



## Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 02:06 am BST

PDB ID : 8B2L / pdb\_00008b2l  
EMDB ID : EMD-15806  
Title : Cryo-EM structure of the plant 80S ribosome  
Authors : Smirnova, J.; Loerke, J.; Kleinau, G.; Schmidt, A.; Buerger, J.; Meyer, E.H.;  
Mielke, T.; Scheerer, P.; Bock, R.; Spahn, C.M.T.; Zoschke, R.  
Deposited on : 2022-09-14  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

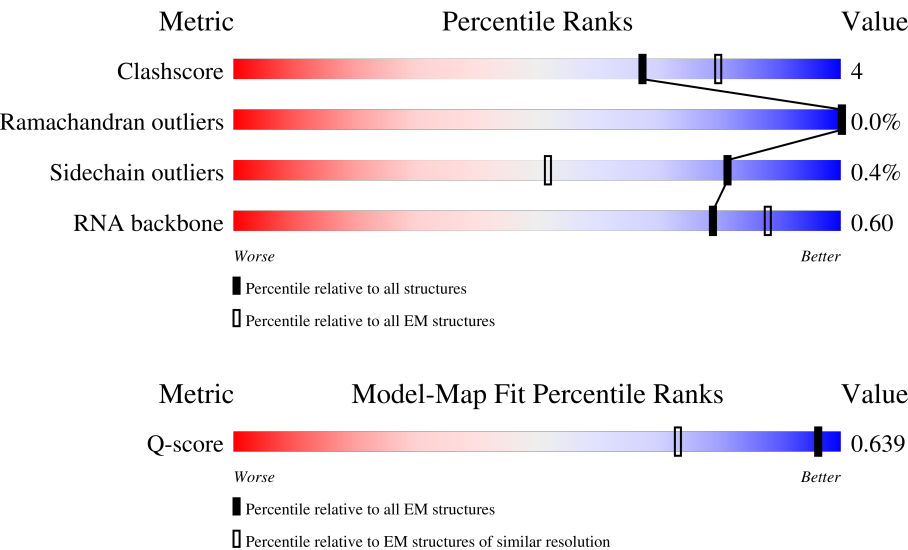
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.20 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.



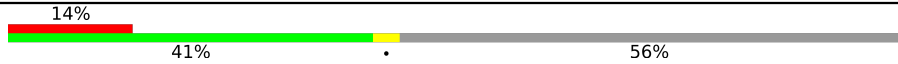
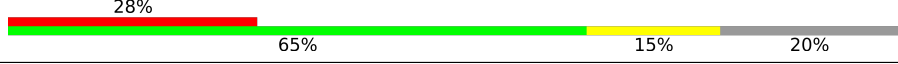
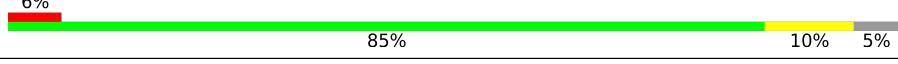
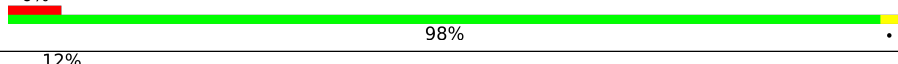
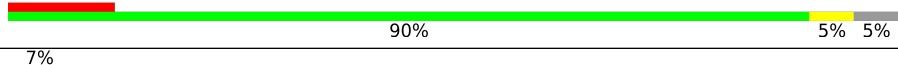
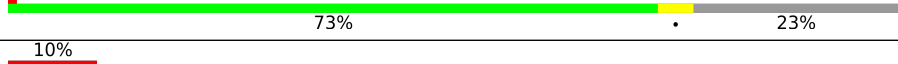
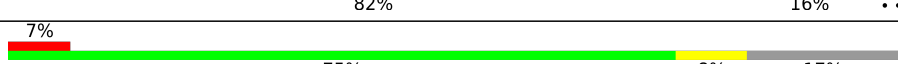
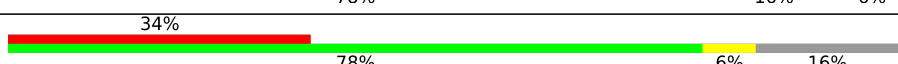
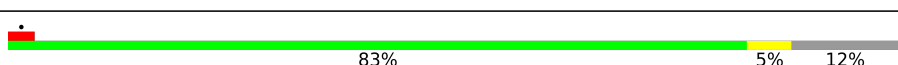
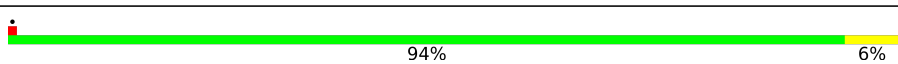
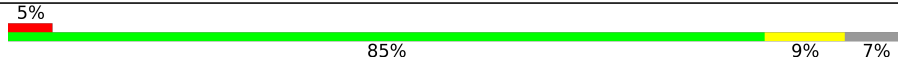
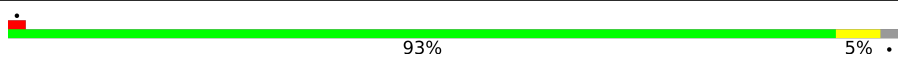
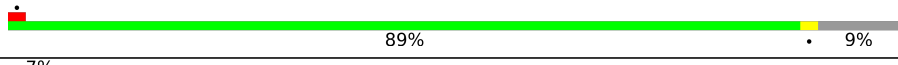
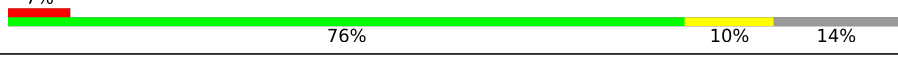
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 3184 ( 1.71 - 2.70 )                                     |

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   | A1    | 264    | <div><div></div><div>91%</div><div>7%</div><div></div></div>                |
| 2   | k1    | 249    | <div><div>21%</div><div>84%</div><div>8%</div><div>8%</div></div>           |
| 3   | h1    | 1808   | <div><div></div><div>59%</div><div>26%</div><div></div><div>10%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | I1    | 208    |    |
| 5   | C1    | 144    |    |
| 6   | D1    | 149    |    |
| 7   | E1    | 143    |    |
| 8   | F1    | 261    |    |
| 9   | G1    | 83     |    |
| 10  | H1    | 133    |    |
| 11  | I1    | 107    |    |
| 12  | J1    | 127    |    |
| 13  | K1    | 86     |    |
| 14  | L1    | 65     |    |
| 15  | M1    | 62     |   |
| 16  | N1    | 156    |  |
| 17  | O1    | 191    |  |
| 18  | P1    | 224    |  |
| 19  | Q1    | 328    |  |
| 20  | R1    | 122    |  |
| 21  | S1    | 150    |  |
| 22  | T1    | 142    |  |
| 23  | U1    | 152    |  |
| 24  | V1    | 56     |  |
| 25  | W1    | 151    |  |
| 26  | X1    | 159    |  |
| 27  | Y1    | 152    |  |
| 28  | Z1    | 336    |  |

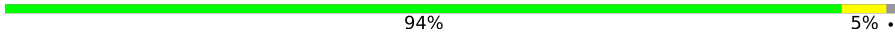
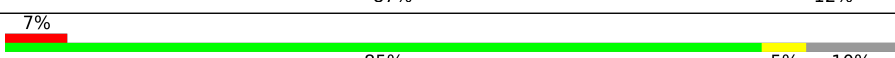
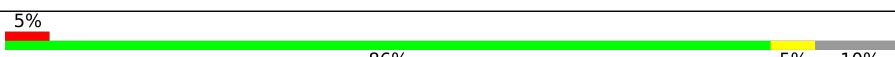
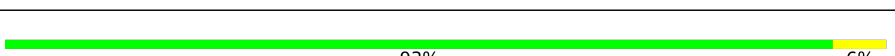
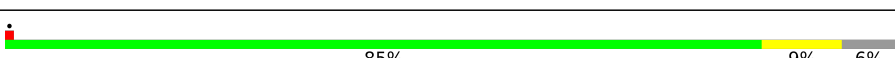
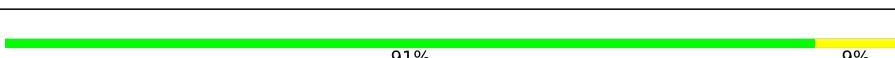
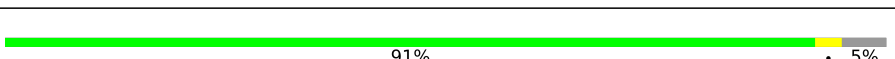
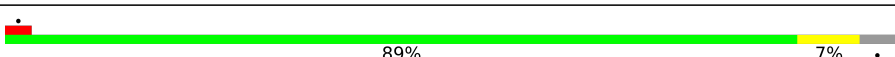
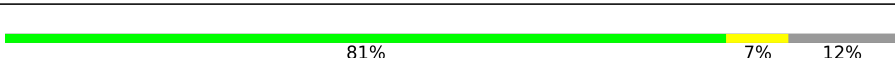
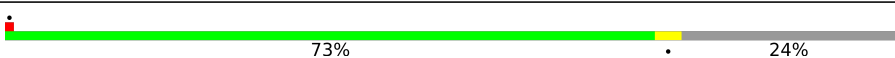
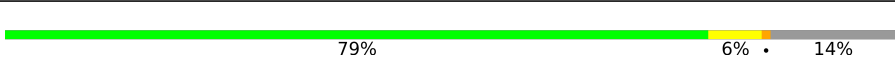
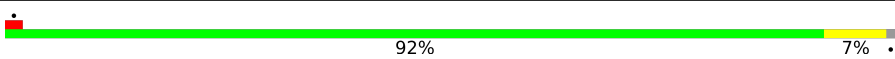
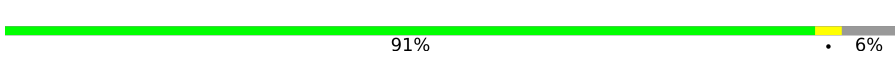
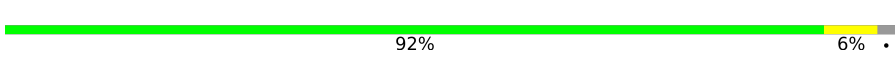
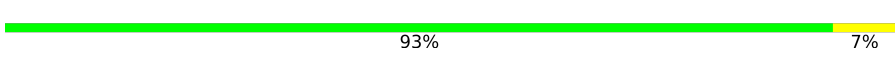
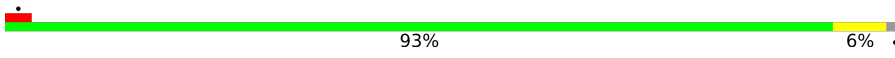
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | a1    | 248    |                  |
| 30  | b1    | 197    |                  |
| 31  | c1    | 280    |                  |
| 32  | d1    | 210    |                  |
| 33  | e1    | 130    |                  |
| 34  | f1    | 147    |                  |
| 35  | B1    | 12     |                  |
| 36  | W2    | 76     |                  |
| 36  | i2    | 76     |                  |
| 37  | C3    | 119    |                  |
| 38  | D3    | 206    |                  |
| 39  | E3    | 134    |                  |
| 40  | F3    | 204    |                  |
| 41  | G3    | 187    |                  |
| 42  | H3    | 214    |                  |
| 43  | I3    | 178    |                  |
| 44  | J3    | 164    |                  |
| 45  | K3    | 127    |                  |
| 46  | L3    | 164    |                  |
| 47  | M3    | 135    |                  |
| 48  | N3    | 143    |                  |
| 49  | O3    | 61     |                  |
| 50  | P3    | 113    |                  |
| 51  | Q3    | 120    |                  |
| 52  | R3    | 133    |                  |

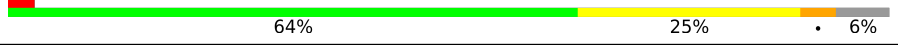
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 53  | S3    | 112    |    |
| 54  | T3    | 120    |    |
| 55  | U3    | 110    |    |
| 56  | V3    | 95     |    |
| 57  | W3    | 69     |    |
| 58  | X3    | 51     |    |
| 59  | Y3    | 128    |    |
| 60  | p3    | 25     |    |
| 61  | Z3    | 105    |    |
| 62  | a3    | 92     |    |
| 63  | b3    | 230    |    |
| 64  | c3    | 258    |   |
| 65  | d3    | 206    |  |
| 66  | e3    | 140    |  |
| 67  | f3    | 148    |  |
| 68  | g3    | 221    |  |
| 69  | h3    | 301    |  |
| 70  | j3    | 175    |  |
| 71  | k3    | 154    |  |
| 72  | m3    | 146    |  |
| 73  | n3    | 123    |  |
| 74  | o3    | 260    |  |
| 75  | q3    | 242    |  |
| 76  | r3    | 389    |  |
| 77  | s3    | 405    |  |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 78  | t3    | 181    |  89% 6% 5%    |
| 79  | u3    | 194    |  88% 10% •    |
| 80  | l3    | 24     |  71% 100%     |
| 81  | A3    | 3390   |  64% 25% • 6% |
| 82  | B3    | 163    |  67% 31% •    |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85  | SPD  | A3    | 3450 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 361205 atoms, of which 151371 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 protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 1   | A1    | 259      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4254  | 1323 | 2180 | 387 | 357 | 7 |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 2   | k1    | 230      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3816  | 1156 | 1965 | 361 | 326 | 8 |         |       |

- Molecule 3 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|-------|------|---------|-------|
| 3   | h1    | 1626     | Total | C     | H     | N    | O     | P    | 0       | 0     |
|     |       |          | 52270 | 15549 | 17529 | 6195 | 11371 | 1626 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S10-1-like.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 4   | l1    | 91       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1549  | 508 | 776 | 125 | 136 | 4 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 5   | C1    | 117      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1778  | 553 | 900 | 153 | 165 | 7 |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S17-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 6   | D1    | 119      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 1989  | 604 | 1026 | 178 | 177 | 4 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S19-3.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 7   | E1    | 136      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2172  | 676 | 1091 | 211 | 190 | 4 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 8   | F1    | 216      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3578  | 1118 | 1818 | 314 | 320 | 8 |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 9   | G1    | 83       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 404 | 643 | 120 | 125 | 3 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 10  | H1    | 127      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2145  | 657 | 1111 | 200 | 174 | 3 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 11  | I1    | 74       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1204  | 365 | 621 | 109 | 106 | 3 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 12  | J1    | 98       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1610  | 491 | 818 | 161 | 132 | 8 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 13  | K1    | 84       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1307  | 404 | 656 | 122 | 118 | 7 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 14  | L1    | 61       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1018  | 303 | 525 | 102 | 86 | 2 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 15  | M1    | 52       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 851   | 249 | 442 | 94 | 65 | 1 |         |       |

- Molecule 16 is a protein called ubiquitin-40S ribosomal protein S27a-like.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 16  | N1    | 69       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1143  | 360 | 581 | 103 | 94 | 5 |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 17  | O1    | 188      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3125  | 972 | 1591 | 281 | 279 | 2 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 18  | P1    | 186      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3081  | 944 | 1570 | 300 | 263 | 4 |         |       |

- Molecule 19 is a protein called guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 19  | Q1    | 309      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4756  | 1512 | 2362 | 414 | 456 | 12 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S20-2.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 20  | R1    | 102      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 505 | 864 | 151 | 145 | 3 |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S14-2.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 21  | S1    | 132      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2026  | 611 | 1028 | 197 | 185 | 5 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 22  | T1    | 141      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2264  | 695 | 1164 | 215 | 187 | 3 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 23  | U1    | 142      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2337  | 718 | 1184 | 227 | 202 | 6 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 24  | V1    | 55       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 871   | 274 | 430 | 90 | 71 | 6 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S15, chloroplastic.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 25  | W1    | 149      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2467  | 762 | 1278 | 223 | 202 | 2 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S11-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 26  | X1    | 145      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2362  | 734 | 1207 | 222 | 194 | 5 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S15-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 27  | Y1    | 131      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2193  | 681 | 1132 | 199 | 176 | 5 |         |       |

- Molecule 28 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 28  | Z1    | 202      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3233  | 1023 | 1623 | 289 | 288 | 10 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S3-2-like.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 29  | a1    | 211      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3413  | 1052 | 1752 | 306 | 295 | 8 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S9-2-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 30  | b1    | 183      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3118  | 964 | 1595 | 301 | 253 | 5 |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S2-3-like.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 31  | c1    | 217      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3472  | 1089 | 1786 | 300 | 289 | 8 |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S5-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 32  | d1    | 194      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3103  | 953 | 1572 | 290 | 280 | 8 |         |       |

- Molecule 33 is a protein called 40S ribosomal protein S15a-1.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 33  | e1    | 129      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2100  | 659 | 1068 | 188 | 180 | 5 |         |       |

- Molecule 34 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 34  | f1    | 141      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2332  | 722 | 1197 | 221 | 188 | 4 |         |       |

- Molecule 35 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|---------|-------|
| 35  | B1    | 12       | Total | C   | H   | N  | O  | P  | 0       | 0     |
|     |       |          | 360   | 108 | 120 | 24 | 96 | 12 |         |       |

- Molecule 36 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 36  | i2    | 76       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 2452  | 726 | 822 | 298 | 530 | 76 |         |       |
| 36  | W2    | 76       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 2451  | 726 | 822 | 298 | 529 | 76 |         |       |

- Molecule 37 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|-----|---------|-------|
| 37  | C3    | 119      | Total | C    | H    | N   | O   | P   | 0       | 0     |
|     |       |          | 3823  | 1133 | 1285 | 457 | 829 | 119 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 38  | D3    | 200      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3296  | 1007 | 1691 | 324 | 270 | 4 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L14-1.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 39  | E3    | 130      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2206  | 678 | 1150 | 196 | 179 | 3 |         |       |

- Molecule 40 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 40  | F3    | 203      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3469  | 1071 | 1768 | 350 | 277 | 3 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L18-2-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 41  | G3    | 186      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3042  | 931 | 1580 | 283 | 245 | 3 |         |       |

- Molecule 42 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 42  | H3    | 182      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3181  | 946 | 1652 | 327 | 247 | 9 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 43  | I3    | 177      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3061  | 969 | 1556 | 277 | 251 | 8 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L21-1-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 44  | J3    | 163      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2672  | 823 | 1366 | 255 | 224 | 4 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L22-2-like.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 45  | K3    | 99       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 515 | 845 | 141 | 150 | 2 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L24-like.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 46  | L3    | 62       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1079  | 341 | 553 | 101 | 81 | 3 |         |       |

- Molecule 47 is a protein called eL27 (60S ribosomal protein L27).

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 47  | M3    | 134      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2283  | 708 | 1184 | 206 | 183 | 2 |         |       |

- Molecule 48 is a protein called eL28 (60S ribosomal protein L28).

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 48  | N3    | 142      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2298  | 701 | 1187 | 207 | 201 | 2 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 49  | O3    | 49       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 831   | 250 | 419 | 95 | 66 | 1 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L30-like.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 50  | P3    | 97       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1526  | 475 | 781 | 130 | 135 | 5 |         |       |

- Molecule 51 is a protein called eL31 (60S ribosomal protein L31).

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 51  | Q3    | 108      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1809  | 549 | 934 | 168 | 156 | 2 |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L32-1.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 52  | R3    | 126      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2151  | 655 | 1115 | 207 | 169 | 5 |         |       |

- Molecule 53 is a protein called eL33 (60S ribosomal protein L35a).

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 53  | S3    | 111      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1832  | 571 | 932 | 171 | 153 | 5 |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 54  | T3    | 114      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 1939  | 579 | 1013 | 193 | 153 | 1 |         |       |

- Molecule 55 is a protein called eL36 (60S ribosomal protein L36).

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 55  | U3    | 98       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 489 | 868 | 162 | 129 | 2 |         |       |

- Molecule 56 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 56  | V3    | 86       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1427  | 429 | 726 | 155 | 112 | 5 |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 57  | W3    | 68       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1160  | 358 | 602 | 99 | 98 | 3 |         |       |

- Molecule 58 is a protein called 60S ribosomal protein L39-3.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 58  | X3    | 50       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 928   | 286 | 480 | 96 | 64 | 2 |         |       |

- Molecule 59 is a protein called ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 59  | Y3    | 51       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 881   | 262 | 460 | 88 | 65 | 6 |         |       |

- Molecule 60 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 60  | p3    | 25       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 527   | 145 | 289 | 62 | 28 | 3 |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 61  | Z3    | 98       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1629  | 494 | 842 | 157 | 131 | 5 |         |       |

- Molecule 62 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 62  | a3    | 91       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1453  | 443 | 745 | 136 | 124 | 5 |         |       |

- Molecule 63 is a protein called eL6 (60S ribosomal protein L6).

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 63  | b3    | 208      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3360  | 1046 | 1749 | 290 | 271 | 4 |         |       |

- Molecule 64 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 64  | c3    | 233      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3907  | 1206 | 2028 | 347 | 319 | 7 |         |       |

- Molecule 65 is a protein called uL13 (60S ribosomal protein L13a).

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 65  | d3    | 205      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3414  | 1046 | 1774 | 318 | 268 | 8 |         |       |

- Molecule 66 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 66  | e3    | 131      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2029  | 623 | 1044 | 183 | 170 | 9 |         |       |

- Molecule 67 is a protein called uL15 (60S ribosomal protein L27a).

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 67  | f3    | 147      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2361  | 740 | 1200 | 228 | 190 | 3 |         |       |

- Molecule 68 is a protein called uL16 (60S ribosomal protein L10).

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 68  | g3    | 209      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3397  | 1058 | 1726 | 329 | 273 | 11 |         |       |

- Molecule 69 is a protein called 60S ribosomal protein L5-like.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 69  | h3    | 288      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4715  | 1481 | 2374 | 426 | 429 | 5 |         |       |

- Molecule 70 is a protein called 50S ribosomal protein L22, chloroplastic.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 70  | j3    | 154      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2515  | 775 | 1270 | 246 | 219 | 5 |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 71  | k3    | 117      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 1980  | 609 | 1030 | 170 | 169 | 2 |         |       |

- Molecule 72 is a protein called uL24 (60S ribosomal protein L26).

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 72  | m3    | 126      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2124  | 634 | 1103 | 209 | 175 | 3 |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L35-like.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 73  | n3    | 122      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2140  | 642 | 1141 | 191 | 165 | 1 |         |       |

- Molecule 74 is a protein called uL2 (60S ribosomal protein L8).

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 74  | o3    | 245      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3791  | 1174 | 1911 | 381 | 315 | 10 |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L7-4-like.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 75  | q3    | 238      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4016  | 1256 | 2058 | 359 | 339 | 4 |         |       |

- Molecule 76 is a protein called uL3 (60S ribosomal protein L3).

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 76  | r3    | 386      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6327  | 1981 | 3223 | 578 | 530 | 15 |         |       |

- Molecule 77 is a protein called uL4 (60S ribosomal protein L4).

