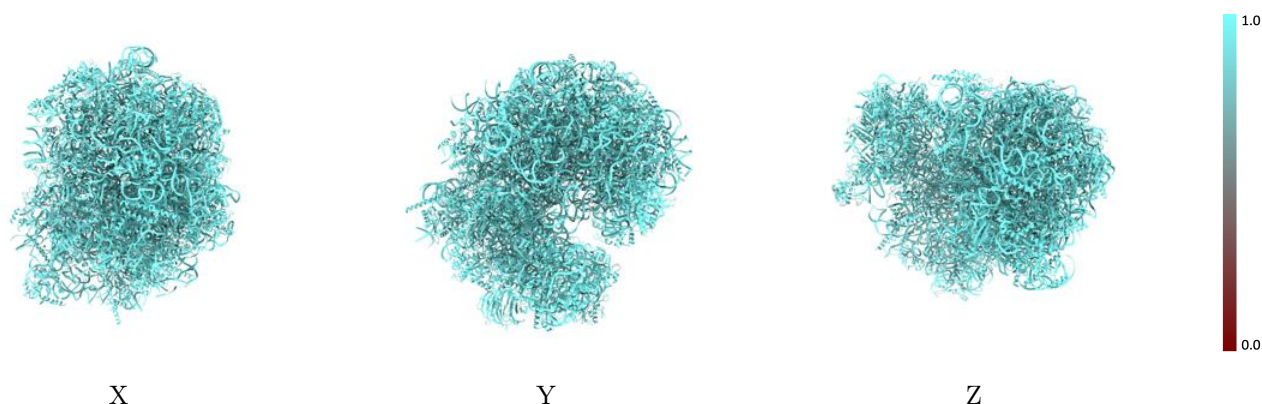


## 9.2 Q-score mapped to coordinate model [i](#)



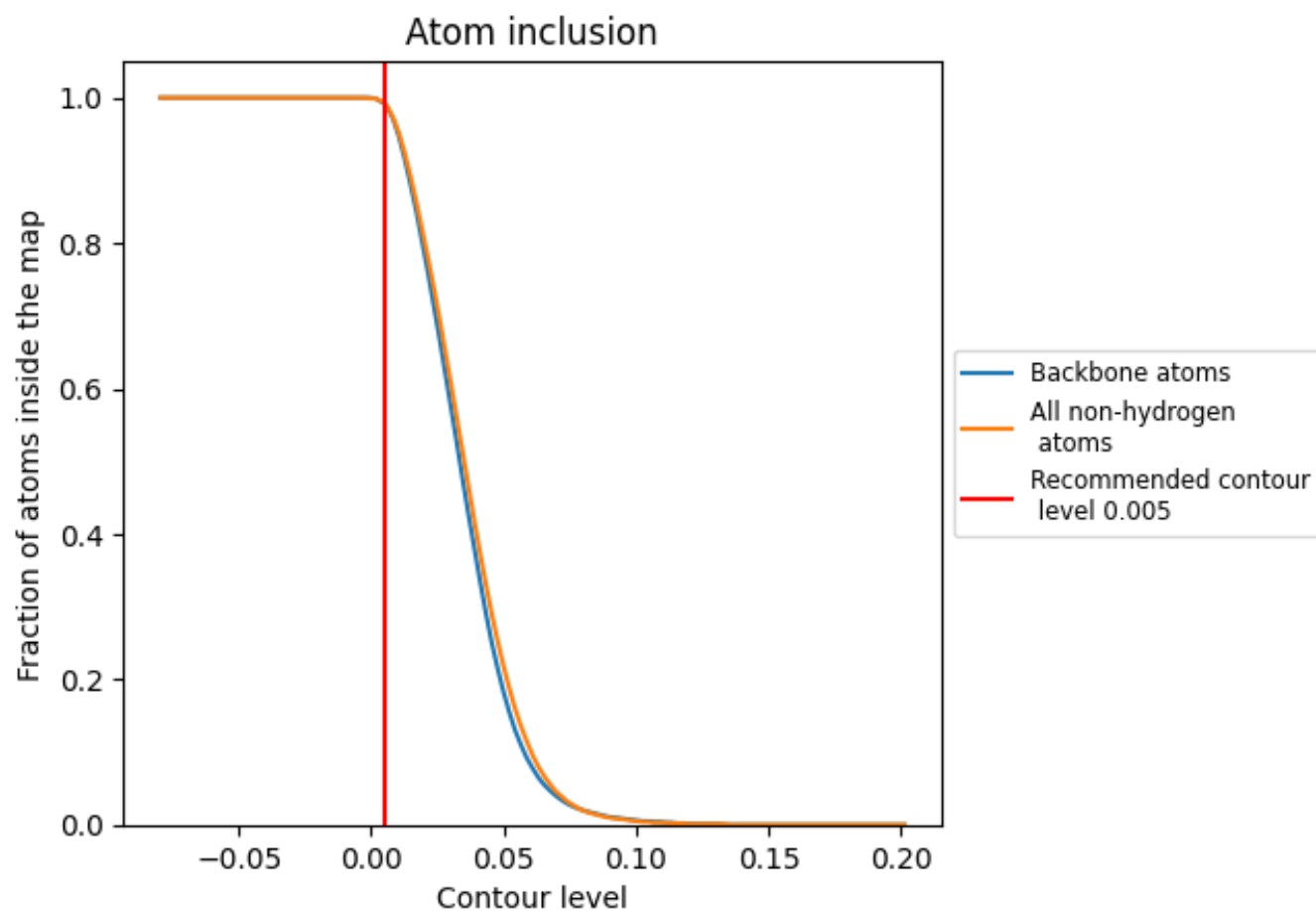
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9930   |  0.6730   |
| L1    |  0.9940   |  0.6770   |
| L2    |  0.9960   |  0.6770   |
| L3    |  0.9940   |  0.6840   |
| L4    |  0.9980   |  0.6920   |
| L5    |  0.9920   |  0.6680   |
| L6    |  0.9900   |  0.6410   |
| L7    |  0.9930   |  0.6880   |
| L8    |  1.0000   |  0.6770   |
| LA    |  0.9990   |  0.7500   |
| LB    |  0.9970   |  0.7260   |
| LC    |  0.9970   |  0.7140   |
| LD    |  0.9960   |  0.6380   |
| LE    |  0.9950   |  0.6900   |
| LF    |  0.9890  |  0.6570  |
| LG    |  0.9900 |  0.6990 |
| LH    |  0.9990 |  0.7100 |
| LI    |  0.9950 |  0.7080 |
| LJ    |  0.9980 |  0.7270 |
| LK    |  0.9950 |  0.6650 |
| LL    |  0.9960 |  0.7220 |
| LM    |  1.0000 |  0.7500 |
| LN    |  0.9960 |  0.6920 |
| LO    |  0.9870 |  0.6550 |
| LP    |  0.9980 |  0.7160 |
| LQ    |  0.9940 |  0.6830 |
| LR    |  0.9980 |  0.6970 |
| LS    |  0.9970 |  0.6890 |
| LT    |  0.9980 |  0.7340 |
| LU    |  0.9950 |  0.6410 |
| LV    |  0.9980 |  0.7280 |
| LW    |  0.9980 |  0.7220 |
| LX    |  0.9930 |  0.6910 |
| LY    |  0.9990 |  0.7010 |
| LZ    |  1.0000 |  0.7060 |





