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 77  | s3    | 398      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6324  | 1956 | 3227 | 583 | 548 | 10 |         |       |

- Molecule 78 is a protein called uL5 (60S ribosomal protein L11).

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 78  | t3    | 172      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2836  | 882 | 1444 | 259 | 244 | 7 |         |       |

- Molecule 79 is a protein called uL6 (60S ribosomal protein L9).

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 79  | u3    | 191      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3124  | 963 | 1604 | 276 | 276 | 5 |         |       |

- Molecule 80 is a protein called nascent chain.

| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|-------|
| 80  | l3    | 24       | Total | C  | H  | N  | O  | 0       | 0     |
|     |       |          | 169   | 72 | 49 | 24 | 24 |         |       |

- Molecule 81 is a RNA chain called 25S rRNA.

| Mol | Chain | Residues | Atoms  |       |       |       |       |      | AltConf | Trace |
|-----|-------|----------|--------|-------|-------|-------|-------|------|---------|-------|
| 81  | A3    | 3196     | Total  | C     | H     | N     | O     | P    | 0       | 0     |
|     |       |          | 103169 | 30602 | 34651 | 12456 | 22264 | 3196 |         |       |

- Molecule 82 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|------|-----|---------|-------|
| 82  | B3    | 163      | Total | C    | H    | N   | O    | P   | 0       | 0     |
|     |       |          | 5243  | 1555 | 1763 | 627 | 1135 | 163 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| B3    | 85      | U        | C      | conflict | GB 1782605526 |

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 83  | h1    | 73       | Total<br>73 | Mg<br>73 | 0       |
| 83  | S1    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 83  | U1    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 83  | B1    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 83  | C3    | 4        | Total<br>4  | Mg<br>4  | 0       |
| 83  | V3    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 83  | e3    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 83  | j3    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 83  | q3    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 83  | r3    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 83  | A3    | 49       | Total<br>49 | Mg<br>49 | 0       |

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

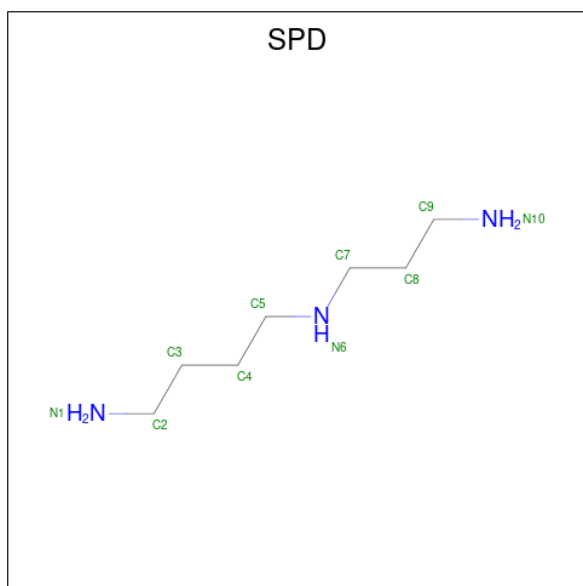
| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 84  | h1    | 42       | Total<br>42 | K<br>42 | 0       |
| 84  | S1    | 1        | Total<br>1  | K<br>1  | 0       |
| 84  | T1    | 1        | Total<br>1  | K<br>1  | 0       |
| 84  | U1    | 1        | Total<br>1  | K<br>1  | 0       |
| 84  | V1    | 1        | Total<br>1  | K<br>1  | 0       |
| 84  | W1    | 1        | Total<br>1  | K<br>1  | 0       |
| 84  | D3    | 1        | Total<br>1  | K<br>1  | 0       |
| 84  | R3    | 1        | Total<br>1  | K<br>1  | 0       |
| 84  | T3    | 1        | Total<br>1  | K<br>1  | 0       |

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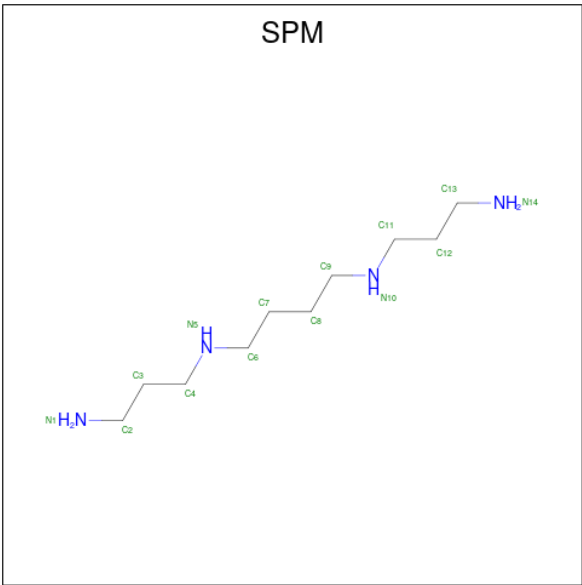
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 84  | Z3    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 84  | f3    | 2        | Total | K  | 0       |
|     |       |          | 2     | 2  |         |
| 84  | g3    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 84  | o3    | 2        | Total | K  | 0       |
|     |       |          | 2     | 2  |         |
| 84  | r3    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 84  | A3    | 83       | Total | K  | 0       |
|     |       |          | 83    | 83 |         |
| 84  | B3    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 85  | h1    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 85  | A3    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 86 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 86  | h1    | 1        | Total | C  | H  | N | 0       |
|     |       |          | 40    | 10 | 26 | 4 |         |
| 86  | h1    | 1        | Total | C  | H  | N | 0       |
|     |       |          | 40    | 10 | 26 | 4 |         |
| 86  | h1    | 1        | Total | C  | H  | N | 0       |
|     |       |          | 40    | 10 | 26 | 4 |         |
| 86  | A3    | 1        | Total | C  | H  | N | 0       |
|     |       |          | 40    | 10 | 26 | 4 |         |
| 86  | A3    | 1        | Total | C  | H  | N | 0       |
|     |       |          | 40    | 10 | 26 | 4 |         |

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 87  | J1    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | N1    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | V1    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | V3    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | Y3    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | Z3    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | a3    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 88 is water.

| Mol | Chain | Residues | Atoms         |           | AltConf |
|-----|-------|----------|---------------|-----------|---------|
| 88  | A1    | 7        | Total<br>7    | O<br>7    | 0       |
| 88  | k1    | 5        | Total<br>5    | O<br>5    | 0       |
| 88  | h1    | 2039     | Total<br>2039 | O<br>2039 | 0       |
| 88  | E1    | 12       | Total<br>12   | O<br>12   | 0       |
| 88  | F1    | 13       | Total<br>13   | O<br>13   | 0       |
| 88  | I1    | 1        | Total<br>1    | O<br>1    | 0       |
| 88  | J1    | 25       | Total<br>25   | O<br>25   | 0       |
| 88  | K1    | 6        | Total<br>6    | O<br>6    | 0       |
| 88  | M1    | 1        | Total<br>1    | O<br>1    | 0       |
| 88  | O1    | 1        | Total<br>1    | O<br>1    | 0       |
| 88  | P1    | 20       | Total<br>20   | O<br>20   | 0       |
| 88  | R1    | 12       | Total<br>12   | O<br>12   | 0       |
| 88  | S1    | 32       | Total<br>32   | O<br>32   | 0       |
| 88  | T1    | 43       | Total<br>43   | O<br>43   | 0       |
| 88  | U1    | 7        | Total<br>7    | O<br>7    | 0       |
| 88  | V1    | 4        | Total<br>4    | O<br>4    | 0       |
| 88  | W1    | 20       | Total<br>20   | O<br>20   | 0       |
| 88  | X1    | 21       | Total<br>21   | O<br>21   | 0       |
| 88  | Y1    | 6        | Total<br>6    | O<br>6    | 0       |
| 88  | Z1    | 1        | Total<br>1    | O<br>1    | 0       |
| 88  | b1    | 11       | Total<br>11   | O<br>11   | 0       |

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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 88  | c1    | 12       | Total<br>12  | O<br>12  | 0       |
| 88  | d1    | 12       | Total<br>12  | O<br>12  | 0       |
| 88  | e1    | 16       | Total<br>16  | O<br>16  | 0       |
| 88  | f1    | 10       | Total<br>10  | O<br>10  | 0       |
| 88  | B1    | 17       | Total<br>17  | O<br>17  | 0       |
| 88  | i2    | 7        | Total<br>7   | O<br>7   | 0       |
| 88  | W2    | 13       | Total<br>13  | O<br>13  | 0       |
| 88  | C3    | 91       | Total<br>91  | O<br>91  | 0       |
| 88  | D3    | 43       | Total<br>43  | O<br>43  | 0       |
| 88  | F3    | 105      | Total<br>105 | O<br>105 | 0       |
| 88  | G3    | 52       | Total<br>52  | O<br>52  | 0       |
| 88  | H3    | 10       | Total<br>10  | O<br>10  | 0       |
| 88  | I3    | 14       | Total<br>14  | O<br>14  | 0       |
| 88  | J3    | 27       | Total<br>27  | O<br>27  | 0       |
| 88  | M3    | 2        | Total<br>2   | O<br>2   | 0       |
| 88  | N3    | 10       | Total<br>10  | O<br>10  | 0       |
| 88  | O3    | 27       | Total<br>27  | O<br>27  | 0       |
| 88  | Q3    | 3        | Total<br>3   | O<br>3   | 0       |
| 88  | R3    | 42       | Total<br>42  | O<br>42  | 0       |
| 88  | S3    | 6        | Total<br>6   | O<br>6   | 0       |
| 88  | T3    | 14       | Total<br>14  | O<br>14  | 0       |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 88  | U3    | 4        | Total<br>4  | O<br>4  | 0       |
| 88  | V3    | 29       | Total<br>29 | O<br>29 | 0       |
| 88  | X3    | 7        | Total<br>7  | O<br>7  | 0       |
| 88  | Y3    | 2        | Total<br>2  | O<br>2  | 0       |
| 88  | p3    | 9        | Total<br>9  | O<br>9  | 0       |
| 88  | Z3    | 21       | Total<br>21 | O<br>21 | 0       |
| 88  | a3    | 6        | Total<br>6  | O<br>6  | 0       |
| 88  | b3    | 1        | Total<br>1  | O<br>1  | 0       |
| 88  | c3    | 10       | Total<br>10 | O<br>10 | 0       |
| 88  | d3    | 13       | Total<br>13 | O<br>13 | 0       |
| 88  | e3    | 12       | Total<br>12 | O<br>12 | 0       |
| 88  | f3    | 48       | Total<br>48 | O<br>48 | 0       |
| 88  | g3    | 16       | Total<br>16 | O<br>16 | 0       |
| 88  | h3    | 15       | Total<br>15 | O<br>15 | 0       |
| 88  | j3    | 16       | Total<br>16 | O<br>16 | 0       |
| 88  | k3    | 14       | Total<br>14 | O<br>14 | 0       |
| 88  | m3    | 9        | Total<br>9  | O<br>9  | 0       |
| 88  | n3    | 15       | Total<br>15 | O<br>15 | 0       |
| 88  | o3    | 56       | Total<br>56 | O<br>56 | 0       |
| 88  | q3    | 29       | Total<br>29 | O<br>29 | 0       |
| 88  | r3    | 27       | Total<br>27 | O<br>27 | 0       |

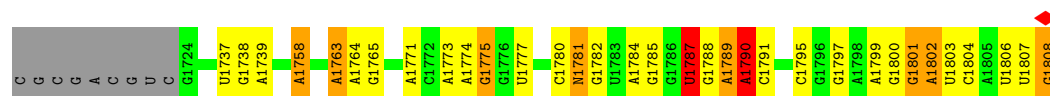
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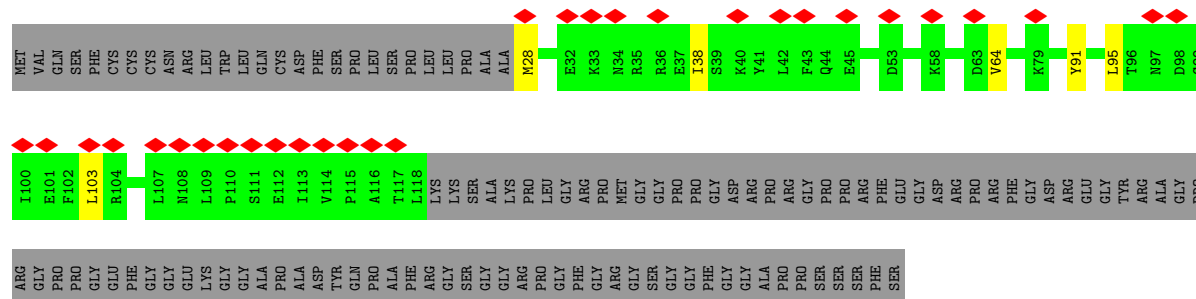
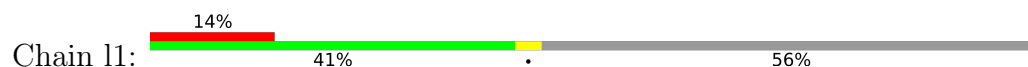
| Mol | Chain | Residues | Atoms         |           | AltConf |
|-----|-------|----------|---------------|-----------|---------|
| 88  | s3    | 65       | Total<br>65   | O<br>65   | 0       |
| 88  | t3    | 1        | Total<br>1    | O<br>1    | 0       |
| 88  | u3    | 2        | Total<br>2    | O<br>2    | 0       |
| 88  | A3    | 3383     | Total<br>3383 | O<br>3383 | 0       |
| 88  | B3    | 162      | Total<br>162  | O<br>162  | 0       |



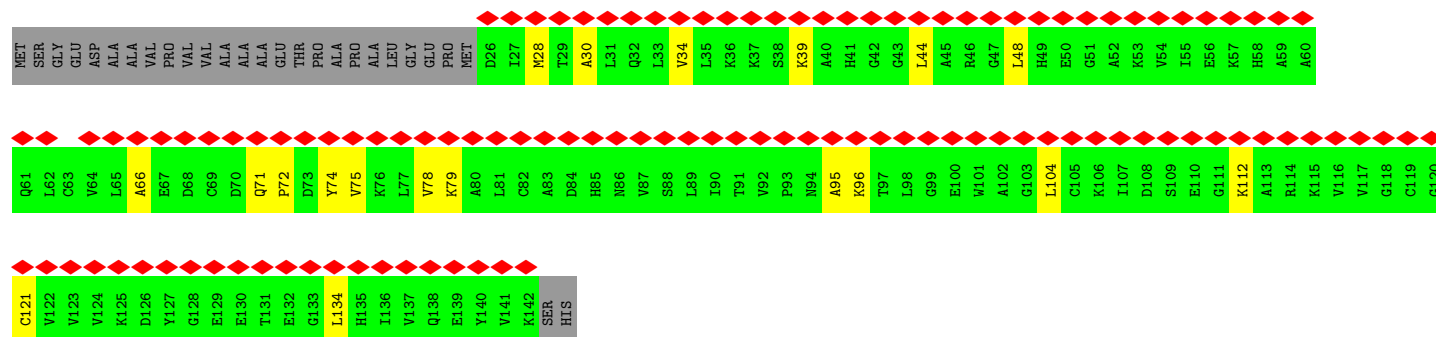
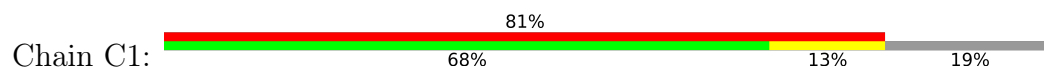




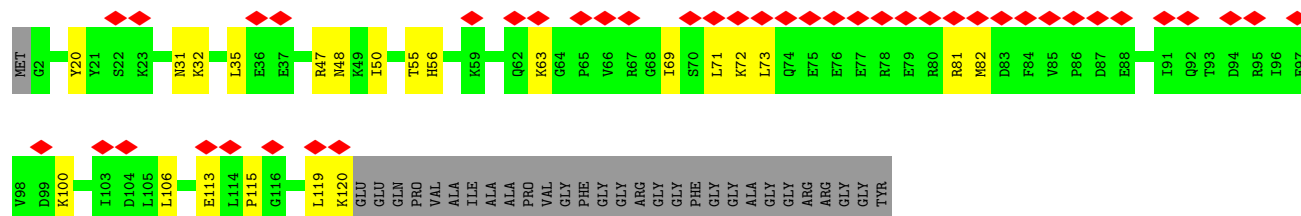
• Molecule 4: 40S ribosomal protein S10-1-like



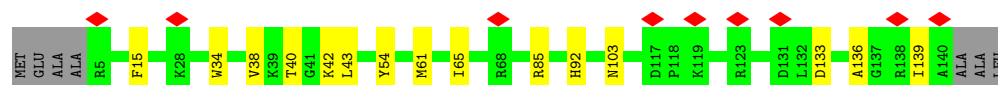
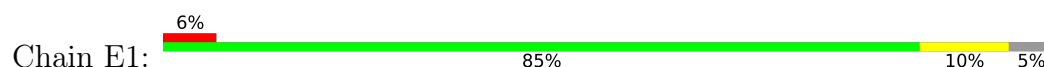
• Molecule 5: 40S ribosomal protein S12



• Molecule 6: 40S ribosomal protein S17-like



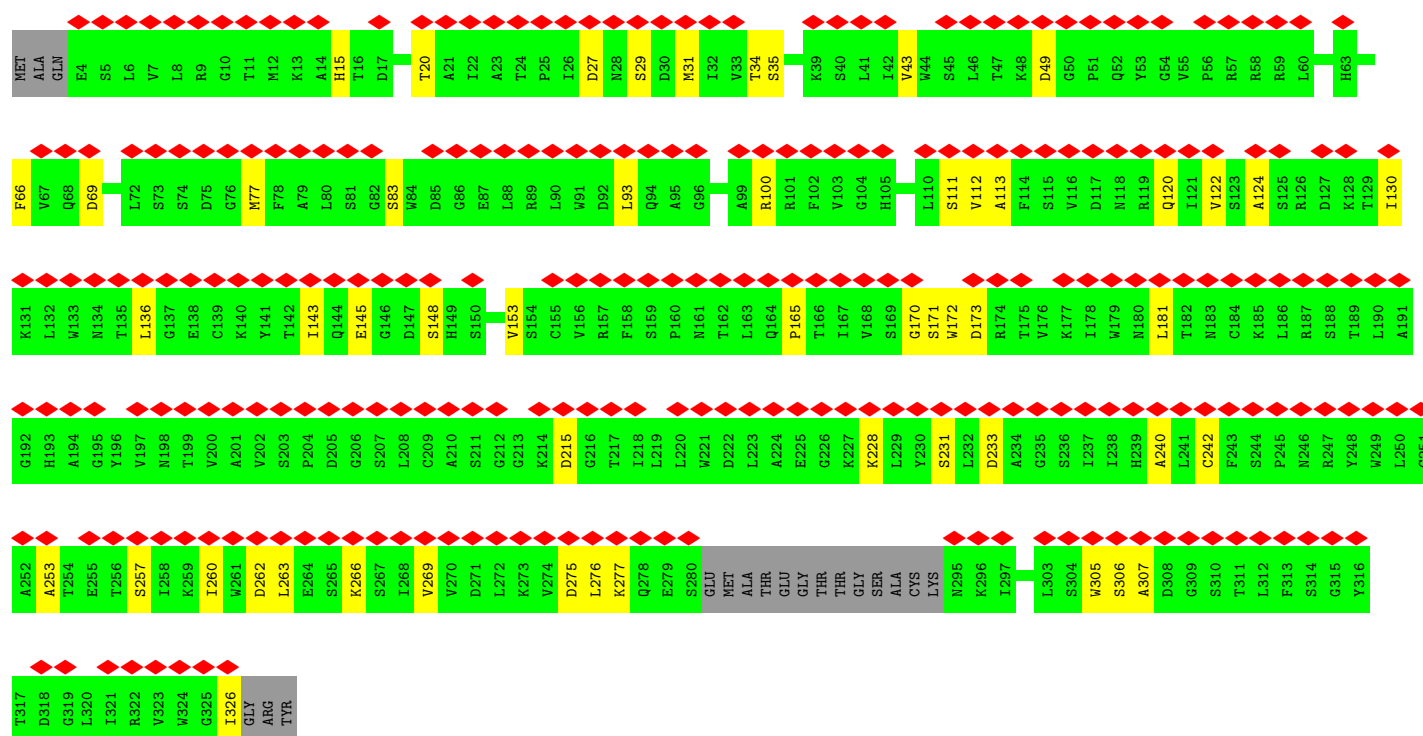
• Molecule 7: 40S ribosomal protein S19-3





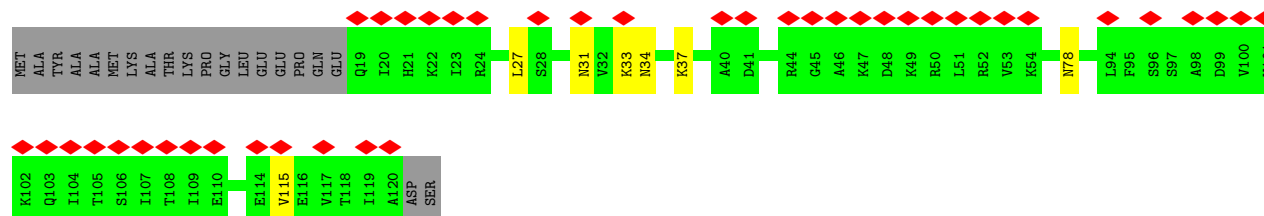


Chain Q1: 



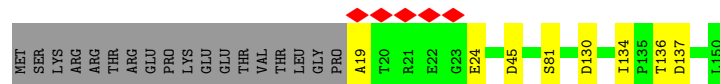
- Molecule 20: 40S ribosomal protein S20-2

Chain R1: 

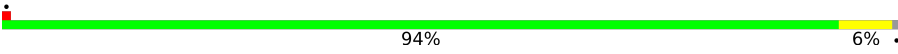


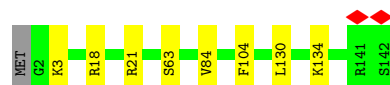
- Molecule 21: 40S ribosomal protein S14-2

Chain S1: 

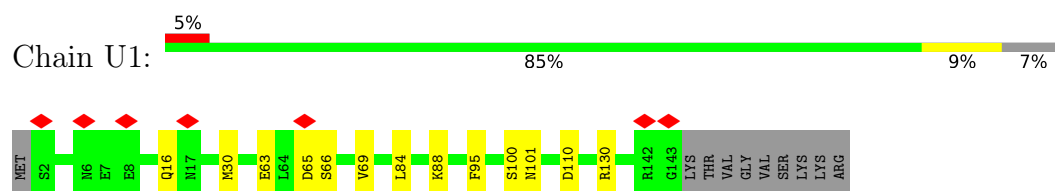


- Molecule 22: 40S ribosomal protein S23

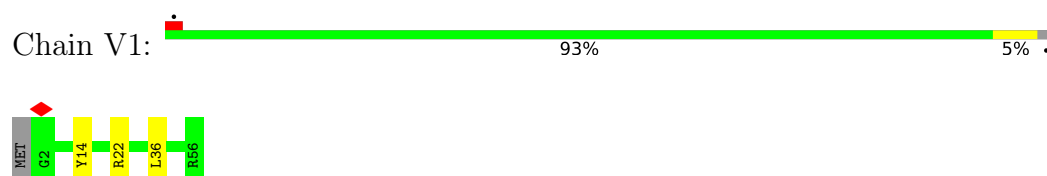
Chain T1: 



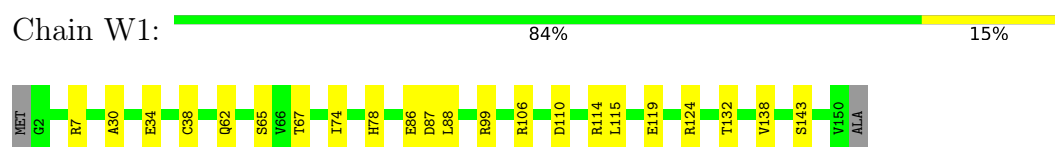
- Molecule 23: 40S ribosomal protein S18



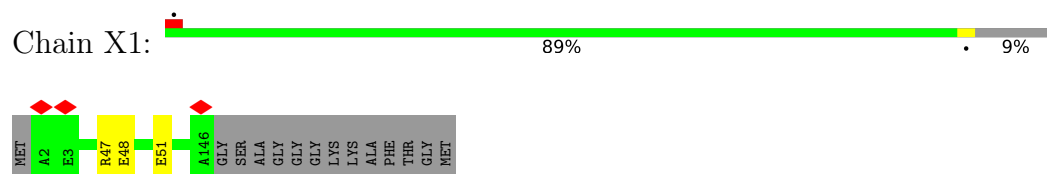
- Molecule 24: 40S ribosomal protein S29



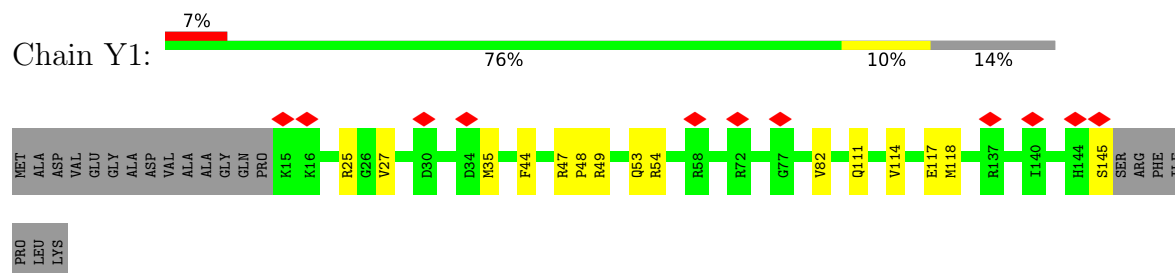
- Molecule 25: 30S ribosomal protein S15, chloroplastic



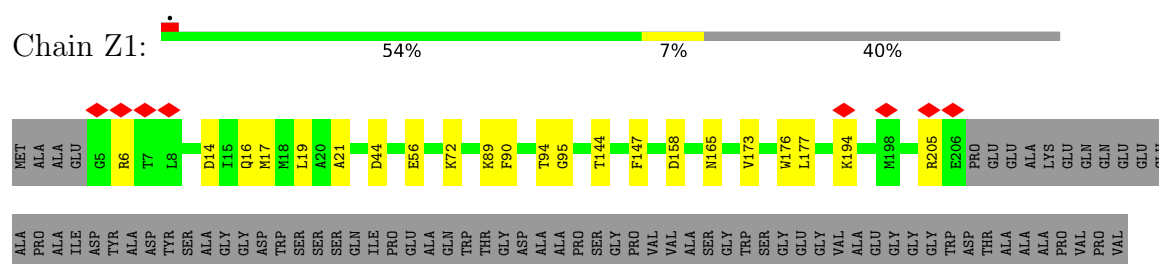
- Molecule 26: 40S ribosomal protein S11-like



- Molecule 27: 40S ribosomal protein S15-like

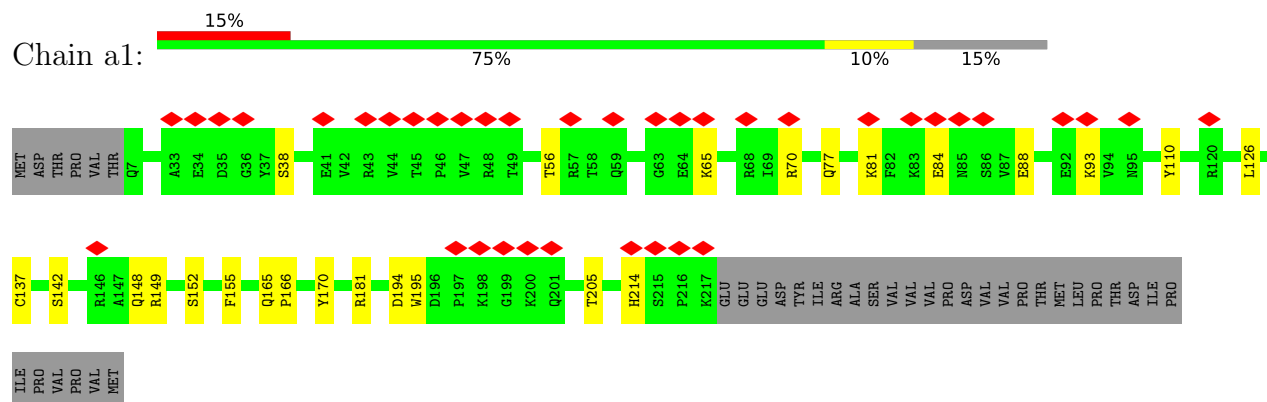


- Molecule 28: 40S ribosomal protein SA

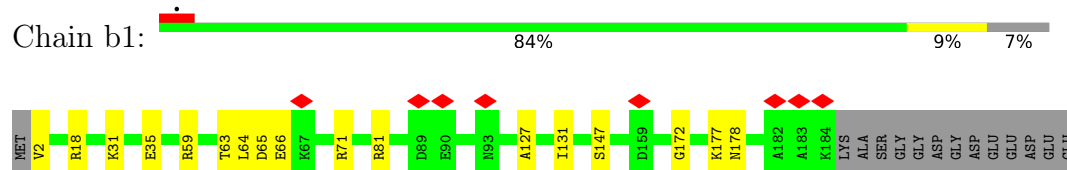


PRO VAL ASP THR SER ASP PRO VAL ALA ALA PRO THR ALA GLY GLY GLY TRP ASP THR ALA ALA ALA PRO VAL PRO VAL PRO VAL SER ASP ALA ALA ALA PRO THR THR GLY TRP GLU

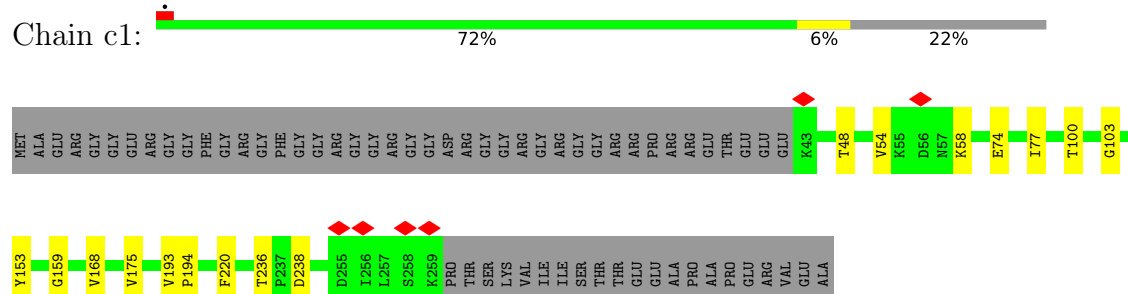
• Molecule 29: 40S ribosomal protein S3-2-like



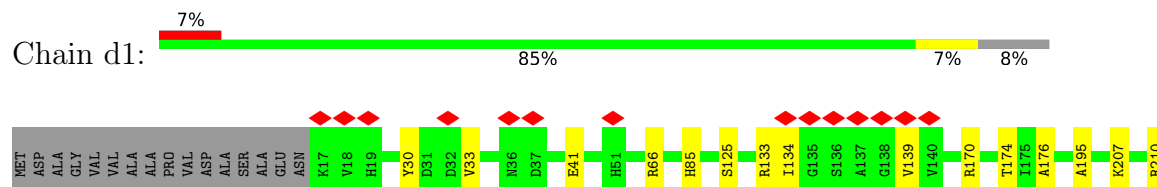
• Molecule 30: 40S ribosomal protein S9-2-like



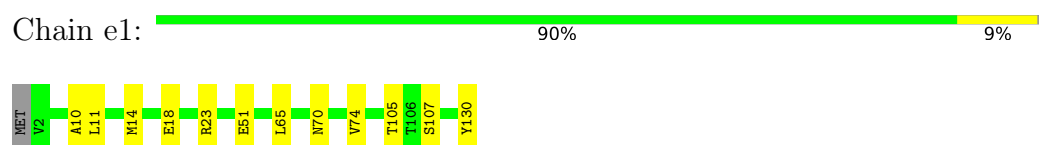
• Molecule 31: 40S ribosomal protein S2-3-like



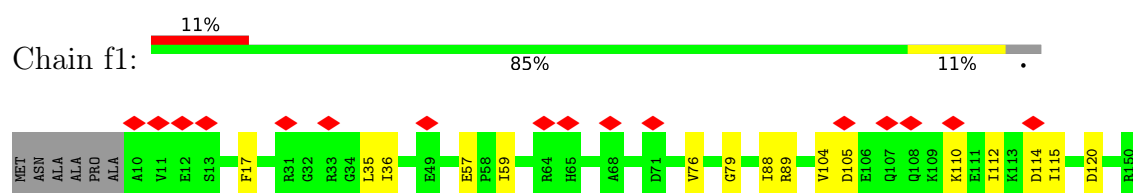
• Molecule 32: 40S ribosomal protein S5-like



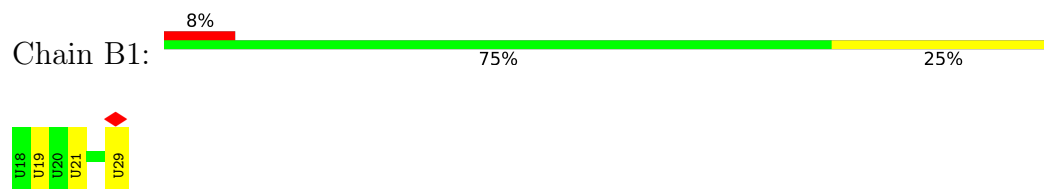
• Molecule 33: 40S ribosomal protein S15a-1



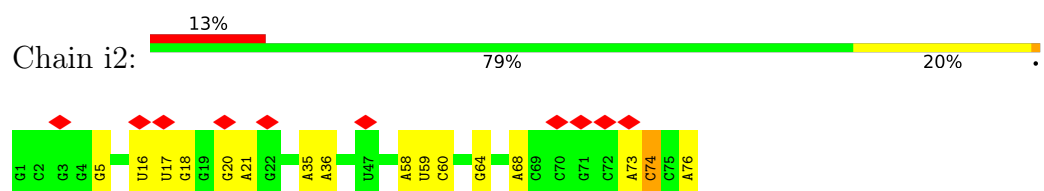
• Molecule 34: 40S ribosomal protein S16



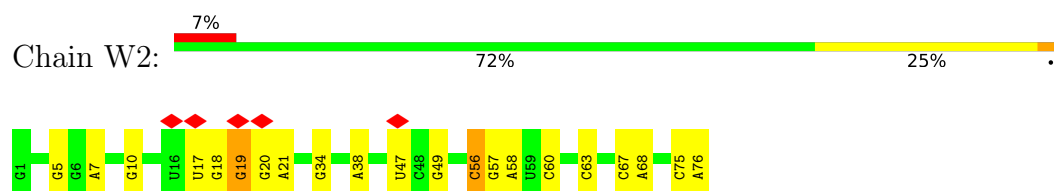
- Molecule 35: mRNA



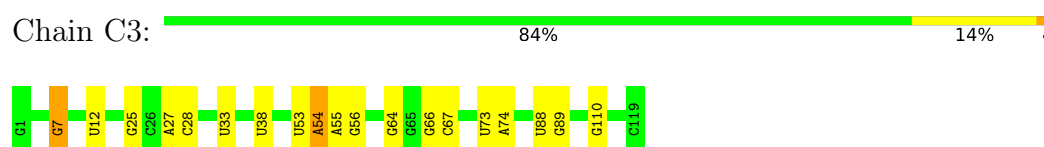
- Molecule 36: tRNA



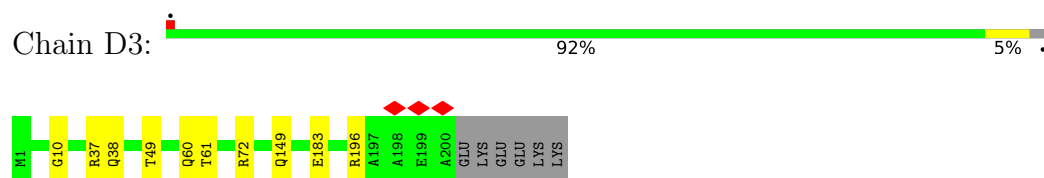
- Molecule 36: tRNA



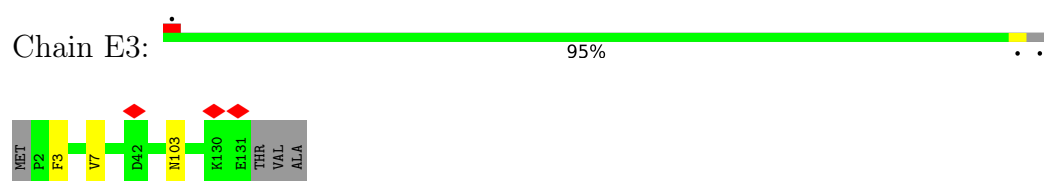
- Molecule 37: 5S rRNA



- Molecule 38: 60S ribosomal protein L13



- Molecule 39: 60S ribosomal protein L14-1

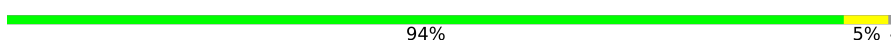


- Molecule 40: Ribosomal protein L15

Chain F3:  91% 9%



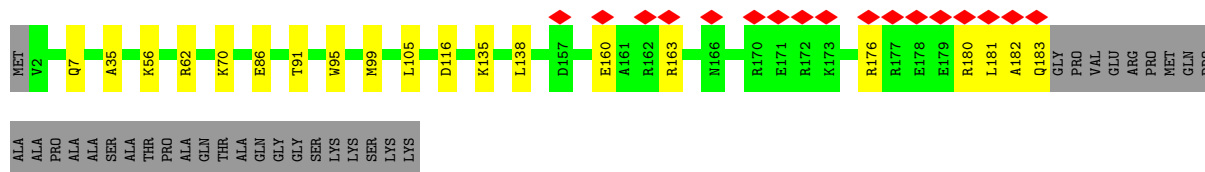
- Molecule 41: 60S ribosomal protein L18-2-like

Chain G3:  94% 5%

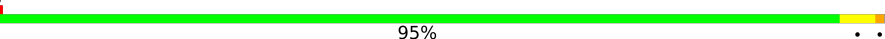


- Molecule 42: Ribosomal protein L19

Chain H3:  8% 76% 9% 15%



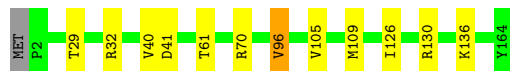
- Molecule 43: 60S ribosomal protein L18a

Chain I3:  95% 5% 2%



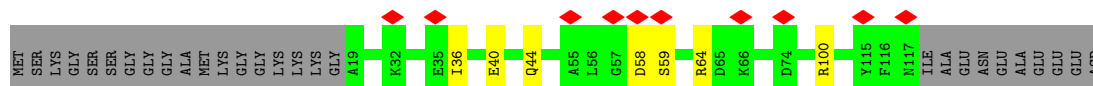
- Molecule 44: 60S ribosomal protein L21-1-like

Chain J3:  92% 7% 1%



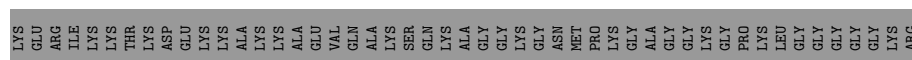
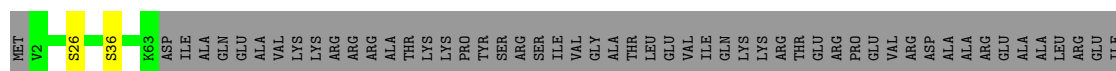
- Molecule 45: 60S ribosomal protein L22-2-like

Chain K3:  8% 72% 6% 22%



- Molecule 46: 60S ribosomal protein L24-like

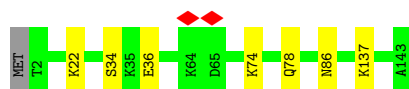
Chain L3:  37% 62%



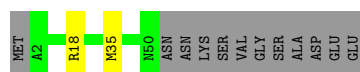
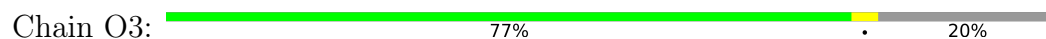
- Molecule 47: eL27 (60S ribosomal protein L27)



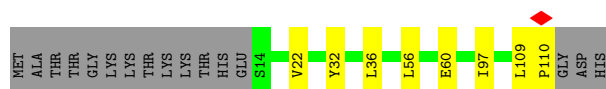
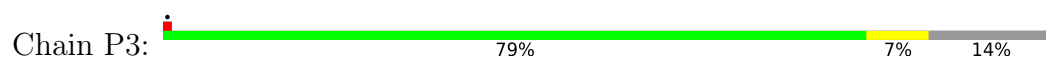
- Molecule 48: eL28 (60S ribosomal protein L28)



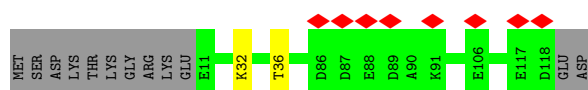
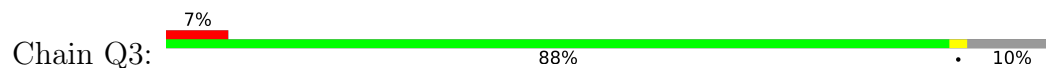
- Molecule 49: 60S ribosomal protein L29



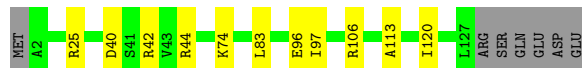
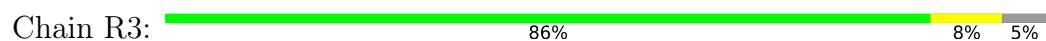
- Molecule 50: 60S ribosomal protein L30-like



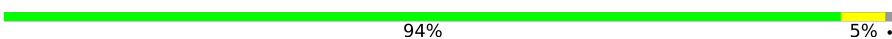
- Molecule 51: eL31 (60S ribosomal protein L31)



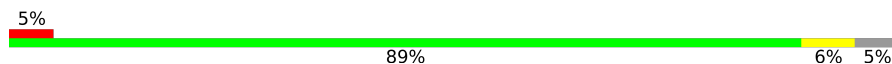
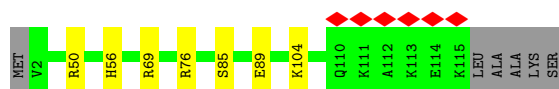
- Molecule 52: 60S ribosomal protein L32-1



## • Molecule 53: eL33 (60S ribosomal protein L35a)

Chain S3:  94% 5%

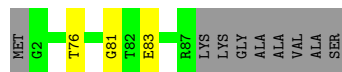
## • Molecule 54: 60S ribosomal protein L34

Chain T3:  5% 89% 6% 5%

## • Molecule 55: eL36 (60S ribosomal protein L36)

Chain U3:  87% 11%

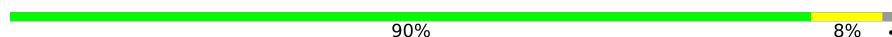
## • Molecule 56: Ribosomal protein L37

Chain V3:  87% 9%

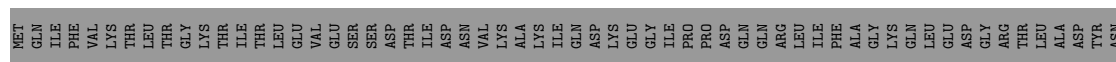
## • Molecule 57: 60S ribosomal protein L38

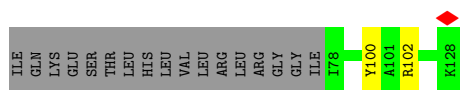
Chain W3:  84% 13%

## • Molecule 58: 60S ribosomal protein L39-3

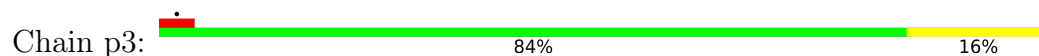
Chain X3:  90% 8%

## • Molecule 59: ubiquitin-60S ribosomal protein L40

Chain Y3:  38% 60%



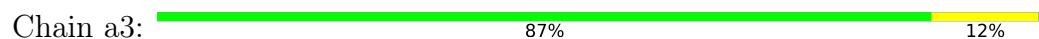
- Molecule 60: 60S ribosomal protein L41



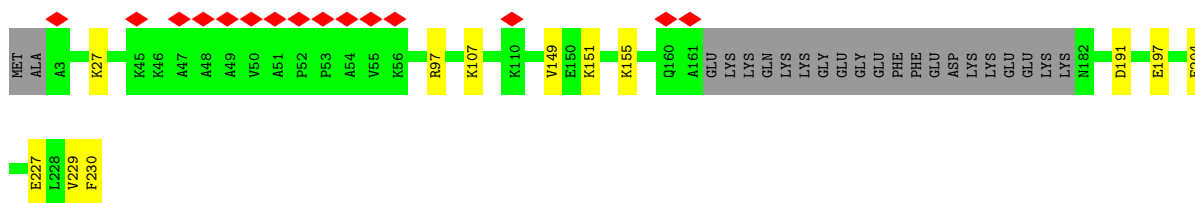
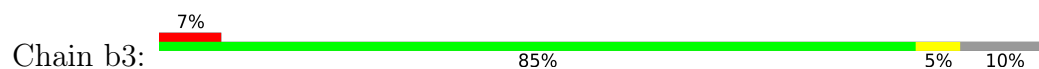
- Molecule 61: 60S ribosomal protein L44