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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| La    |  0.9980   |  0.7020   |
| Lb    |  0.9960   |  0.7090   |
| Lc    |  0.9990   |  0.7030   |
| Ld    |  0.9940   |  0.7210   |
| Le    |  0.9900   |  0.6880   |
| Lf    |  0.9980   |  0.7080   |
| Lg    |  0.9980   |  0.6990   |
| Lh    |  0.9920   |  0.6980   |
| Li    |  0.9960   |  0.6970   |
| Lj    |  0.9980   |  0.7490   |
| Lk    |  0.9950   |  0.6970   |
| Ll    |  1.0000   |  0.7440   |
| Lm    |  0.9980   |  0.6910   |
| Ln    |  1.0000   |  0.7130   |
| Lo    |  0.9940   |  0.7420   |
| Lp    |  0.9970   |  0.6930   |
| S1    |  0.9910   |  0.6530   |
| S2    |  0.9540   |  0.4430   |
| S3    |  0.9860   |  0.5550   |
| S4    |  0.9540  |  0.3780  |
| S5    |  0.9560 |  0.5120 |
| SA    |  0.9910 |  0.7080 |
| SB    |  0.9930 |  0.6860 |
| SC    |  0.9910 |  0.6410 |
| SD    |  0.9950 |  0.6930 |
| SE    |  0.9950 |  0.7030 |
| SF    |  0.9890 |  0.7090 |
| SG    |  0.9960 |  0.6600 |
| SH    |  0.9930 |  0.6860 |
| SI    |  0.9940 |  0.6910 |
| SJ    |  0.9970 |  0.7330 |
| SK    |  0.9960 |  0.6880 |
| SL    |  0.9980 |  0.6960 |
| SM    |  0.9870 |  0.6450 |
| SN    |  0.9870 |  0.5820 |
| SO    |  0.9960 |  0.7270 |
| SP    |  0.9960 |  0.7100 |
| SQ    |  0.8850 |  0.3870 |
| SR    |  0.9940 |  0.6490 |
| SS    |  0.9930 |  0.6900 |
| ST    |  0.9960 |  0.7330 |
| SU    |  0.9920 |  0.6870 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| SV    |  0.9810 |  0.6380 |
| SW    |  0.9830 |  0.6280 |
| SX    |  0.9950 |  0.6700 |
| SY    |  0.9940 |  0.6940 |
| SZ    |  0.9900 |  0.6680 |
| Sa    |  0.9790 |  0.6320 |
| Sb    |  0.9990 |  0.7320 |
| Sc    |  0.9840 |  0.6730 |
| Sd    |  0.9810 |  0.6530 |
| Se    |  0.9790 |  0.6280 |
| Sf    |  0.9180 |  0.4020 |
| Sg    |  0.9740 |  0.5940 |
| Sh    |  0.9220 |  0.4270 |