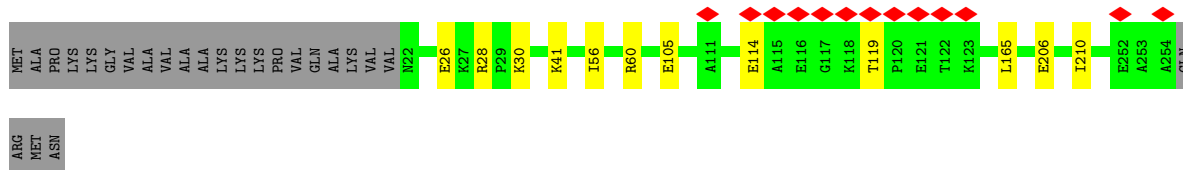
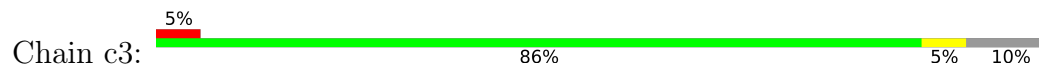
- Molecule 62: 60S ribosomal protein L37a



- Molecule 63: eL6 (60S ribosomal protein L6)



- Molecule 64: 60S ribosomal protein L7a

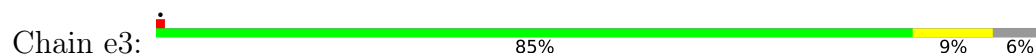


- Molecule 65: uL13 (60S ribosomal protein L13a)





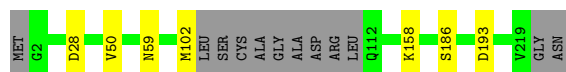
- Molecule 66: 60S ribosomal protein L23



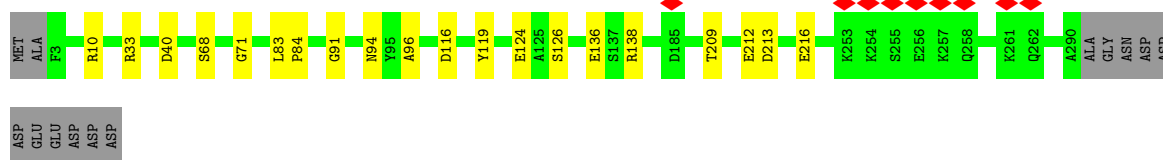
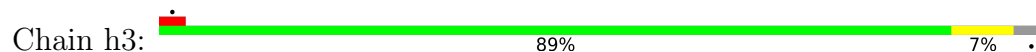
- Molecule 67: uL15 (60S ribosomal protein L27a)



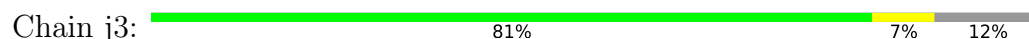
- Molecule 68: uL16 (60S ribosomal protein L10)



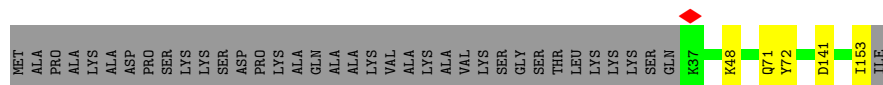
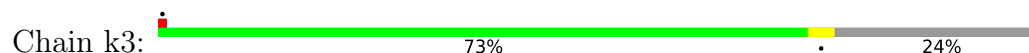
- Molecule 69: 60S ribosomal protein L5-like



- Molecule 70: 50S ribosomal protein L22, chloroplastic



- Molecule 71: 60S ribosomal protein L23a



- Molecule 72: uL24 (60S ribosomal protein L26)

Chain m3:  79% 6% 14%



- Molecule 73: 60S ribosomal protein L35-like

Chain n3:  92% 7%



- Molecule 74: uL2 (60S ribosomal protein L8)

Chain o3:  91% 6%



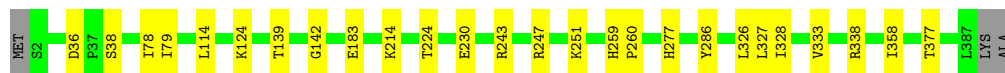
- Molecule 75: 60S ribosomal protein L7-4-like

Chain q3:  92% 6%



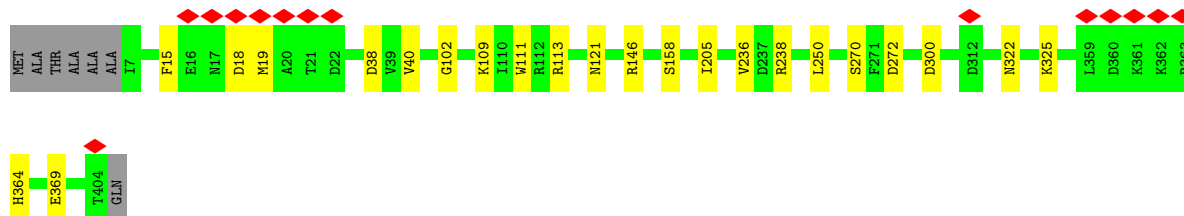
- Molecule 76: uL3 (60S ribosomal protein L3)

Chain r3:  93% 7%



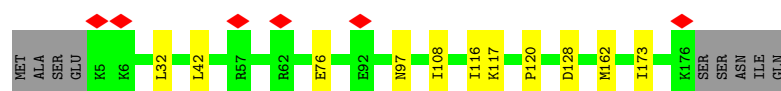
- Molecule 77: uL4 (60S ribosomal protein L4)

Chain s3:  93% 6%



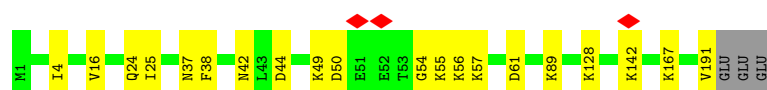
- Molecule 78: uL5 (60S ribosomal protein L11)

Chain t3:  89% 6% 5%



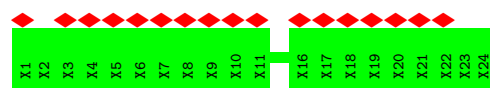
- Molecule 79: uL6 (60S ribosomal protein L9)

Chain u3:  88% 10% 2%



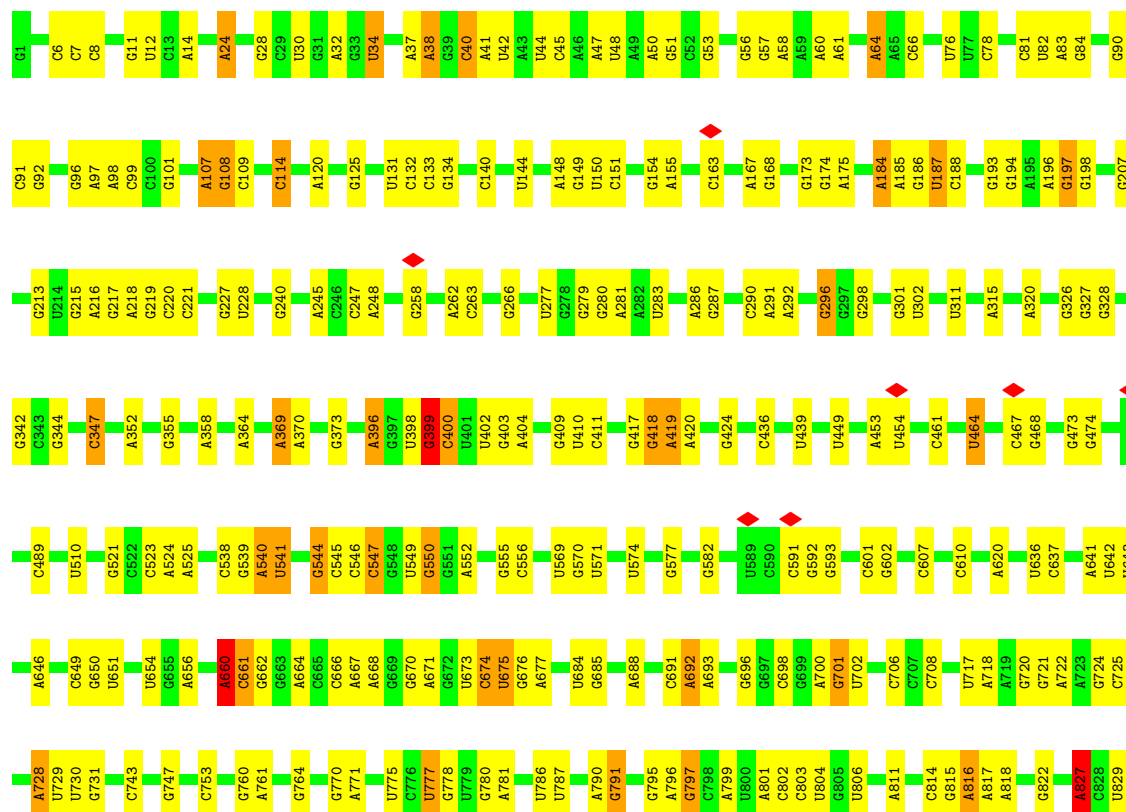
- Molecule 80: nascent chain

Chain l3:  71% 100%

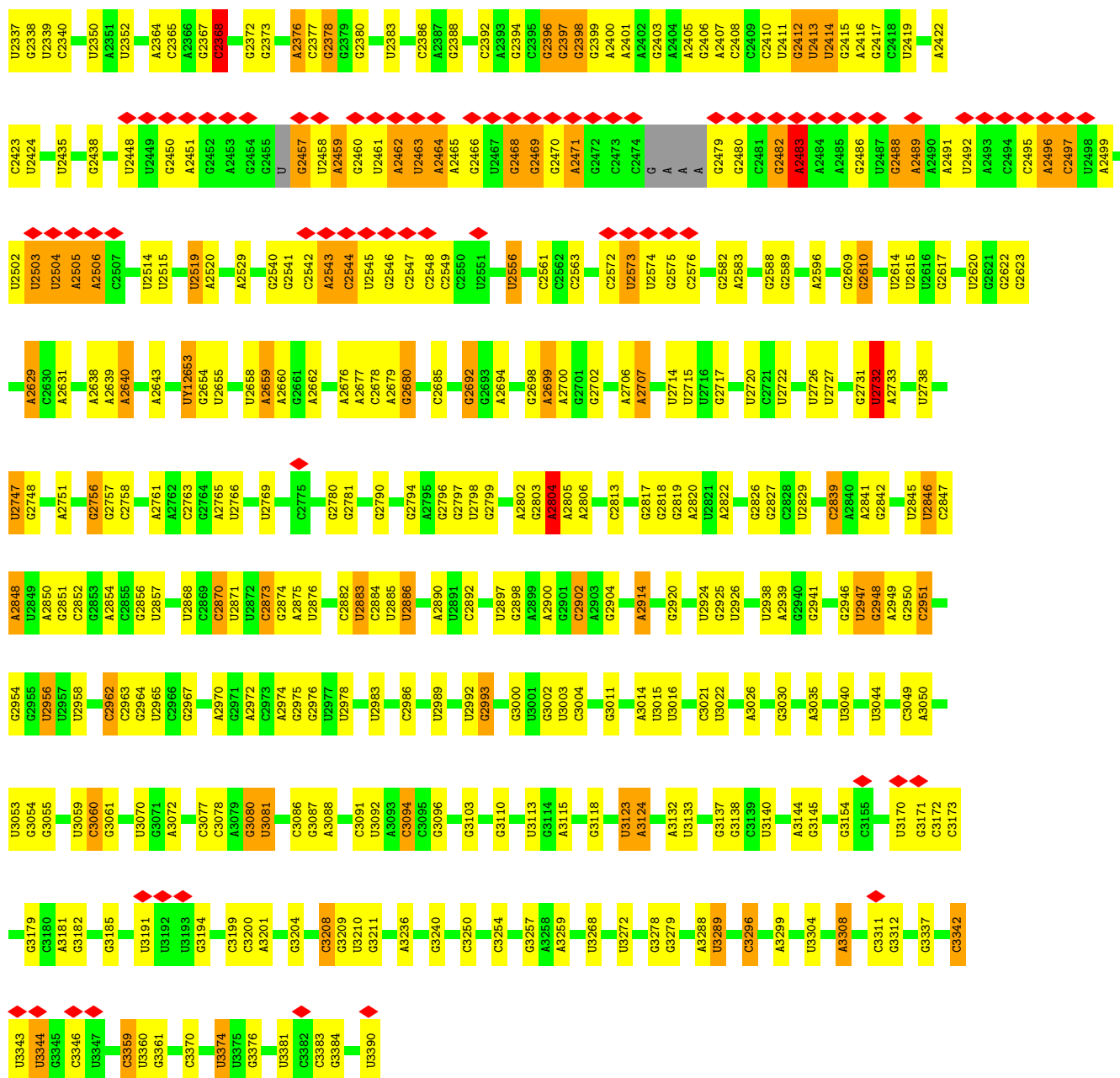


- Molecule 81: 25S rRNA

Chain A3:  64% 25% 6%

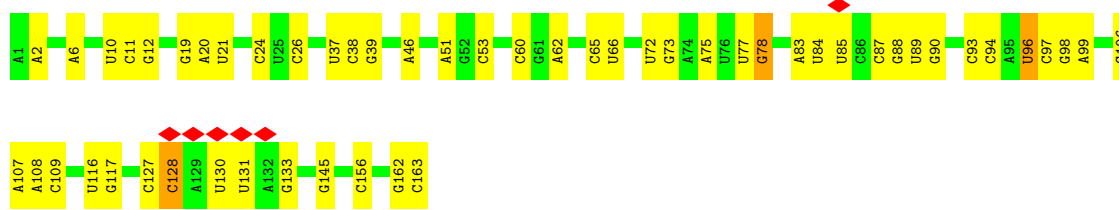






### • Molecule 82: 5.8S rRNA

Chain B3: 67% 31%



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 335291              | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 27                  | Depositor |
| Minimum defocus (nm)                 | 1000                | Depositor |
| Maximum defocus (nm)                 | 2500                | Depositor |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 14.499              | Depositor |
| Minimum map value                    | -6.970              | Depositor |
| Average map value                    | 0.031               | Depositor |
| Map value standard deviation         | 0.323               | Depositor |
| Recommended contour level            | 0.6                 | Depositor |
| Map size ( $\text{\AA}$ )            | 381.6, 381.6, 381.6 | wwPDB     |
| Map dimensions                       | 450, 450, 450       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.848, 0.848, 0.848 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMU, 1MA, MA6, B8N, A2M, PSU, UY1, K, UR3, SPD, OMC, ZN, 5MC, 6MZ, 4AC, OMG, SPM

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   | A1    | 0.11         | 0/2114         | 0.27        | 0/2837      |
| 2   | k1    | 0.12         | 0/1875         | 0.30        | 0/2494      |
| 3   | h1    | 0.14         | 1/36945 (0.0%) | 0.23        | 0/57563     |
| 4   | l1    | 0.11         | 0/794          | 0.25        | 0/1074      |
| 5   | C1    | 0.14         | 0/889          | 0.37        | 0/1198      |
| 6   | D1    | 0.15         | 0/973          | 0.31        | 0/1299      |
| 7   | E1    | 0.12         | 0/1103         | 0.24        | 0/1480      |
| 8   | F1    | 0.10         | 0/1790         | 0.26        | 0/2402      |
| 9   | G1    | 0.10         | 0/662          | 0.25        | 0/891       |
| 10  | H1    | 0.11         | 0/1049         | 0.26        | 0/1391      |
| 11  | I1    | 0.10         | 0/589          | 0.24        | 0/789       |
| 12  | J1    | 0.12         | 0/805          | 0.26        | 0/1076      |
| 13  | K1    | 0.13         | 0/662          | 0.25        | 0/892       |
| 14  | L1    | 0.13         | 0/496          | 0.32        | 0/661       |
| 15  | M1    | 0.15         | 0/414          | 0.26        | 0/544       |
| 16  | N1    | 0.14         | 0/574          | 0.29        | 0/763       |
| 17  | O1    | 0.14         | 0/1560         | 0.33        | 0/2097      |
| 18  | P1    | 0.12         | 0/1535         | 0.28        | 0/2050      |
| 19  | Q1    | 0.12         | 0/2446         | 0.33        | 0/3324      |
| 20  | R1    | 0.12         | 0/813          | 0.26        | 0/1095      |
| 21  | S1    | 0.12         | 0/1010         | 0.27        | 0/1352      |
| 22  | T1    | 0.12         | 0/1119         | 0.25        | 0/1487      |
| 23  | U1    | 0.12         | 0/1170         | 0.28        | 0/1562      |
| 24  | V1    | 0.14         | 0/453          | 0.23        | 0/605       |
| 25  | W1    | 0.13         | 0/1214         | 0.26        | 0/1632      |
| 26  | X1    | 0.11         | 0/1180         | 0.27        | 0/1579      |
| 27  | Y1    | 0.12         | 0/1084         | 0.27        | 0/1450      |
| 28  | Z1    | 0.14         | 0/1644         | 0.30        | 0/2223      |
| 29  | a1    | 0.13         | 0/1684         | 0.30        | 0/2257      |
| 30  | b1    | 0.10         | 0/1550         | 0.23        | 0/2073      |
| 31  | c1    | 0.11         | 0/1721         | 0.29        | 0/2320      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 32  | d1    | 0.11         | 0/1553  | 0.28        | 0/2095  |
| 33  | e1    | 0.11         | 0/1050  | 0.26        | 0/1405  |
| 34  | f1    | 0.12         | 0/1154  | 0.27        | 0/1542  |
| 35  | B1    | 0.07         | 0/263   | 0.20        | 0/404   |
| 36  | W2    | 0.10         | 0/1822  | 0.24        | 0/2840  |
| 36  | i2    | 0.08         | 0/1823  | 0.23        | 0/2840  |
| 37  | C3    | 0.08         | 0/2837  | 0.22        | 0/4420  |
| 38  | D3    | 0.10         | 0/1635  | 0.25        | 0/2194  |
| 39  | E3    | 0.09         | 0/1069  | 0.23        | 0/1427  |
| 40  | F3    | 0.13         | 0/1740  | 0.30        | 0/2333  |
| 41  | G3    | 0.12         | 0/1487  | 0.27        | 0/1989  |
| 42  | H3    | 0.11         | 0/1548  | 0.28        | 0/2042  |
| 43  | I3    | 0.10         | 0/1544  | 0.25        | 0/2071  |
| 44  | J3    | 0.09         | 0/1331  | 0.25        | 0/1784  |
| 45  | K3    | 0.11         | 0/819   | 0.27        | 0/1098  |
| 46  | L3    | 0.12         | 0/539   | 0.26        | 0/716   |
| 47  | M3    | 0.11         | 0/1118  | 0.24        | 0/1492  |
| 48  | N3    | 0.11         | 0/1126  | 0.29        | 0/1508  |
| 49  | O3    | 0.13         | 0/422   | 0.31        | 0/558   |
| 50  | P3    | 0.14         | 0/757   | 0.29        | 0/1018  |
| 51  | Q3    | 0.13         | 0/885   | 0.30        | 0/1184  |
| 52  | R3    | 0.11         | 0/1053  | 0.27        | 0/1408  |
| 53  | S3    | 0.11         | 0/920   | 0.26        | 0/1232  |
| 54  | T3    | 0.10         | 0/939   | 0.24        | 0/1251  |
| 55  | U3    | 0.11         | 0/791   | 0.25        | 0/1047  |
| 56  | V3    | 0.14         | 0/714   | 0.29        | 0/949   |
| 57  | W3    | 0.16         | 0/566   | 0.36        | 0/752   |
| 58  | X3    | 0.09         | 0/460   | 0.21        | 0/611   |
| 59  | Y3    | 0.12         | 0/427   | 0.27        | 0/562   |
| 60  | p3    | 0.12         | 0/239   | 0.32        | 0/302   |
| 61  | Z3    | 0.12         | 0/801   | 0.23        | 0/1058  |
| 62  | a3    | 0.11         | 0/717   | 0.25        | 0/952   |
| 63  | b3    | 0.12         | 0/1645  | 0.28        | 0/2210  |
| 64  | c3    | 0.12         | 0/1912  | 0.27        | 0/2562  |
| 65  | d3    | 0.12         | 0/1669  | 0.26        | 0/2235  |
| 66  | e3    | 0.11         | 0/1001  | 0.29        | 0/1345  |
| 67  | f3    | 0.13         | 0/1190  | 0.30        | 0/1591  |
| 68  | g3    | 0.11         | 0/1707  | 0.26        | 0/2283  |
| 69  | h3    | 0.11         | 0/2386  | 0.28        | 0/3200  |
| 70  | j3    | 0.12         | 0/1270  | 0.32        | 0/1704  |
| 71  | k3    | 0.10         | 0/965   | 0.25        | 0/1295  |
| 72  | m3    | 0.09         | 0/1035  | 0.26        | 0/1383  |
| 73  | n3    | 0.11         | 0/1009  | 0.22        | 0/1343  |

| Mol | Chain | Bond lengths |                 | Bond angles |          |
|-----|-------|--------------|-----------------|-------------|----------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5  |
| 74  | o3    | 0.11         | 0/1924          | 0.30        | 0/2585   |
| 75  | q3    | 0.14         | 0/1992          | 0.29        | 0/2670   |
| 76  | r3    | 0.10         | 0/3172          | 0.28        | 0/4249   |
| 77  | s3    | 0.10         | 0/3159          | 0.26        | 0/4259   |
| 78  | t3    | 0.12         | 0/1414          | 0.30        | 0/1890   |
| 79  | u3    | 0.10         | 0/1539          | 0.29        | 0/2059   |
| 81  | A3    | 0.15         | 4/73585 (0.0%)  | 0.26        | 0/114781 |
| 82  | B3    | 0.13         | 1/3772 (0.0%)   | 0.26        | 0/5878   |
| All | All   | 0.13         | 6/212412 (0.0%) | 0.26        | 0/311066 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 81  | A3    | 675  | OMU  | O3'-P  | 5.26  | 1.61        | 1.56     |
| 81  | A3    | 2284 | A2M  | O3'-P  | 5.11  | 1.61        | 1.56     |
| 82  | B3    | 46   | A2M  | O3'-P  | 5.10  | 1.61        | 1.56     |
| 81  | A3    | 2483 | A    | C1'-N9 | -5.05 | 1.40        | 1.48     |
| 3   | h1    | 440  | A2M  | O3'-P  | 5.03  | 1.61        | 1.56     |
| 81  | A3    | 2949 | A2M  | O3'-P  | 5.00  | 1.61        | 1.56     |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A1    | 2074  | 2180     | 2181     | 14      | 0            |
| 2   | k1    | 1851  | 1965     | 1969     | 19      | 0            |
| 3   | h1    | 34741 | 17529    | 17528    | 280     | 0            |
| 4   | l1    | 773   | 776      | 776      | 4       | 0            |
| 5   | C1    | 878   | 900      | 905      | 15      | 0            |
| 6   | D1    | 963   | 1026     | 1025     | 18      | 0            |
| 7   | E1    | 1081  | 1091     | 1091     | 11      | 0            |
| 8   | F1    | 1760  | 1818     | 1820     | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | G1    | 652   | 643      | 645      | 2       | 0            |
| 10  | H1    | 1034  | 1111     | 1110     | 4       | 0            |
| 11  | I1    | 583   | 621      | 620      | 2       | 0            |
| 12  | J1    | 792   | 818      | 820      | 5       | 0            |
| 13  | K1    | 651   | 656      | 661      | 7       | 0            |
| 14  | L1    | 493   | 525      | 524      | 7       | 0            |
| 15  | M1    | 409   | 442      | 440      | 2       | 0            |
| 16  | N1    | 562   | 581      | 580      | 3       | 0            |
| 17  | O1    | 1534  | 1591     | 1590     | 22      | 0            |
| 18  | P1    | 1511  | 1570     | 1570     | 18      | 0            |
| 19  | Q1    | 2394  | 2362     | 2368     | 38      | 0            |
| 20  | R1    | 804   | 864      | 865      | 6       | 0            |
| 21  | S1    | 998   | 1028     | 1028     | 7       | 0            |
| 22  | T1    | 1100  | 1164     | 1165     | 6       | 0            |
| 23  | U1    | 1153  | 1184     | 1184     | 10      | 0            |
| 24  | V1    | 441   | 430      | 430      | 3       | 0            |
| 25  | W1    | 1189  | 1278     | 1277     | 15      | 0            |
| 26  | X1    | 1155  | 1207     | 1210     | 2       | 0            |
| 27  | Y1    | 1061  | 1132     | 1131     | 10      | 0            |
| 28  | Z1    | 1610  | 1623     | 1624     | 17      | 0            |
| 29  | a1    | 1661  | 1752     | 1754     | 17      | 0            |
| 30  | b1    | 1523  | 1595     | 1595     | 12      | 0            |
| 31  | c1    | 1686  | 1786     | 1789     | 8       | 0            |
| 32  | d1    | 1531  | 1572     | 1573     | 9       | 0            |
| 33  | e1    | 1032  | 1068     | 1068     | 8       | 0            |
| 34  | f1    | 1135  | 1197     | 1198     | 10      | 0            |
| 35  | B1    | 240   | 120      | 121      | 2       | 0            |
| 36  | W2    | 1629  | 822      | 823      | 23      | 0            |
| 36  | i2    | 1630  | 822      | 823      | 9       | 0            |
| 37  | C3    | 2538  | 1285     | 1285     | 10      | 0            |
| 38  | D3    | 1605  | 1691     | 1691     | 7       | 0            |
| 39  | E3    | 1056  | 1150     | 1150     | 2       | 0            |
| 40  | F3    | 1701  | 1768     | 1769     | 13      | 0            |
| 41  | G3    | 1462  | 1580     | 1581     | 7       | 0            |
| 42  | H3    | 1529  | 1652     | 1652     | 18      | 0            |
| 43  | I3    | 1505  | 1556     | 1557     | 7       | 0            |
| 44  | J3    | 1306  | 1366     | 1367     | 9       | 0            |
| 45  | K3    | 808   | 845      | 845      | 4       | 0            |
| 46  | L3    | 526   | 553      | 554      | 1       | 0            |
| 47  | M3    | 1099  | 1184     | 1184     | 6       | 0            |
| 48  | N3    | 1111  | 1187     | 1186     | 5       | 0            |
| 49  | O3    | 412   | 419      | 418      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 50  | P3    | 745   | 781      | 783      | 5       | 0            |
| 51  | Q3    | 875   | 934      | 934      | 1       | 0            |
| 52  | R3    | 1036  | 1115     | 1116     | 11      | 0            |
| 53  | S3    | 900   | 932      | 933      | 4       | 0            |
| 54  | T3    | 926   | 1013     | 1013     | 5       | 0            |
| 55  | U3    | 782   | 868      | 867      | 2       | 0            |
| 56  | V3    | 701   | 726      | 724      | 2       | 0            |
| 57  | W3    | 558   | 602      | 604      | 9       | 0            |
| 58  | X3    | 448   | 480      | 480      | 3       | 0            |
| 59  | Y3    | 421   | 460      | 459      | 2       | 0            |
| 60  | p3    | 238   | 289      | 289      | 3       | 0            |
| 61  | Z3    | 787   | 842      | 842      | 5       | 0            |
| 62  | a3    | 708   | 745      | 744      | 8       | 0            |
| 63  | b3    | 1611  | 1749     | 1749     | 10      | 0            |
| 64  | c3    | 1879  | 2028     | 2030     | 11      | 0            |
| 65  | d3    | 1640  | 1774     | 1776     | 8       | 0            |
| 66  | e3    | 985   | 1044     | 1046     | 8       | 0            |
| 67  | f3    | 1161  | 1200     | 1200     | 12      | 0            |
| 68  | g3    | 1671  | 1726     | 1731     | 5       | 0            |
| 69  | h3    | 2341  | 2374     | 2374     | 14      | 0            |
| 70  | j3    | 1245  | 1270     | 1272     | 7       | 0            |
| 71  | k3    | 950   | 1030     | 1029     | 5       | 0            |
| 72  | m3    | 1021  | 1103     | 1103     | 7       | 0            |
| 73  | n3    | 999   | 1141     | 1140     | 7       | 0            |
| 74  | o3    | 1880  | 1911     | 1915     | 8       | 0            |
| 75  | q3    | 1958  | 2058     | 2058     | 12      | 0            |
| 76  | r3    | 3104  | 3223     | 3229     | 17      | 0            |
| 77  | s3    | 3097  | 3227     | 3228     | 21      | 0            |
| 78  | t3    | 1392  | 1444     | 1446     | 9       | 0            |
| 79  | u3    | 1520  | 1604     | 1605     | 11      | 0            |
| 80  | l3    | 120   | 49       | 34       | 0       | 0            |
| 81  | A3    | 68518 | 34651    | 34634    | 525     | 0            |
| 82  | B3    | 3480  | 1763     | 1764     | 22      | 0            |
| 83  | A3    | 49    | 0        | 0        | 0       | 0            |
| 83  | B1    | 1     | 0        | 0        | 0       | 0            |
| 83  | C3    | 4     | 0        | 0        | 0       | 0            |
| 83  | S1    | 1     | 0        | 0        | 0       | 0            |
| 83  | U1    | 1     | 0        | 0        | 0       | 0            |
| 83  | V3    | 1     | 0        | 0        | 0       | 0            |
| 83  | e3    | 1     | 0        | 0        | 0       | 0            |
| 83  | h1    | 73    | 0        | 0        | 0       | 0            |
| 83  | j3    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 83  | q3    | 1     | 0        | 0        | 0       | 0            |
| 83  | r3    | 2     | 0        | 0        | 0       | 0            |
| 84  | A3    | 83    | 0        | 0        | 0       | 0            |
| 84  | B3    | 1     | 0        | 0        | 0       | 0            |
| 84  | D3    | 1     | 0        | 0        | 0       | 0            |
| 84  | R3    | 1     | 0        | 0        | 0       | 0            |
| 84  | S1    | 1     | 0        | 0        | 0       | 0            |
| 84  | T1    | 1     | 0        | 0        | 0       | 0            |
| 84  | T3    | 1     | 0        | 0        | 0       | 0            |
| 84  | U1    | 1     | 0        | 0        | 0       | 0            |
| 84  | V1    | 1     | 0        | 0        | 0       | 0            |
| 84  | W1    | 1     | 0        | 0        | 0       | 0            |
| 84  | Z3    | 1     | 0        | 0        | 0       | 0            |
| 84  | f3    | 2     | 0        | 0        | 0       | 0            |
| 84  | g3    | 1     | 0        | 0        | 0       | 0            |
| 84  | h1    | 42    | 0        | 0        | 0       | 0            |
| 84  | o3    | 2     | 0        | 0        | 0       | 0            |
| 84  | r3    | 1     | 0        | 0        | 0       | 0            |
| 85  | A3    | 10    | 0        | 19       | 6       | 0            |
| 85  | h1    | 10    | 0        | 19       | 2       | 0            |
| 86  | A3    | 28    | 52       | 52       | 1       | 0            |
| 86  | h1    | 42    | 78       | 78       | 3       | 0            |
| 87  | J1    | 1     | 0        | 0        | 0       | 0            |
| 87  | N1    | 1     | 0        | 0        | 0       | 0            |
| 87  | V1    | 1     | 0        | 0        | 0       | 0            |
| 87  | V3    | 1     | 0        | 0        | 0       | 0            |
| 87  | Y3    | 1     | 0        | 0        | 0       | 0            |
| 87  | Z3    | 1     | 0        | 0        | 0       | 0            |
| 87  | a3    | 1     | 0        | 0        | 0       | 0            |
| 88  | A1    | 7     | 0        | 0        | 0       | 0            |
| 88  | A3    | 3383  | 0        | 0        | 160     | 0            |
| 88  | B1    | 17    | 0        | 0        | 1       | 0            |
| 88  | B3    | 162   | 0        | 0        | 8       | 0            |
| 88  | C3    | 91    | 0        | 0        | 4       | 0            |
| 88  | D3    | 43    | 0        | 0        | 1       | 0            |
| 88  | E1    | 12    | 0        | 0        | 0       | 0            |
| 88  | F1    | 13    | 0        | 0        | 0       | 0            |
| 88  | F3    | 105   | 0        | 0        | 3       | 0            |
| 88  | G3    | 52    | 0        | 0        | 0       | 0            |
| 88  | H3    | 10    | 0        | 0        | 0       | 0            |
| 88  | I1    | 1     | 0        | 0        | 0       | 0            |
| 88  | I3    | 14    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 88  | J1    | 25    | 0        | 0        | 1       | 0            |
| 88  | J3    | 27    | 0        | 0        | 0       | 0            |
| 88  | K1    | 6     | 0        | 0        | 1       | 0            |
| 88  | M1    | 1     | 0        | 0        | 0       | 0            |
| 88  | M3    | 2     | 0        | 0        | 0       | 0            |
| 88  | N3    | 10    | 0        | 0        | 1       | 0            |
| 88  | O1    | 1     | 0        | 0        | 0       | 0            |
| 88  | O3    | 27    | 0        | 0        | 2       | 0            |
| 88  | P1    | 20    | 0        | 0        | 1       | 0            |
| 88  | Q3    | 3     | 0        | 0        | 0       | 0            |
| 88  | R1    | 12    | 0        | 0        | 1       | 0            |
| 88  | R3    | 42    | 0        | 0        | 5       | 0            |
| 88  | S1    | 32    | 0        | 0        | 1       | 0            |
| 88  | S3    | 6     | 0        | 0        | 0       | 0            |
| 88  | T1    | 43    | 0        | 0        | 3       | 0            |
| 88  | T3    | 14    | 0        | 0        | 0       | 0            |
| 88  | U1    | 7     | 0        | 0        | 0       | 0            |
| 88  | U3    | 4     | 0        | 0        | 0       | 0            |
| 88  | V1    | 4     | 0        | 0        | 0       | 0            |
| 88  | V3    | 29    | 0        | 0        | 0       | 0            |
| 88  | W1    | 20    | 0        | 0        | 2       | 0            |
| 88  | W2    | 13    | 0        | 0        | 0       | 0            |
| 88  | X1    | 21    | 0        | 0        | 0       | 0            |
| 88  | X3    | 7     | 0        | 0        | 0       | 0            |
| 88  | Y1    | 6     | 0        | 0        | 0       | 0            |
| 88  | Y3    | 2     | 0        | 0        | 1       | 0            |
| 88  | Z1    | 1     | 0        | 0        | 0       | 0            |
| 88  | Z3    | 21    | 0        | 0        | 1       | 0            |
| 88  | a3    | 6     | 0        | 0        | 1       | 0            |
| 88  | b1    | 11    | 0        | 0        | 0       | 0            |
| 88  | b3    | 1     | 0        | 0        | 0       | 0            |
| 88  | c1    | 12    | 0        | 0        | 0       | 0            |
| 88  | c3    | 10    | 0        | 0        | 1       | 0            |
| 88  | d1    | 12    | 0        | 0        | 0       | 0            |
| 88  | d3    | 13    | 0        | 0        | 0       | 0            |
| 88  | e1    | 16    | 0        | 0        | 1       | 0            |
| 88  | e3    | 12    | 0        | 0        | 0       | 0            |
| 88  | f1    | 10    | 0        | 0        | 0       | 0            |
| 88  | f3    | 48    | 0        | 0        | 2       | 0            |
| 88  | g3    | 16    | 0        | 0        | 1       | 0            |
| 88  | h1    | 2039  | 0        | 0        | 72      | 0            |
| 88  | h3    | 15    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 88  | i2    | 7      | 0        | 0        | 0       | 0            |
| 88  | j3    | 16     | 0        | 0        | 1       | 0            |
| 88  | k1    | 5      | 0        | 0        | 0       | 0            |
| 88  | k3    | 14     | 0        | 0        | 1       | 0            |
| 88  | m3    | 9      | 0        | 0        | 0       | 0            |
| 88  | n3    | 15     | 0        | 0        | 0       | 0            |
| 88  | o3    | 56     | 0        | 0        | 1       | 0            |
| 88  | p3    | 9      | 0        | 0        | 0       | 0            |
| 88  | q3    | 29     | 0        | 0        | 2       | 0            |
| 88  | r3    | 27     | 0        | 0        | 2       | 0            |
| 88  | s3    | 65     | 0        | 0        | 4       | 0            |
| 88  | t3    | 1      | 0        | 0        | 0       | 0            |
| 88  | u3    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 209834 | 151371   | 151439   | 1332    | 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 4.

All (1332) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:W2:56:C:N4     | 81:A3:2458:U:H3    | 1.60                     | 0.99              |
| 81:A3:2468:G:O2'  | 81:A3:2469:G:O5'   | 1.83                     | 0.96              |
| 3:h1:392:OMG:OP2  | 3:h1:427:G:O2'     | 1.84                     | 0.95              |
| 81:A3:884:U:OP2   | 81:A3:1913:C:O2'   | 1.85                     | 0.94              |
| 3:h1:76:C:O2'     | 3:h1:77:A:O4'      | 1.88                     | 0.91              |
| 52:R3:25:ARG:NH2  | 88:R3:301:HOH:O    | 2.04                     | 0.90              |
| 36:W2:19:G:O6     | 81:A3:2489:A:N1    | 2.05                     | 0.89              |
| 81:A3:3094:C:O2'  | 81:A3:3096:G:OP2   | 1.91                     | 0.89              |
| 3:h1:856:G:OP1    | 42:H3:180:ARG:NH2  | 2.06                     | 0.89              |
| 36:i2:20:G:O6     | 36:i2:59:U:O4      | 1.93                     | 0.87              |
| 3:h1:96:G:HO2'    | 3:h1:464:A:HO2'    | 1.17                     | 0.87              |
| 81:A3:2188:G:O2'  | 81:A3:2317:PSU:OP2 | 1.93                     | 0.86              |
| 37:C3:66:G:OP1    | 69:h3:10:ARG:NH1   | 2.09                     | 0.86              |
| 81:A3:40:OMC:HM22 | 81:A3:2806:A:H61   | 1.40                     | 0.86              |
| 81:A3:866:G:O2'   | 81:A3:867:G:O5'    | 1.93                     | 0.86              |
| 81:A3:700:A:N7    | 81:A3:702:U:O2'    | 2.10                     | 0.85              |
| 19:Q1:100:ARG:NH1 | 19:Q1:136:LEU:O    | 2.11                     | 0.84              |
| 81:A3:2870:C:OP1  | 88:A3:3601:HOH:O   | 1.95                     | 0.84              |
| 81:A3:975:A:OP2   | 88:A3:3602:HOH:O   | 1.96                     | 0.83              |
| 2:k1:4:ASN:OD1    | 3:h1:150:U:O2'     | 1.96                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:E1:54:TYR:OH    | 7:E1:103:ASN:OD1  | 1.97                     | 0.83              |
| 81:A3:661:C:OP1   | 88:A3:3603:HOH:O  | 1.97                     | 0.82              |
| 81:A3:2104:A:O2'  | 81:A3:2105:C:O4'  | 1.96                     | 0.82              |
| 81:A3:3044:U:OP2  | 81:A3:3094:C:N4   | 2.11                     | 0.82              |
| 48:N3:86:ASN:ND2  | 81:A3:461:C:O2'   | 2.13                     | 0.81              |
| 81:A3:3199:C:OP2  | 81:A3:3200:C:N4   | 2.12                     | 0.81              |
| 3:h1:1376:G:O2'   | 3:h1:1379:A:OP2   | 1.97                     | 0.81              |
| 81:A3:342:G:OP2   | 88:A3:3604:HOH:O  | 1.98                     | 0.81              |
| 31:c1:236:THR:OG1 | 31:c1:238:ASP:OD2 | 1.97                     | 0.81              |
| 81:A3:1074:G:O2'  | 81:A3:1109:A:OP1  | 1.98                     | 0.81              |
| 3:h1:1195:C:OP2   | 3:h1:1196:A:O2'   | 1.99                     | 0.80              |
| 57:W3:68:ASP:O    | 57:W3:69:LEU:HD23 | 1.82                     | 0.80              |
| 81:A3:2620:U:OP2  | 88:A3:3606:HOH:O  | 1.99                     | 0.80              |
| 3:h1:782:C:O2'    | 3:h1:783:U:O5'    | 2.00                     | 0.80              |
| 40:F3:5:THR:OG1   | 81:A3:114:C:OP1   | 2.00                     | 0.80              |
| 81:A3:2856:G:O6   | 88:A3:3608:HOH:O  | 2.00                     | 0.79              |
| 81:A3:2376:A:OP1  | 88:A3:3605:HOH:O  | 1.99                     | 0.79              |
| 3:h1:514:A:OP2    | 30:b1:178:ASN:ND2 | 2.16                     | 0.79              |
| 17:O1:17:THR:OG1  | 17:O1:20:GLU:OE1  | 2.01                     | 0.79              |
| 3:h1:392:OMG:OP1  | 88:h1:2101:HOH:O  | 2.00                     | 0.79              |
| 81:A3:2299:A:OP1  | 88:A3:3607:HOH:O  | 2.00                     | 0.79              |
| 3:h1:1275:U:O2'   | 3:h1:1278:A:OP2   | 2.00                     | 0.78              |
| 81:A3:352:A:OP2   | 88:A3:3611:HOH:O  | 2.01                     | 0.78              |
| 81:A3:101:G:OP2   | 88:A3:3615:HOH:O  | 2.01                     | 0.78              |
| 81:A3:660:A2M:OP2 | 81:A3:2871:U:O2'  | 1.99                     | 0.78              |
| 81:A3:2756:G:OP1  | 88:A3:3614:HOH:O  | 2.01                     | 0.78              |
| 81:A3:2769:U:OP2  | 88:A3:3613:HOH:O  | 2.01                     | 0.78              |
| 81:A3:2876:U:OP2  | 88:A3:3603:HOH:O  | 2.00                     | 0.78              |
| 81:A3:2766:U:O2   | 85:A3:3450:SPD:N1 | 2.15                     | 0.78              |
| 81:A3:3088:A:OP1  | 88:A3:3612:HOH:O  | 2.01                     | 0.78              |
| 3:h1:648:U:O2     | 3:h1:688:G:O6     | 2.01                     | 0.78              |
| 3:h1:1613:G:OP2   | 85:h1:2016:SPD:N1 | 2.16                     | 0.78              |
| 42:H3:62:ARG:NH1  | 81:A3:3072:A:OP1  | 2.17                     | 0.78              |
| 81:A3:1885:A:OP2  | 88:A3:3610:HOH:O  | 2.01                     | 0.78              |
| 3:h1:1597:C:OP1   | 88:h1:2102:HOH:O  | 2.02                     | 0.78              |
| 29:a1:56:THR:O    | 29:a1:93:LYS:NZ   | 2.17                     | 0.78              |
| 81:A3:2503:U:O2'  | 81:A3:2504:U:OP1  | 2.01                     | 0.77              |
| 81:A3:691:C:OP2   | 88:A3:3609:HOH:O  | 2.00                     | 0.77              |
| 81:A3:2900:A:OP2  | 81:A3:2902:C:N4   | 2.17                     | 0.77              |
| 17:O1:39:SER:OG   | 17:O1:40:GLU:OE1  | 2.01                     | 0.77              |
| 71:k3:48:LYS:NZ   | 88:k3:201:HOH:O   | 2.18                     | 0.77              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A1:141:THR:OG1   | 1:A1:143:ASP:OD1  | 2.01                     | 0.77              |
| 36:i2:20:G:C6      | 36:i2:59:U:O4     | 2.36                     | 0.77              |
| 81:A3:3342:C:O2'   | 81:A3:3344:U:OP2  | 2.01                     | 0.77              |
| 81:A3:1368:G:OP1   | 88:A3:3617:HOH:O  | 2.02                     | 0.77              |
| 1:A1:130:GLN:N     | 1:A1:130:GLN:OE1  | 2.17                     | 0.77              |
| 36:W2:56:C:N3      | 81:A3:2489:A:C2   | 2.52                     | 0.77              |
| 81:A3:56:G:OP1     | 88:A3:3618:HOH:O  | 2.02                     | 0.76              |
| 81:A3:1460:A2M:OP1 | 88:A3:3620:HOH:O  | 2.02                     | 0.76              |
| 81:A3:57:G:OP2     | 88:A3:3619:HOH:O  | 2.02                     | 0.76              |
| 81:A3:918:OMG:OP1  | 88:A3:3623:HOH:O  | 2.03                     | 0.76              |
| 81:A3:2623:G:OP1   | 88:A3:3629:HOH:O  | 2.04                     | 0.76              |
| 3:h1:945:G:OP2     | 88:h1:2103:HOH:O  | 2.03                     | 0.76              |
| 81:A3:880:A:OP1    | 88:A3:3625:HOH:O  | 2.04                     | 0.76              |
| 82:B3:12:G:OP1     | 88:B3:301:HOH:O   | 2.04                     | 0.76              |
| 82:B3:60:C:OP2     | 88:B3:302:HOH:O   | 2.04                     | 0.76              |
| 27:Y1:117:GLU:N    | 27:Y1:117:GLU:OE2 | 2.19                     | 0.76              |
| 81:A3:540:A:O2'    | 81:A3:541:U:O5'   | 2.00                     | 0.76              |
| 81:A3:2285:U:OP1   | 81:A3:2976:G:O2'  | 2.04                     | 0.76              |
| 81:A3:1641:A:OP1   | 88:A3:3633:HOH:O  | 2.05                     | 0.75              |
| 81:A3:2496:A:O2'   | 81:A3:2497:C:OP1  | 2.04                     | 0.75              |
| 81:A3:2640:A:OP1   | 88:A3:3631:HOH:O  | 2.04                     | 0.75              |
| 81:A3:2757:G:OP1   | 88:A3:3621:HOH:O  | 2.03                     | 0.75              |
| 81:A3:2765:A:OP2   | 88:A3:3628:HOH:O  | 2.04                     | 0.75              |
| 81:A3:83:A:OP1     | 88:A3:3627:HOH:O  | 2.04                     | 0.75              |
| 81:A3:2275:G:OP2   | 81:A3:2275:G:N2   | 2.18                     | 0.75              |
| 74:o3:223:SER:HG   | 81:A3:2247:A:HO2' | 1.33                     | 0.75              |
| 52:R3:40:ASP:OD1   | 88:R3:302:HOH:O   | 2.04                     | 0.75              |
| 37:C3:55:A:OP2     | 88:C3:301:HOH:O   | 2.04                     | 0.75              |
| 81:A3:2401:A:OP1   | 88:A3:3622:HOH:O  | 2.03                     | 0.75              |
| 81:A3:1959:G:O4'   | 81:A3:2096:A:N6   | 2.19                     | 0.74              |
| 81:A3:2189:U:OP1   | 88:A3:3630:HOH:O  | 2.04                     | 0.74              |
| 36:i2:64:G:O2'     | 68:g3:28:ASP:OD2  | 2.01                     | 0.74              |
| 3:h1:344:U:OP2     | 88:h1:2104:HOH:O  | 2.05                     | 0.74              |
| 81:A3:1482:PSU:OP2 | 88:A3:3636:HOH:O  | 2.06                     | 0.74              |
| 81:A3:2411:U:OP1   | 88:A3:3626:HOH:O  | 2.04                     | 0.74              |
| 81:A3:816:A:OP1    | 88:A3:3624:HOH:O  | 2.03                     | 0.74              |
| 81:A3:2732:OMU:OP2 | 88:A3:3637:HOH:O  | 2.06                     | 0.74              |
| 34:f1:57:GLU:OE1   | 34:f1:89:ARG:NH1  | 2.19                     | 0.74              |
| 81:A3:984:G:OP2    | 88:A3:3634:HOH:O  | 2.05                     | 0.74              |
| 81:A3:2403:G:O6    | 88:A3:3632:HOH:O  | 2.04                     | 0.74              |
| 82:B3:145:G:N7     | 88:B3:307:HOH:O   | 2.19                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 81:A3:2352:U:OP1  | 88:A3:3620:HOH:O   | 2.05                     | 0.74              |
| 58:X3:45:ARG:NH2  | 81:A3:1847:A:O2'   | 2.20                     | 0.74              |
| 88:R3:301:HOH:O   | 81:A3:2364:A:N3    | 2.19                     | 0.73              |
| 81:A3:1837:U:O2'  | 82:B3:117:G:OP1    | 2.04                     | 0.73              |
| 3:h1:880:G:OP1    | 88:h1:2105:HOH:O   | 2.06                     | 0.73              |
| 65:d3:206:TYR:OH  | 81:A3:3204:G:OP1   | 2.05                     | 0.73              |
| 81:A3:692:A:O2'   | 81:A3:708:C:N4     | 2.20                     | 0.73              |
| 3:h1:1194:B8N:OP1 | 88:h1:2109:HOH:O   | 2.07                     | 0.73              |
| 36:W2:19:G:C8     | 81:A3:2458:U:H2'   | 2.24                     | 0.73              |
| 3:h1:1644:G:OP1   | 88:h1:2106:HOH:O   | 2.07                     | 0.73              |
| 3:h1:390:G:OP2    | 88:h1:2107:HOH:O   | 2.07                     | 0.73              |
| 66:e3:117:ILE:O   | 66:e3:137:ASN:ND2  | 2.21                     | 0.73              |
| 81:A3:2572:C:O2'  | 81:A3:2573:U:O4'   | 2.04                     | 0.73              |
| 13:K1:25:ARG:O    | 88:K1:101:HOH:O    | 2.07                     | 0.73              |
| 81:A3:219:G:OP2   | 88:A3:3644:HOH:O   | 2.07                     | 0.73              |
| 81:A3:1850:C:OP1  | 88:A3:3638:HOH:O   | 2.06                     | 0.73              |
| 36:W2:56:C:H42    | 81:A3:2458:U:H3    | 0.80                     | 0.73              |
| 81:A3:2332:C:OP1  | 88:A3:3639:HOH:O   | 2.06                     | 0.73              |
| 3:h1:1048:C:OP1   | 88:h1:2108:HOH:O   | 2.07                     | 0.72              |
| 81:A3:418:G:O6    | 81:A3:2386:C:O2'   | 2.07                     | 0.72              |
| 81:A3:2790:G:OP1  | 88:A3:3641:HOH:O   | 2.07                     | 0.72              |
| 19:Q1:69:ASP:OD1  | 19:Q1:112:VAL:N    | 2.21                     | 0.72              |
| 81:A3:780:G:OP2   | 88:A3:3635:HOH:O   | 2.06                     | 0.72              |
| 3:h1:857:U:OP2    | 42:H3:180:ARG:NH1  | 2.23                     | 0.72              |
| 38:D3:10:GLY:O    | 88:D3:401:HOH:O    | 2.07                     | 0.72              |
| 3:h1:1799:A:OP1   | 88:h1:2113:HOH:O   | 2.07                     | 0.72              |
| 18:P1:151:SER:O   | 18:P1:155:LEU:HD12 | 1.90                     | 0.72              |
| 76:r3:243:ARG:NH2 | 81:A3:1913:C:O2    | 2.22                     | 0.72              |
| 3:h1:29:U:OP2     | 88:h1:2114:HOH:O   | 2.07                     | 0.72              |
| 3:h1:1600:G:OP1   | 88:h1:2110:HOH:O   | 2.07                     | 0.72              |
| 50:P3:32:TYR:OH   | 50:P3:60:GLU:OE1   | 2.07                     | 0.72              |
| 81:A3:32:A:OP2    | 88:A3:3643:HOH:O   | 2.07                     | 0.72              |
| 3:h1:261:C:O2     | 18:P1:193:ARG:NH1  | 2.22                     | 0.72              |
| 81:A3:1501:A:OP2  | 88:A3:3650:HOH:O   | 2.08                     | 0.72              |
| 2:k1:152:GLU:OE2  | 2:k1:152:GLU:N     | 2.23                     | 0.71              |
| 81:A3:670:G:OP1   | 88:A3:3642:HOH:O   | 2.07                     | 0.71              |
| 81:A3:674:OMC:OP1 | 88:A3:3654:HOH:O   | 2.08                     | 0.71              |
| 81:A3:1153:G:OP1  | 88:A3:3640:HOH:O   | 2.07                     | 0.71              |
| 3:h1:1196:A:OP1   | 88:h1:2112:HOH:O   | 2.07                     | 0.71              |
| 79:u3:50:ASP:OD2  | 79:u3:57:LYS:NZ    | 2.22                     | 0.71              |
| 81:A3:969:C:OP2   | 88:A3:3649:HOH:O   | 2.08                     | 0.71              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 77:s3:238:ARG:O   | 88:s3:501:HOH:O  | 2.09                     | 0.71              |
| 81:A3:1027:A:O2'  | 81:A3:1028:U:OP1 | 2.06                     | 0.71              |
| 81:A3:1444:A:OP2  | 88:A3:3646:HOH:O | 2.08                     | 0.71              |
| 81:A3:1601:C:O2'  | 81:A3:1700:A:N3  | 2.23                     | 0.71              |
| 81:A3:1946:G:OP2  | 88:A3:3648:HOH:O | 2.08                     | 0.71              |
| 81:A3:28:G:N7     | 88:A3:3754:HOH:O | 2.22                     | 0.71              |
| 81:A3:1947:C:OP2  | 88:A3:3657:HOH:O | 2.09                     | 0.71              |
| 25:W1:86:GLU:OE1  | 88:W1:301:HOH:O  | 2.07                     | 0.71              |
| 42:H3:62:ARG:NH2  | 81:A3:3070:U:OP2 | 2.24                     | 0.71              |
| 81:A3:28:G:OP1    | 88:A3:3647:HOH:O | 2.08                     | 0.71              |
| 81:A3:832:G:OP1   | 88:A3:3655:HOH:O | 2.08                     | 0.71              |
| 3:h1:521:A:O2'    | 3:h1:522:C:O5'   | 2.07                     | 0.71              |
| 3:h1:96:G:O6      | 88:h1:2115:HOH:O | 2.07                     | 0.71              |
| 3:h1:551:G:OP2    | 88:h1:2122:HOH:O | 2.09                     | 0.71              |
| 3:h1:1025:C:OP1   | 88:h1:2120:HOH:O | 2.09                     | 0.71              |
| 3:h1:1167:G:OP2   | 88:h1:2123:HOH:O | 2.09                     | 0.71              |
| 36:W2:56:C:N4     | 81:A3:2458:U:N3  | 2.26                     | 0.71              |
| 81:A3:806:U:OP2   | 88:A3:3653:HOH:O | 2.08                     | 0.71              |
| 3:h1:878:G:OP2    | 88:h1:2121:HOH:O | 2.09                     | 0.70              |
| 81:A3:1072:U:OP2  | 88:A3:3651:HOH:O | 2.08                     | 0.70              |
| 81:A3:2414:U:OP1  | 88:A3:3645:HOH:O | 2.08                     | 0.70              |
| 3:h1:15:U:OP2     | 88:h1:2125:HOH:O | 2.09                     | 0.70              |
| 77:s3:15:PHE:N    | 77:s3:18:ASP:OD2 | 2.24                     | 0.70              |
| 3:h1:777:C:OP2    | 88:h1:2117:HOH:O | 2.08                     | 0.70              |
| 36:W2:58:A:O2'    | 36:W2:60:C:OP2   | 2.05                     | 0.70              |
| 81:A3:1489:C:OP2  | 88:A3:3661:HOH:O | 2.09                     | 0.70              |
| 3:h1:93:A:N3      | 88:h1:2184:HOH:O | 2.23                     | 0.70              |
| 3:h1:961:PSU:OP1  | 88:h1:2129:HOH:O | 2.10                     | 0.70              |
| 3:h1:1201:G:O6    | 88:h1:2111:HOH:O | 2.07                     | 0.70              |
| 44:J3:41:ASP:OD1  | 44:J3:61:THR:OG1 | 2.08                     | 0.70              |
| 70:j3:5:SER:OG    | 88:j3:301:HOH:O  | 2.08                     | 0.70              |
| 81:A3:98:A:OP2    | 88:A3:3662:HOH:O | 2.09                     | 0.70              |
| 81:A3:2733:A:OP1  | 88:A3:3656:HOH:O | 2.09                     | 0.70              |
| 3:h1:1139:U:OP2   | 88:h1:2118:HOH:O | 2.08                     | 0.70              |
| 3:h1:1194:B8N:N34 | 36:W2:34:G:OP1   | 2.24                     | 0.70              |
| 82:B3:24:C:OP1    | 88:B3:303:HOH:O  | 2.10                     | 0.70              |
| 81:A3:1127:G:OP1  | 88:A3:3670:HOH:O | 2.10                     | 0.70              |
| 64:c3:26:GLU:N    | 64:c3:26:GLU:OE1 | 2.24                     | 0.70              |
| 81:A3:1462:C:OP1  | 88:A3:3658:HOH:O | 2.09                     | 0.70              |
| 3:h1:1471:G:O2'   | 3:h1:1608:C:OP1  | 2.10                     | 0.69              |
| 81:A3:1552:G:OP2  | 88:A3:3659:HOH:O | 2.09                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 81:A3:963:G:OP2   | 88:A3:3660:HOH:O  | 2.09                     | 0.69              |
| 81:A3:984:G:N7    | 88:A3:3761:HOH:O  | 2.23                     | 0.69              |
| 25:W1:7:ARG:NH2   | 88:W1:302:HOH:O   | 2.24                     | 0.69              |
| 81:A3:1550:U:O4   | 81:A3:1563:G:O2'  | 2.10                     | 0.69              |
| 3:h1:450:A:OP1    | 88:h1:2128:HOH:O  | 2.10                     | 0.69              |
| 81:A3:34:PSU:O2   | 81:A3:45:C:O2'    | 2.03                     | 0.69              |
| 81:A3:696:G:OP2   | 88:A3:3665:HOH:O  | 2.10                     | 0.69              |
| 77:s3:38:ASP:OD1  | 88:s3:502:HOH:O   | 2.10                     | 0.69              |
| 81:A3:78:C:OP2    | 88:A3:3669:HOH:O  | 2.10                     | 0.69              |
| 74:o3:215:ASN:ND2 | 81:A3:2972:A:N7   | 2.41                     | 0.69              |
| 3:h1:1780:C:OP2   | 88:h1:2132:HOH:O  | 2.10                     | 0.69              |
| 23:U1:88:LYS:O    | 27:Y1:25:ARG:NH1  | 2.26                     | 0.69              |
| 81:A3:818:A:N7    | 88:A3:3778:HOH:O  | 2.24                     | 0.69              |
| 3:h1:1011:G:OP2   | 88:h1:2136:HOH:O  | 2.11                     | 0.69              |
| 64:c3:30:LYS:NZ   | 81:A3:2563:C:OP1  | 2.26                     | 0.69              |
| 81:A3:40:OMC:CM2  | 81:A3:2806:A:H61  | 2.06                     | 0.69              |
| 81:A3:1357:G:N7   | 88:A3:3802:HOH:O  | 2.26                     | 0.69              |
| 81:A3:3145:G:N7   | 88:A3:3795:HOH:O  | 2.26                     | 0.69              |
| 3:h1:46:A:OP2     | 88:h1:2131:HOH:O  | 2.10                     | 0.68              |
| 81:A3:2678:C:OP2  | 81:A3:2679:A:O2'  | 2.06                     | 0.68              |
| 3:h1:774:A:OP2    | 88:h1:2124:HOH:O  | 2.09                     | 0.68              |
| 3:h1:1176:C:OP1   | 23:U1:130:ARG:NH2 | 2.26                     | 0.68              |
| 81:A3:706:C:OP2   | 88:A3:3677:HOH:O  | 2.12                     | 0.68              |
| 81:A3:1357:G:N3   | 88:A3:3774:HOH:O  | 2.24                     | 0.68              |
| 3:h1:1559:G:O2'   | 24:V1:14:TYR:OH   | 2.06                     | 0.68              |
| 6:D1:115:PRO:O    | 28:Z1:16:GLN:NE2  | 2.27                     | 0.68              |
| 38:D3:60:GLN:O    | 38:D3:61:THR:OG1  | 2.10                     | 0.68              |
| 81:A3:2582:G:OP2  | 81:A3:2583:A:O2'  | 2.09                     | 0.68              |
| 3:h1:993:C:OP2    | 88:h1:2127:HOH:O  | 2.10                     | 0.68              |
| 3:h1:1030:A:N7    | 88:h1:2200:HOH:O  | 2.25                     | 0.68              |
| 3:h1:1174:A:OP2   | 88:h1:2134:HOH:O  | 2.11                     | 0.68              |
| 3:h1:1789:MA6:OP1 | 88:h1:2130:HOH:O  | 2.10                     | 0.68              |
| 18:P1:36:THR:OG1  | 18:P1:58:ALA:O    | 2.09                     | 0.68              |
| 33:e1:107:SER:OG  | 88:e1:201:HOH:O   | 2.09                     | 0.68              |
| 64:c3:60:ARG:NH1  | 88:c3:302:HOH:O   | 2.26                     | 0.68              |
| 76:r3:124:LYS:NZ  | 81:A3:3289:OMU:O4 | 2.26                     | 0.68              |
| 81:A3:37:A:OP2    | 88:A3:3681:HOH:O  | 2.12                     | 0.68              |
| 81:A3:2176:U:OP2  | 88:A3:3664:HOH:O  | 2.10                     | 0.68              |
| 3:h1:1801:G:OP2   | 88:h1:2135:HOH:O  | 2.11                     | 0.68              |
| 81:A3:664:A:OP2   | 88:A3:3663:HOH:O  | 2.10                     | 0.68              |
| 81:A3:3110:G:O6   | 88:A3:3666:HOH:O  | 2.10                     | 0.68              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 81:A3:673:U:OP1    | 88:A3:3673:HOH:O  | 2.11                     | 0.68              |
| 81:A3:1639:G:N2    | 81:A3:1642:A:OP2  | 2.24                     | 0.68              |
| 48:N3:22:LYS:O     | 88:N3:201:HOH:O   | 2.12                     | 0.68              |
| 81:A3:364:A:OP2    | 88:A3:3675:HOH:O  | 2.11                     | 0.68              |
| 81:A3:3359:C:OP2   | 81:A3:3360:U:O2'  | 2.11                     | 0.68              |
| 3:h1:206:U:O3'     | 18:P1:185:SER:OG  | 2.10                     | 0.67              |
| 81:A3:2398:OMG:OP2 | 88:A3:3671:HOH:O  | 2.11                     | 0.67              |
| 81:A3:2261:PSU:OP2 | 88:A3:3668:HOH:O  | 2.10                     | 0.67              |
| 81:A3:1128:G:OP2   | 88:A3:3680:HOH:O  | 2.12                     | 0.67              |
| 81:A3:1450:U:OP2   | 88:A3:3676:HOH:O  | 2.11                     | 0.67              |
| 3:h1:1806:U:O2     | 3:h1:1808:G:O2'   | 2.11                     | 0.67              |
| 47:M3:57:ASP:O     | 47:M3:62:GLN:NE2  | 2.28                     | 0.67              |
| 52:R3:40:ASP:O     | 88:R3:303:HOH:O   | 2.13                     | 0.67              |
| 81:A3:2883:PSU:OP2 | 88:A3:3672:HOH:O  | 2.11                     | 0.67              |
| 49:O3:35:MET:O     | 88:O3:101:HOH:O   | 2.13                     | 0.67              |
| 81:A3:1800:U:OP2   | 88:A3:3684:HOH:O  | 2.13                     | 0.67              |
| 3:h1:1003:C:OP2    | 88:h1:2140:HOH:O  | 2.12                     | 0.67              |
| 17:O1:175:ARG:NE   | 17:O1:181:ASP:OD2 | 2.28                     | 0.67              |
| 66:e3:123:LYS:NZ   | 66:e3:127:ASP:OD2 | 2.26                     | 0.67              |
| 40:F3:56:LYS:NZ    | 81:A3:148:A:OP1   | 2.28                     | 0.67              |
| 81:A3:57:G:OP1     | 88:A3:3674:HOH:O  | 2.11                     | 0.67              |
| 82:B3:162:G:O2'    | 82:B3:163:C:H5'   | 1.94                     | 0.67              |
| 3:h1:338:G:OP1     | 88:h1:2142:HOH:O  | 2.13                     | 0.67              |
| 3:h1:630:C:OP1     | 88:h1:2138:HOH:O  | 2.12                     | 0.67              |
| 81:A3:2288:C:OP2   | 81:A3:2289:U:O2'  | 2.03                     | 0.67              |
| 81:A3:2413:OMU:OP2 | 88:A3:3688:HOH:O  | 2.13                     | 0.67              |
| 81:A3:1869:G:OP2   | 88:A3:3687:HOH:O  | 2.13                     | 0.66              |
| 81:A3:2199:C:O2'   | 81:A3:2273:A:N3   | 2.27                     | 0.66              |
| 81:A3:2702:G:OP1   | 88:A3:3689:HOH:O  | 2.13                     | 0.66              |
| 3:h1:385:C:OP1     | 88:h1:2137:HOH:O  | 2.12                     | 0.66              |
| 81:A3:347:C:O2     | 88:A3:3682:HOH:O  | 2.13                     | 0.66              |
| 81:A3:916:A:O2'    | 81:A3:917:G:OP2   | 2.12                     | 0.66              |
| 40:F3:103:GLU:OE2  | 88:F3:301:HOH:O   | 2.13                     | 0.66              |
| 3:h1:384:U:OP1     | 88:h1:2148:HOH:O  | 2.14                     | 0.66              |
| 81:A3:1353:U:O2'   | 88:A3:3691:HOH:O  | 2.13                     | 0.66              |
| 81:A3:3059:U:OP1   | 81:A3:3060:C:O2'  | 2.09                     | 0.66              |
| 81:A3:2805:A:OP2   | 88:A3:3696:HOH:O  | 2.14                     | 0.66              |
| 3:h1:1130:G:OP1    | 88:h1:2143:HOH:O  | 2.13                     | 0.66              |
| 18:P1:13:ALA:O     | 88:P1:301:HOH:O   | 2.14                     | 0.66              |
| 19:Q1:77:MET:HE2   | 19:Q1:77:MET:HA   | 1.77                     | 0.66              |
| 72:m3:125:ARG:NH2  | 81:A3:184:A:OP1   | 2.27                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 81:A3:424:G:H22   | 81:A3:643:U:H3    | 1.42                     | 0.66              |
| 81:A3:662:G:O2'   | 81:A3:1446:A:OP1  | 2.12                     | 0.66              |
| 81:A3:2227:A:OP1  | 88:A3:3685:HOH:O  | 2.13                     | 0.66              |
| 9:G1:32:VAL:HG21  | 28:Z1:158:ASP:OD2 | 1.95                     | 0.66              |
| 31:c1:58:LYS:HE3  | 31:c1:58:LYS:HA   | 1.78                     | 0.66              |
| 61:Z3:67:LYS:O    | 88:Z3:301:HOH:O   | 2.12                     | 0.66              |
| 81:A3:220:C:OP2   | 88:A3:3694:HOH:O  | 2.14                     | 0.66              |
| 81:A3:925:A:OP1   | 88:A3:3683:HOH:O  | 2.13                     | 0.66              |
| 81:A3:2610:G:OP2  | 88:A3:3690:HOH:O  | 2.13                     | 0.66              |
| 82:B3:51:A:O2'    | 82:B3:53:C:OP2    | 2.09                     | 0.66              |
| 37:C3:7:G:OP1     | 69:h3:33:ARG:NH1  | 2.29                     | 0.66              |
| 69:h3:124:GLU:OE1 | 69:h3:126:SER:OG  | 2.08                     | 0.66              |
| 81:A3:2397:G:OP1  | 88:A3:3692:HOH:O  | 2.14                     | 0.66              |
| 3:h1:1488:A:N3    | 3:h1:1613:G:O2'   | 2.28                     | 0.65              |
| 21:S1:137:ASP:O   | 88:S1:301:HOH:O   | 2.14                     | 0.65              |
| 81:A3:2989:U:OP2  | 88:A3:3698:HOH:O  | 2.14                     | 0.65              |
| 3:h1:1782:G:OP1   | 88:h1:2147:HOH:O  | 2.13                     | 0.65              |
| 29:a1:149:ARG:NH1 | 35:B1:29:U:O2'    | 2.28                     | 0.65              |
| 3:h1:1530:A:N3    | 3:h1:1596:G:O2'   | 2.29                     | 0.65              |
| 25:W1:38:CYS:SG   | 25:W1:78:HIS:ND1  | 2.69                     | 0.65              |
| 36:W2:19:G:N7     | 81:A3:2458:U:H2'  | 2.12                     | 0.65              |
| 62:a3:9:GLY:O     | 81:A3:846:A:O2'   | 2.14                     | 0.65              |
| 63:b3:107:LYS:NZ  | 63:b3:149:VAL:O   | 2.30                     | 0.65              |
| 35:B1:21:U:OP2    | 88:B1:1802:HOH:O  | 2.15                     | 0.65              |
| 81:A3:53:G:N7     | 88:A3:3839:HOH:O  | 2.29                     | 0.65              |
| 1:A1:167:ASN:ND2  | 3:h1:125:A:OP1    | 2.30                     | 0.65              |
| 81:A3:801:A:N3    | 88:A3:3831:HOH:O  | 2.29                     | 0.65              |
| 81:A3:66:C:OP2    | 81:A3:298:G:N2    | 2.29                     | 0.65              |
| 81:A3:125:G:N7    | 88:A3:3825:HOH:O  | 2.28                     | 0.65              |
| 81:A3:2761:A:OP1  | 88:A3:3701:HOH:O  | 2.15                     | 0.65              |
| 3:h1:100:C:OP2    | 88:h1:2145:HOH:O  | 2.13                     | 0.65              |
| 3:h1:1476:A:OP2   | 32:d1:170:ARG:NH1 | 2.30                     | 0.65              |
| 81:A3:1447:U:OP1  | 88:A3:3695:HOH:O  | 2.14                     | 0.65              |
| 20:R1:31:ASN:ND2  | 20:R1:34:ASN:OD1  | 2.30                     | 0.64              |
| 38:D3:37:ARG:NH2  | 81:A3:696:G:OP1   | 2.26                     | 0.64              |
| 64:c3:114:GLU:OE2 | 64:c3:119:THR:OG1 | 2.14                     | 0.64              |
| 8:F1:219:LYS:NZ   | 62:a3:92:SER:O    | 2.19                     | 0.64              |
| 81:A3:1451:G:OP2  | 88:A3:3697:HOH:O  | 2.14                     | 0.64              |
| 81:A3:3208:C:O2'  | 81:A3:3250:C:O2'  | 2.15                     | 0.64              |
| 3:h1:5:U:OP1      | 88:h1:2144:HOH:O  | 2.13                     | 0.64              |
| 12:J1:4:LYS:O     | 88:J1:301:HOH:O   | 2.14                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:N1:99:LYS:HE2   | 16:N1:99:LYS:HA    | 1.79                     | 0.64              |
| 3:h1:1342:C:O2'    | 3:h1:1344:G:N7     | 2.29                     | 0.64              |
| 45:K3:100:ARG:NH2  | 81:A3:1762:C:OP1   | 2.29                     | 0.64              |
| 81:A3:1322:G:OP2   | 88:A3:3700:HOH:O   | 2.15                     | 0.64              |
| 81:A3:1838:C:OP2   | 88:A3:3699:HOH:O   | 2.15                     | 0.64              |
| 3:h1:1278:A:O2'    | 29:a1:148:GLN:O    | 2.11                     | 0.64              |
| 5:C1:96:LYS:HE2    | 5:C1:96:LYS:H      | 1.62                     | 0.64              |
| 26:X1:47:ARG:NH1   | 26:X1:51:GLU:OE1   | 2.30                     | 0.64              |
| 52:R3:44:ARG:O     | 88:R3:304:HOH:O    | 2.14                     | 0.64              |
| 76:r3:183:GLU:OE2  | 81:A3:3004:C:O2'   | 2.13                     | 0.64              |
| 19:Q1:260:ILE:O    | 19:Q1:269:VAL:N    | 2.31                     | 0.64              |
| 32:d1:207:LYS:HD2  | 32:d1:210:ARG:HH21 | 1.63                     | 0.63              |
| 81:A3:814:C:OP2    | 88:A3:3704:HOH:O   | 2.16                     | 0.63              |
| 81:A3:2156:A:N7    | 88:A3:3849:HOH:O   | 2.30                     | 0.63              |
| 81:A3:2412:OMG:OP2 | 88:A3:3702:HOH:O   | 2.15                     | 0.63              |
| 3:h1:614:OMU:OP2   | 88:h1:2150:HOH:O   | 2.15                     | 0.63              |
| 3:h1:903:A:OP2     | 88:h1:2151:HOH:O   | 2.15                     | 0.63              |
| 42:H3:70:LYS:NZ    | 88:A3:3687:HOH:O   | 2.32                     | 0.63              |
| 52:R3:106:ARG:NH2  | 81:A3:1423:G:OP1   | 2.30                     | 0.63              |
| 3:h1:1600:G:OP2    | 3:h1:1602:C:N4     | 2.31                     | 0.63              |
| 67:f3:76:ASP:O     | 88:f3:301:HOH:O    | 2.15                     | 0.63              |
| 81:A3:941:C:O2'    | 88:A3:3678:HOH:O   | 2.12                     | 0.63              |
| 81:A3:2543:A:O2'   | 81:A3:2544:C:O5'   | 2.04                     | 0.63              |
| 1:A1:247:SER:N     | 1:A1:250:GLU:OE1   | 2.31                     | 0.62              |
| 40:F3:204:ARG:O    | 88:F3:302:HOH:O    | 2.16                     | 0.62              |
| 36:W2:56:C:C2      | 81:A3:2489:A:C2    | 2.88                     | 0.62              |
| 81:A3:3080:G:O2'   | 81:A3:3081:U:OP1   | 2.15                     | 0.62              |
| 77:s3:19:MET:HE3   | 77:s3:19:MET:H     | 1.64                     | 0.62              |
| 77:s3:19:MET:HE3   | 77:s3:19:MET:N     | 2.14                     | 0.62              |
| 3:h1:995:A:OP1     | 86:h1:2019:SPM:N14 | 2.32                     | 0.62              |
| 81:A3:418:G:O2'    | 81:A3:2368:OMC:OP2 | 2.15                     | 0.62              |
| 40:F3:175:ARG:NH2  | 88:F3:303:HOH:O    | 2.32                     | 0.62              |
| 81:A3:2146:A:OP2   | 88:A3:3706:HOH:O   | 2.16                     | 0.62              |
| 3:h1:1440:G:O6     | 4:l1:91:TYR:OH     | 2.11                     | 0.62              |
| 82:B3:127:C:C4     | 82:B3:128:C:N4     | 2.67                     | 0.62              |
| 68:g3:102:MET:HA   | 68:g3:102:MET:HE2  | 1.80                     | 0.62              |
| 6:D1:47:ARG:NH1    | 6:D1:48:ASN:OD1    | 2.33                     | 0.62              |
| 36:W2:56:C:C4      | 81:A3:2489:A:C2    | 2.88                     | 0.62              |
| 3:h1:1392:G:OP1    | 6:D1:32:LYS:NZ     | 2.31                     | 0.61              |
| 8:F1:38:PHE:O      | 8:F1:41:LYS:NZ     | 2.33                     | 0.61              |
| 42:H3:56:LYS:NZ    | 81:A3:1879:U:OP2   | 2.34                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:T3:69:ARG:NH1  | 81:A3:1649:G:OP1   | 2.30                     | 0.61              |
| 74:o3:69:TYR:OH   | 81:A3:2561:C:OP1   | 2.13                     | 0.61              |
| 3:h1:1307:G:OP2   | 3:h1:1308:PSU:O2'  | 2.12                     | 0.61              |
| 78:t3:162:MET:HG2 | 78:t3:173:ILE:HD13 | 1.81                     | 0.61              |
| 3:h1:1361:A:O2'   | 7:E1:133:ASP:OD2   | 2.13                     | 0.61              |
| 75:q3:162:ALA:O   | 88:q3:401:HOH:O    | 2.16                     | 0.61              |
| 3:h1:639:A:OP2    | 88:h1:2152:HOH:O   | 2.16                     | 0.61              |
| 81:A3:370:A:OP2   | 88:A3:3708:HOH:O   | 2.16                     | 0.61              |
| 81:A3:959:C:OP2   | 88:A3:3707:HOH:O   | 2.16                     | 0.61              |
| 41:G3:67:LEU:HD11 | 41:G3:79:VAL:HG21  | 1.81                     | 0.61              |
| 79:u3:50:ASP:O    | 79:u3:54:GLY:N     | 2.29                     | 0.61              |
| 81:A3:198:G:OP1   | 81:A3:217:G:O2'    | 2.14                     | 0.61              |
| 6:D1:31:ASN:ND2   | 6:D1:55:THR:OG1    | 2.33                     | 0.61              |
| 21:S1:19:ALA:N    | 21:S1:24:GLU:OE1   | 2.33                     | 0.61              |
| 57:W3:68:ASP:C    | 57:W3:69:LEU:HD23  | 2.25                     | 0.61              |
| 6:D1:82:MET:HE2   | 6:D1:82:MET:N      | 2.16                     | 0.60              |
| 59:Y3:102:ARG:O   | 88:Y3:301:HOH:O    | 2.16                     | 0.60              |
| 78:t3:128:ASP:OD2 | 81:A3:2676:A:O2'   | 2.13                     | 0.60              |
| 81:A3:38:A:OP1    | 85:A3:3450:SPD:H92 | 2.00                     | 0.60              |
| 81:A3:1674:C:O2'  | 81:A3:1866:G:OP1   | 2.19                     | 0.60              |
| 1:A1:117:GLU:OE2  | 1:A1:117:GLU:N     | 2.31                     | 0.60              |
| 57:W3:35:LYS:NZ   | 81:A3:1753:G:OP1   | 2.23                     | 0.60              |
| 3:h1:1641:A:OP1   | 88:h1:2153:HOH:O   | 2.16                     | 0.60              |
| 44:J3:126:ILE:O   | 81:A3:1106:C:O2'   | 2.17                     | 0.60              |
| 81:A3:3374:U:O2'  | 81:A3:3376:G:N7    | 2.26                     | 0.60              |
| 38:D3:72:ARG:NH2  | 81:A3:108:G:OP2    | 2.32                     | 0.60              |
| 61:Z3:33:ASP:OD2  | 81:A3:2769:U:O2'   | 2.20                     | 0.60              |
| 3:h1:1161:C:O2'   | 3:h1:1587:C:OP2    | 2.19                     | 0.60              |
| 36:W2:75:C:O2'    | 61:Z3:56:PRO:O     | 2.17                     | 0.60              |
| 3:h1:67:G:O2'     | 3:h1:69:A:OP1      | 2.14                     | 0.60              |
| 3:h1:817:U:O2'    | 42:H3:163:ARG:NH2  | 2.35                     | 0.60              |
| 3:h1:1025:C:O2'   | 3:h1:1128:A:N1     | 2.35                     | 0.60              |
| 81:A3:950:G:OP2   | 88:A3:3710:HOH:O   | 2.17                     | 0.60              |
| 3:h1:782:C:HO2'   | 3:h1:783:U:P       | 2.22                     | 0.60              |
| 20:R1:78:ASN:ND2  | 88:R1:202:HOH:O    | 2.34                     | 0.60              |
| 81:A3:2503:U:HO2' | 81:A3:2504:U:P     | 2.25                     | 0.60              |
| 6:D1:113:GLU:OE2  | 28:Z1:6:ARG:NH2    | 2.35                     | 0.59              |
| 81:A3:962:A:OP2   | 88:A3:3705:HOH:O   | 2.16                     | 0.59              |
| 17:O1:30:MET:HE2  | 17:O1:30:MET:HA    | 1.84                     | 0.59              |
| 3:h1:1559:G:HO2'  | 24:V1:14:TYR:HH    | 1.36                     | 0.59              |
| 41:G3:146:GLU:N   | 81:A3:797:G:OP1    | 2.36                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:k3:153:ILE:HG22 | 73:n3:37:THR:HG22  | 1.84                     | 0.59              |
| 2:k1:181:GLN:NE2   | 3:h1:65:A:OP1      | 2.33                     | 0.59              |
| 77:s3:364:HIS:NE2  | 81:A3:549:U:O2'    | 2.28                     | 0.59              |
| 36:i2:20:G:O6      | 36:i2:59:U:C4      | 2.56                     | 0.59              |
| 74:o3:223:SER:OG   | 81:A3:2247:A:O2'   | 2.06                     | 0.59              |
| 77:s3:236:VAL:O    | 88:s3:503:HOH:O    | 2.16                     | 0.59              |
| 81:A3:2383:U:OP2   | 88:A3:3711:HOH:O   | 2.17                     | 0.59              |
| 3:h1:1616:G:OP2    | 88:h1:2154:HOH:O   | 2.17                     | 0.59              |
| 56:V3:81:GLY:N     | 82:B3:99:A:OP1     | 2.34                     | 0.59              |
| 9:G1:32:VAL:HG22   | 9:G1:60:ARG:HD2    | 1.85                     | 0.59              |
| 65:d3:49:SER:OG    | 81:A3:1327:U:OP2   | 2.15                     | 0.59              |
| 5:C1:66:ALA:CB     | 5:C1:95:ALA:HB2    | 2.33                     | 0.58              |
| 81:A3:396:A:OP1    | 88:A3:3703:HOH:O   | 2.16                     | 0.58              |
| 81:A3:770:G:O2'    | 81:A3:771:A:OP2    | 2.20                     | 0.58              |
| 81:A3:2763:C:OP2   | 88:A3:3713:HOH:O   | 2.17                     | 0.58              |
| 68:g3:193:ASP:OD1  | 81:A3:1022:G:N2    | 2.37                     | 0.58              |
| 76:r3:214:LYS:NZ   | 76:r3:358:ILE:O    | 2.34                     | 0.58              |
| 3:h1:1758:A2M:H4'  | 60:p3:13:LEU:HD21  | 1.85                     | 0.58              |
| 54:T3:76:ARG:NH1   | 81:A3:1643:C:OP2   | 2.37                     | 0.58              |
| 82:B3:39:G:O6      | 88:B3:305:HOH:O    | 2.12                     | 0.58              |
| 3:h1:1389:A:OP1    | 20:R1:33:LYS:NZ    | 2.36                     | 0.58              |
| 62:a3:5:THR:OG1    | 81:A3:847:A:OP1    | 2.22                     | 0.58              |
| 2:k1:44:GLU:OE2    | 2:k1:44:GLU:N      | 2.28                     | 0.58              |
| 77:s3:40:VAL:HG21  | 77:s3:250:LEU:HD21 | 1.86                     | 0.58              |
| 3:h1:1789:MA6:H92  | 3:h1:1790:MA6:H93  | 1.86                     | 0.57              |
| 19:Q1:43:VAL:HG21  | 19:Q1:93:LEU:HD12  | 1.86                     | 0.57              |
| 28:Z1:194:LYS:HE3  | 28:Z1:194:LYS:HA   | 1.86                     | 0.57              |
| 81:A3:2904:G:O2'   | 81:A3:3026:A:N1    | 2.37                     | 0.57              |
| 29:a1:126:LEU:HD11 | 29:a1:155:PHE:HB3  | 1.84                     | 0.57              |
| 6:D1:106:LEU:HD21  | 28:Z1:19:LEU:HD11  | 1.86                     | 0.57              |
| 7:E1:15:PHE:HA     | 7:E1:139:ILE:HD11  | 1.86                     | 0.57              |
| 81:A3:2336:C:OP2   | 88:A3:3715:HOH:O   | 2.18                     | 0.57              |
| 81:A3:1234:G:O2'   | 81:A3:1235:A:OP2   | 2.23                     | 0.57              |
| 3:h1:1493:G:O2'    | 3:h1:1501:C:O2     | 2.18                     | 0.57              |
| 19:Q1:143:ILE:HD12 | 19:Q1:143:ILE:O    | 2.05                     | 0.57              |
| 63:b3:27:LYS:NZ    | 81:A3:593:G:OP2    | 2.36                     | 0.57              |
| 19:Q1:145:GLU:O    | 19:Q1:148:SER:OG   | 2.19                     | 0.57              |
| 3:h1:385:C:O2'     | 3:h1:759:A:N1      | 2.36                     | 0.57              |
| 73:n3:10:ARG:NH1   | 73:n3:63:GLN:OE1   | 2.37                     | 0.57              |
| 81:A3:344:G:OP2    | 88:A3:3712:HOH:O   | 2.17                     | 0.57              |
| 3:h1:21:U:O2       | 88:h1:2139:HOH:O   | 2.12                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:h1:1483:U:OP1    | 7:E1:40:THR:OG1    | 2.11                     | 0.57              |
| 3:h1:1194:B8N:OP1  | 88:h1:2156:HOH:O   | 2.17                     | 0.57              |
| 78:t3:117:LYS:HE2  | 78:t3:117:LYS:HA   | 1.86                     | 0.57              |
| 30:b1:59:ARG:O     | 30:b1:63:THR:HG23  | 2.05                     | 0.56              |
| 13:K1:69:THR:OG1   | 13:K1:72:ARG:O     | 2.22                     | 0.56              |
| 79:u3:16:VAL:O     | 79:u3:56:LYS:NZ    | 2.37                     | 0.56              |
| 82:B3:106:G:OP2    | 82:B3:108:A:O2'    | 2.22                     | 0.56              |
| 3:h1:533:C:O2      | 10:H1:63:ARG:NH1   | 2.37                     | 0.56              |
| 5:C1:112:LYS:HD2   | 5:C1:112:LYS:C     | 2.31                     | 0.56              |
| 81:A3:2873:5MC:O2' | 88:A3:3693:HOH:O   | 2.14                     | 0.56              |
| 3:h1:556:G:OP2     | 3:h1:557:C:O2'     | 2.17                     | 0.56              |
| 81:A3:60:A:N7      | 88:A3:3891:HOH:O   | 2.32                     | 0.56              |
| 81:A3:1382:G:OP2   | 88:A3:3720:HOH:O   | 2.18                     | 0.56              |
| 82:B3:108:A:OP1    | 88:B3:306:HOH:O    | 2.18                     | 0.56              |
| 68:g3:59:ASN:O     | 88:g3:401:HOH:O    | 2.17                     | 0.56              |
| 81:A3:1504:G:N2    | 81:A3:1504:G:OP2   | 2.36                     | 0.56              |
| 42:H3:135:LYS:NZ   | 81:A3:1955:G:OP2   | 2.36                     | 0.56              |
| 76:r3:286:TYR:N    | 76:r3:327:LEU:O    | 2.37                     | 0.56              |
| 3:h1:1548:G:OP1    | 7:E1:85:ARG:NH2    | 2.39                     | 0.56              |
| 81:A3:1187:C:OP2   | 81:A3:1188:A:O2'   | 2.15                     | 0.56              |
| 69:h3:116:ASP:OD2  | 69:h3:116:ASP:N    | 2.38                     | 0.55              |
| 3:h1:17:C:O2'      | 3:h1:1140:A:N1     | 2.36                     | 0.55              |
| 71:k3:153:ILE:HG22 | 73:n3:37:THR:CG2   | 2.36                     | 0.55              |
| 43:I3:175:ASN:ND2  | 81:A3:3199:C:O2    | 2.37                     | 0.55              |
| 81:A3:92:G:O5'     | 85:A3:3450:SPD:H21 | 2.07                     | 0.55              |
| 81:A3:1163:G:OP2   | 81:A3:1163:G:N2    | 2.35                     | 0.55              |
| 3:h1:1406:A:OP1    | 6:D1:56:HIS:NE2    | 2.38                     | 0.55              |
| 6:D1:119:LEU:HD23  | 6:D1:120:LYS:N     | 2.21                     | 0.55              |
| 30:b1:127:ALA:O    | 30:b1:131:ILE:HG13 | 2.07                     | 0.55              |
| 59:Y3:100:TYR:O    | 81:A3:2898:G:O2'   | 2.25                     | 0.55              |
| 81:A3:720:G:N3     | 81:A3:764:G:O2'    | 2.40                     | 0.55              |
| 42:H3:7:GLN:NE2    | 42:H3:35:ALA:O     | 2.39                     | 0.55              |
| 64:c3:105:GLU:OE1  | 64:c3:105:GLU:C    | 2.50                     | 0.55              |
| 66:e3:139:ILE:O    | 66:e3:140:VAL:HB   | 2.06                     | 0.55              |
| 78:t3:76:GLU:OE1   | 78:t3:76:GLU:HA    | 2.07                     | 0.55              |
| 81:A3:1596:G:N7    | 88:A3:3907:HOH:O   | 2.34                     | 0.55              |
| 81:A3:2519:U:OP2   | 81:A3:2589:G:N2    | 2.39                     | 0.55              |
| 3:h1:1491:G:O6     | 3:h1:1529:G:N2     | 2.39                     | 0.54              |
| 7:E1:61:MET:O      | 7:E1:65:ILE:HG13   | 2.07                     | 0.54              |
| 81:A3:40:OMC:HM22  | 81:A3:2806:A:N6    | 2.17                     | 0.54              |
| 81:A3:2707:A:OP1   | 88:A3:3719:HOH:O   | 2.18                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:h1:874:A:H2'     | 3:h1:875:G:C8      | 2.42                     | 0.54              |
| 8:F1:89:GLU:OE1    | 8:F1:89:GLU:N      | 2.39                     | 0.54              |
| 27:Y1:53:GLN:C     | 27:Y1:53:GLN:OE1   | 2.50                     | 0.54              |
| 29:a1:65:LYS:O     | 29:a1:70:ARG:NH2   | 2.41                     | 0.54              |
| 29:a1:81:LYS:HD2   | 29:a1:81:LYS:C     | 2.33                     | 0.54              |
| 76:r3:36:ASP:OD2   | 76:r3:38:SER:OG    | 2.22                     | 0.54              |
| 36:W2:19:G:O5'     | 81:A3:2458:U:O2'   | 2.25                     | 0.54              |
| 81:A3:464:PSU:OP2  | 88:A3:3716:HOH:O   | 2.18                     | 0.54              |
| 19:Q1:233:ASP:OD2  | 19:Q1:233:ASP:C    | 2.51                     | 0.54              |
| 32:d1:30:TYR:O     | 32:d1:33:VAL:HG12  | 2.07                     | 0.54              |
| 3:h1:275:C:O2'     | 3:h1:276:G:O4'     | 2.26                     | 0.54              |
| 19:Q1:228:LYS:NZ   | 19:Q1:231:SER:OG   | 2.40                     | 0.54              |
| 3:h1:1067:G:O2'    | 8:F1:204:ILE:O     | 2.25                     | 0.54              |
| 5:C1:28:MET:HA     | 5:C1:28:MET:HE2    | 1.90                     | 0.54              |
| 76:r3:224:THR:HG22 | 76:r3:333:VAL:HG23 | 1.89                     | 0.54              |
| 31:c1:100:THR:OG1  | 31:c1:103:GLY:O    | 2.20                     | 0.54              |
| 52:R3:74:LYS:NZ    | 52:R3:96:GLU:OE1   | 2.24                     | 0.53              |
| 81:A3:2392:C:O2'   | 81:A3:3299:A:N1    | 2.39                     | 0.53              |
| 77:s3:113:ARG:NH2  | 81:A3:801:A:OP1    | 2.35                     | 0.53              |
| 3:h1:1093:C:OP1    | 12:J1:6:ARG:NH1    | 2.39                     | 0.53              |
| 19:Q1:27:ASP:C     | 19:Q1:27:ASP:OD2   | 2.50                     | 0.53              |
| 81:A3:1517:G:N7    | 88:A3:3905:HOH:O   | 2.33                     | 0.53              |
| 3:h1:185:G:O2'     | 3:h1:195:A:N6      | 2.39                     | 0.53              |
| 76:r3:338:ARG:NH2  | 81:A3:3296:C:O2'   | 2.42                     | 0.53              |
| 3:h1:100:C:OP2     | 3:h1:382:A:O2'     | 2.23                     | 0.53              |
| 31:c1:54:VAL:HG21  | 31:c1:77:ILE:HG23  | 1.89                     | 0.53              |
| 69:h3:136:GLU:OE1  | 69:h3:136:GLU:N    | 2.27                     | 0.53              |
| 75:q3:125:ASN:ND2  | 81:A3:999:C:OP1    | 2.40                     | 0.53              |
| 81:A3:2468:G:O2'   | 81:A3:2469:G:P     | 2.67                     | 0.53              |
| 3:h1:86:A:N3       | 3:h1:146:A:O2'     | 2.39                     | 0.53              |
| 36:W2:18:G:O2'     | 36:W2:57:G:N2      | 2.33                     | 0.53              |
| 17:O1:20:GLU:OE1   | 17:O1:20:GLU:N     | 2.36                     | 0.53              |
| 69:h3:216:GLU:OE1  | 69:h3:216:GLU:N    | 2.38                     | 0.53              |
| 81:A3:958:C:O2     | 88:A3:3714:HOH:O   | 2.17                     | 0.53              |
| 11:I1:43:ASP:OD1   | 11:I1:44:LYS:N     | 2.41                     | 0.53              |
| 19:Q1:111:SER:HB3  | 19:Q1:124:ALA:HB3  | 1.91                     | 0.53              |
| 81:A3:1699:U:O2'   | 81:A3:1754:A:N1    | 2.36                     | 0.53              |
| 3:h1:114:U:O2      | 88:h1:2158:HOH:O   | 2.18                     | 0.53              |
| 3:h1:1232:G:N2     | 3:h1:1258:G:O2'    | 2.39                     | 0.53              |
| 42:H3:105:LEU:HD23 | 42:H3:138:LEU:HD12 | 1.91                     | 0.53              |
| 53:S3:82:ASN:OD1   | 81:A3:1338:A:O2'   | 2.27                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 78:t3:42:LEU:HD13 | 78:t3:116:ILE:HD11 | 1.91                     | 0.53              |
| 19:Q1:20:THR:OG1  | 19:Q1:35:SER:OG    | 2.27                     | 0.53              |
| 19:Q1:27:ASP:OD2  | 19:Q1:29:SER:OG    | 2.27                     | 0.53              |
| 81:A3:56:G:OP2    | 88:A3:3724:HOH:O   | 2.19                     | 0.53              |
| 81:A3:2376:A:N3   | 81:A3:2827:G:O2'   | 2.30                     | 0.53              |
| 3:h1:503:C:O2'    | 3:h1:504:U:P       | 2.67                     | 0.52              |
| 19:Q1:215:ASP:OD1 | 19:Q1:215:ASP:N    | 2.42                     | 0.52              |
| 81:A3:186:G:N7    | 88:A3:3911:HOH:O   | 2.34                     | 0.52              |
| 81:A3:1634:U:H2'  | 81:A3:1635:G:C4    | 2.44                     | 0.52              |
| 81:A3:926:G:H5'   | 81:A3:927:A:OP1    | 2.09                     | 0.52              |
| 3:h1:128:G:OP1    | 3:h1:201:G:O2'     | 2.18                     | 0.52              |
| 82:B3:116:U:O2'   | 88:B3:304:HOH:O    | 2.11                     | 0.52              |
| 3:h1:393:G:OP1    | 88:h1:2164:HOH:O   | 2.19                     | 0.52              |
| 3:h1:1102:U:OP2   | 88:h1:2163:HOH:O   | 2.19                     | 0.52              |
| 5:C1:39:LYS:HA    | 5:C1:44:LEU:HD22   | 1.90                     | 0.52              |
| 5:C1:96:LYS:HE2   | 5:C1:96:LYS:N      | 2.24                     | 0.52              |
| 8:F1:47:LEU:HD23  | 8:F1:47:LEU:H      | 1.74                     | 0.52              |
| 33:e1:18:GLU:OE2  | 33:e1:18:GLU:HA    | 2.09                     | 0.52              |
| 38:D3:196:ARG:NH2 | 81:A3:777:U:OP1    | 2.39                     | 0.52              |
| 63:b3:155:LYS:N   | 63:b3:155:LYS:HE2  | 2.23                     | 0.52              |
| 81:A3:84:G:O2'    | 81:A3:96:G:O6      | 2.26                     | 0.52              |
| 81:A3:2541:G:C5   | 81:A3:2542:C:N4    | 2.77                     | 0.52              |
| 3:h1:625:A:OP2    | 88:h1:2162:HOH:O   | 2.19                     | 0.52              |
| 7:E1:43:LEU:HD23  | 7:E1:43:LEU:H      | 1.74                     | 0.52              |
| 73:n3:27:GLU:HA   | 73:n3:27:GLU:OE1   | 2.10                     | 0.52              |
| 81:A3:2662:A:OP1  | 88:A3:3722:HOH:O   | 2.19                     | 0.52              |
| 88:h1:2139:HOH:O  | 30:b1:18:ARG:NH2   | 2.42                     | 0.52              |
| 5:C1:75:VAL:O     | 5:C1:79:LYS:HG3    | 2.10                     | 0.52              |
| 81:A3:2396:G:O2'  | 81:A3:2397:G:OP2   | 2.23                     | 0.52              |
| 81:A3:2797:G:O2'  | 81:A3:2798:U:OP2   | 2.24                     | 0.52              |
| 3:h1:294:G:C2     | 3:h1:295:C:C5      | 2.98                     | 0.52              |
| 3:h1:1569:G:OP1   | 7:E1:42:LYS:NZ     | 2.43                     | 0.52              |
| 81:A3:673:U:H2'   | 81:A3:674:OMC:C6   | 2.44                     | 0.52              |
| 81:A3:2461:U:O2'  | 81:A3:2462:A:O4'   | 2.27                     | 0.52              |
| 1:A1:32:SER:OG    | 1:A1:81:THR:OG1    | 2.21                     | 0.52              |
| 3:h1:781:C:C2'    | 3:h1:782:C:O5'     | 2.58                     | 0.52              |
| 39:E3:3:PHE:CE1   | 43:I3:178:MET:HE2  | 2.45                     | 0.52              |
| 76:r3:247:ARG:O   | 76:r3:251:LYS:NZ   | 2.35                     | 0.52              |
| 3:h1:521:A:HO2'   | 3:h1:522:C:P       | 2.29                     | 0.52              |
| 81:A3:3288:A:H2'  | 81:A3:3289:OMU:H6  | 1.92                     | 0.52              |
| 16:N1:92:LYS:HE2  | 16:N1:92:LYS:HA    | 1.91                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 75:q3:70:ARG:NH1   | 81:A3:524:A:OP2     | 2.43                     | 0.52              |
| 81:A3:2505:A:O2'   | 81:A3:2506:A:OP2    | 2.22                     | 0.52              |
| 38:D3:183:GLU:OE2  | 38:D3:183:GLU:HA    | 2.09                     | 0.51              |
| 42:H3:86:GLU:OE2   | 42:H3:91:THR:HG22   | 2.10                     | 0.51              |
| 51:Q3:32:LYS:O     | 51:Q3:36:THR:OG1    | 2.14                     | 0.51              |
| 63:b3:151:LYS:NZ   | 63:b3:191:ASP:OD1   | 2.35                     | 0.51              |
| 65:d3:59:TYR:OH    | 65:d3:78:PHE:O      | 2.28                     | 0.51              |
| 81:A3:2468:G:HO2'  | 81:A3:2469:G:P      | 2.30                     | 0.51              |
| 32:d1:174:THR:HG22 | 32:d1:176:ALA:H     | 1.75                     | 0.51              |
| 61:Z3:41:ARG:NH1   | 81:A3:281:A:OP2     | 2.42                     | 0.51              |
| 81:A3:654:U:O2'    | 81:A3:1164:A:N1     | 2.37                     | 0.51              |
| 81:A3:2714:U:O2'   | 81:A3:2747:PSU:OP1  | 2.26                     | 0.51              |
| 3:h1:192:G:N7      | 18:P1:156:ARG:NH2   | 2.58                     | 0.51              |
| 17:O1:25:GLN:NE2   | 17:O1:29:ASP:OD2    | 2.44                     | 0.51              |
| 41:G3:121:THR:OG1  | 41:G3:123:ASP:OD1   | 2.26                     | 0.51              |
| 81:A3:64:A:OP1     | 88:A3:3723:HOH:O    | 2.19                     | 0.51              |
| 2:k1:53:MET:HE2    | 2:k1:53:MET:HA      | 1.92                     | 0.51              |
| 81:A3:2819:G:O4'   | 81:A3:2873:5MC:HM52 | 2.09                     | 0.51              |
| 3:h1:50:C:OP2      | 88:h1:2160:HOH:O    | 2.19                     | 0.51              |
| 3:h1:77:A:O2'      | 3:h1:78:G:O4'       | 2.28                     | 0.51              |
| 81:A3:2540:G:H2'   | 81:A3:2541:G:C8     | 2.45                     | 0.51              |
| 3:h1:610:G:H21     | 3:h1:617:C:H5''     | 1.76                     | 0.51              |
| 19:Q1:276:LEU:HD12 | 19:Q1:277:LYS:N     | 2.25                     | 0.51              |
| 63:b3:204:GLU:HA   | 63:b3:204:GLU:OE2   | 2.10                     | 0.51              |
| 3:h1:889:U:O2'     | 21:S1:134:ILE:O     | 2.29                     | 0.51              |
| 22:T1:84:VAL:O     | 88:T1:302:HOH:O     | 2.19                     | 0.51              |
| 29:a1:170:TYR:OH   | 29:a1:205:THR:O     | 2.28                     | 0.51              |
| 36:W2:19:G:C6      | 81:A3:2458:U:O2     | 2.64                     | 0.51              |
| 81:A3:692:A:N6     | 81:A3:708:C:H2'     | 2.26                     | 0.51              |
| 8:F1:127:VAL:HG21  | 8:F1:176:ALA:CB     | 2.41                     | 0.51              |
| 19:Q1:275:ASP:C    | 19:Q1:275:ASP:OD1   | 2.53                     | 0.51              |
| 19:Q1:306:SER:OG   | 19:Q1:307:ALA:N     | 2.44                     | 0.51              |
| 29:a1:88:GLU:C     | 29:a1:88:GLU:OE1    | 2.53                     | 0.51              |
| 81:A3:2900:A:O2'   | 81:A3:2902:C:OP1    | 2.25                     | 0.51              |
| 81:A3:955:C:H2'    | 81:A3:956:C:C6      | 2.46                     | 0.51              |
| 81:A3:1440:G:O6    | 88:A3:3717:HOH:O    | 2.18                     | 0.51              |
| 6:D1:63:LYS:C      | 6:D1:63:LYS:HD3     | 2.36                     | 0.50              |
| 3:h1:959:U:OP1     | 3:h1:1075:C:O2'     | 2.28                     | 0.50              |
| 28:Z1:90:PHE:O     | 28:Z1:94:THR:OG1    | 2.23                     | 0.50              |
| 40:F3:45:PRO:O     | 40:F3:49:ARG:HG3    | 2.10                     | 0.50              |
| 81:A3:2941:G:N7    | 88:A3:3912:HOH:O    | 2.34                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A1:54:TYR:O     | 10:H1:16:ASN:ND2   | 2.44                     | 0.50              |
| 3:h1:476:U:O2'    | 3:h1:773:A:N3      | 2.42                     | 0.50              |
| 46:L3:26:SER:N    | 66:e3:99:GLU:OE1   | 2.41                     | 0.50              |
| 49:O3:18:ARG:NE   | 88:O3:104:HOH:O    | 2.44                     | 0.50              |
| 57:W3:17:ARG:NH2  | 81:A3:1830:C:O3'   | 2.44                     | 0.50              |
| 17:O1:67:TYR:O    | 17:O1:70:ARG:NH1   | 2.40                     | 0.50              |
| 32:d1:125:SER:OG  | 32:d1:195:ALA:HB1  | 2.12                     | 0.50              |
| 81:A3:2946:G:H2'  | 81:A3:2947:PSU:O4' | 2.12                     | 0.50              |
| 3:h1:542:G:OP2    | 3:h1:542:G:N2      | 2.36                     | 0.50              |
| 3:h1:1173:G:C2    | 3:h1:1174:A:C8     | 2.99                     | 0.50              |
| 8:F1:171:ILE:HG21 | 8:F1:197:ILE:HG13  | 1.93                     | 0.50              |
| 17:O1:128:GLU:OE1 | 17:O1:128:GLU:O    | 2.30                     | 0.50              |
| 81:A3:1160:G:O6   | 88:A3:3721:HOH:O   | 2.18                     | 0.50              |
| 70:j3:37:ARG:NH2  | 82:B3:6:A:OP1      | 2.39                     | 0.50              |
| 3:h1:325:C:N4     | 3:h1:1673:G:OP1    | 2.45                     | 0.50              |
| 3:h1:1186:A:OP2   | 88:h1:2161:HOH:O   | 2.19                     | 0.50              |
| 3:h1:849:G:O6     | 3:h1:850:A:N6      | 2.45                     | 0.50              |
| 11:I1:91:MET:SD   | 11:I1:94:ALA:HB2   | 2.51                     | 0.50              |
| 69:h3:68:SER:OG   | 69:h3:71:GLY:O     | 2.27                     | 0.50              |
| 77:s3:102:GLY:O   | 88:s3:504:HOH:O    | 2.20                     | 0.50              |
| 78:t3:97:ASN:ND2  | 81:A3:2676:A:OP1   | 2.42                     | 0.50              |
| 81:A3:540:A:HO2'  | 81:A3:541:U:P      | 2.28                     | 0.50              |
| 3:h1:319:A:C2     | 3:h1:357:A:C5      | 3.00                     | 0.50              |
| 36:i2:5:G:H22     | 36:i2:68:A:H2      | 1.59                     | 0.50              |
| 73:n3:12:LYS:O    | 73:n3:64:LYS:NZ    | 2.45                     | 0.50              |
| 81:A3:1015:A:N1   | 81:A3:1061:C:O2'   | 2.34                     | 0.50              |
| 81:A3:1189:A:N3   | 81:A3:1340:C:O2'   | 2.45                     | 0.50              |
| 3:h1:617:C:OP2    | 22:T1:3:LYS:NZ     | 2.41                     | 0.49              |
| 37:C3:12:U:OP2    | 37:C3:67:C:O2'     | 2.28                     | 0.49              |
| 47:M3:127:ARG:O   | 47:M3:131:THR:HG23 | 2.12                     | 0.49              |
| 70:j3:10:ASN:OD1  | 70:j3:12:THR:OG1   | 2.29                     | 0.49              |
| 79:u3:24:GLN:OE1  | 79:u3:37:ASN:ND2   | 2.45                     | 0.49              |
| 81:A3:2471:A:N6   | 81:A3:2483:A:OP1   | 2.45                     | 0.49              |
| 81:A3:2541:G:H2'  | 81:A3:2542:C:C6    | 2.47                     | 0.49              |
| 81:A3:2547:C:H2'  | 81:A3:2548:C:C6    | 2.47                     | 0.49              |
| 81:A3:2967:G:N2   | 81:A3:2970:A:OP2   | 2.37                     | 0.49              |
| 17:O1:76:ILE:HD12 | 17:O1:76:ILE:O     | 2.12                     | 0.49              |
| 44:J3:40:VAL:HB   | 44:J3:96:VAL:HG22  | 1.94                     | 0.49              |
| 45:K3:40:GLU:O    | 45:K3:44:GLN:HG3   | 2.12                     | 0.49              |
| 48:N3:74:LYS:O    | 48:N3:78:GLN:NE2   | 2.44                     | 0.49              |
| 50:P3:109:LEU:HB2 | 50:P3:110:PRO:HD3  | 1.94                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 81:A3:2122:C:H2'    | 81:A3:2123:A:O4'   | 2.11                     | 0.49              |
| 81:A3:2222:A:H2'    | 81:A3:2223:A2M:H8  | 1.94                     | 0.49              |
| 81:A3:2488:G:N2     | 81:A3:2491:A:N7    | 2.60                     | 0.49              |
| 7:E1:34:TRP:O       | 7:E1:38:VAL:HG22   | 2.11                     | 0.49              |
| 67:f3:85:GLU:CD     | 67:f3:85:GLU:H     | 2.20                     | 0.49              |
| 79:u3:25:ILE:HD13   | 79:u3:38:PHE:HD2   | 1.76                     | 0.49              |
| 81:A3:938:C:OP1     | 88:A3:3729:HOH:O   | 2.19                     | 0.49              |
| 14:L1:32:ASP:OD1    | 14:L1:33:ASP:N     | 2.45                     | 0.49              |
| 18:P1:78:ARG:HB3    | 18:P1:78:ARG:NH1   | 2.28                     | 0.49              |
| 29:a1:126:LEU:HD11  | 29:a1:155:PHE:CB   | 2.42                     | 0.49              |
| 34:f1:104:VAL:HG12  | 34:f1:105:ASP:N    | 2.28                     | 0.49              |
| 52:R3:42:ARG:NH2    | 81:A3:646:A:O2'    | 2.45                     | 0.49              |
| 81:A3:883:C:H4'     | 81:A3:884:U:OP2    | 2.12                     | 0.49              |
| 81:A3:970:PSU:OP1   | 88:A3:3731:HOH:O   | 2.20                     | 0.49              |
| 81:A3:82:U:OP1      | 88:A3:3726:HOH:O   | 2.19                     | 0.49              |
| 81:A3:2141:U:OP2    | 81:A3:2146:A:N6    | 2.39                     | 0.49              |
| 19:Q1:242:CYS:HG    | 19:Q1:305:TRP:CD1  | 2.31                     | 0.49              |
| 78:t3:108:ILE:C     | 78:t3:108:ILE:HD12 | 2.38                     | 0.49              |
| 3:h1:1216:G:O2'     | 3:h1:1247:A:N7     | 2.45                     | 0.49              |
| 17:O1:68:ARG:NH1    | 42:H3:181:LEU:HD21 | 2.27                     | 0.49              |
| 23:U1:30:MET:HA     | 23:U1:30:MET:HE3   | 1.94                     | 0.49              |
| 36:W2:56:C:N4       | 81:A3:2458:U:C4    | 2.80                     | 0.49              |
| 3:h1:1621:C:OP1     | 32:d1:66:ARG:NH2   | 2.45                     | 0.49              |
| 36:W2:19:G:C8       | 81:A3:2458:U:C2'   | 2.95                     | 0.49              |
| 81:A3:2482:G:O2'    | 81:A3:2483:A:OP1   | 2.27                     | 0.49              |
| 18:P1:94:THR:HG22   | 18:P1:94:THR:O     | 2.11                     | 0.49              |
| 28:Z1:17:MET:HE1    | 28:Z1:176:TRP:CZ3  | 2.48                     | 0.49              |
| 65:d3:28:LEU:HD22   | 65:d3:38:VAL:HG11  | 1.95                     | 0.49              |
| 68:g3:158:LYS:NZ    | 81:A3:2839:OMC:O2  | 2.46                     | 0.49              |
| 77:s3:270:SER:OG    | 77:s3:272:ASP:OD1  | 2.16                     | 0.49              |
| 81:A3:30:U:OP1      | 88:A3:3732:HOH:O   | 2.20                     | 0.49              |
| 81:A3:666:C:H2'     | 81:A3:667:A:H8     | 1.78                     | 0.49              |
| 81:A3:2542:C:H2'    | 81:A3:2543:A:C4    | 2.48                     | 0.49              |
| 81:A3:2962:OMC:HM22 | 81:A3:2963:C:O4'   | 2.13                     | 0.49              |
| 10:H1:44:LYS:O      | 10:H1:48:MET:HG3   | 2.12                     | 0.48              |
| 23:U1:16:GLN:OE1    | 23:U1:100:SER:OG   | 2.21                     | 0.48              |
| 52:R3:113:ALA:CB    | 52:R3:120:ILE:HD11 | 2.43                     | 0.48              |
| 81:A3:151:C:OP2     | 88:A3:3730:HOH:O   | 2.20                     | 0.48              |
| 81:A3:419:A:N1      | 81:A3:2365:C:O2'   | 2.39                     | 0.48              |
| 82:B3:75:A:OP2      | 88:B3:308:HOH:O    | 2.20                     | 0.48              |
| 6:D1:119:LEU:HD23   | 6:D1:120:LYS:H     | 1.78                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:c1:153:TYR:OH   | 31:c1:159:GLY:O    | 2.29                     | 0.48              |
| 1:A1:165:GLU:OE2   | 1:A1:165:GLU:HA    | 2.13                     | 0.48              |
| 3:h1:1147:U:HO2'   | 3:h1:1304:PSU:HO2' | 1.61                     | 0.48              |
| 27:Y1:44:PHE:O     | 27:Y1:49:ARG:NH2   | 2.46                     | 0.48              |
| 65:d3:21:LEU:O     | 65:d3:25:SER:OG    | 2.25                     | 0.48              |
| 81:A3:279:G:OP1    | 86:A3:3451:SPM:N14 | 2.45                     | 0.48              |
| 81:A3:1555:G:OP2   | 88:A3:3733:HOH:O   | 2.20                     | 0.48              |
| 3:h1:825:C:H3'     | 3:h1:826:G:H21     | 1.77                     | 0.48              |
| 3:h1:933:A:OP1     | 12:J1:32:LYS:NZ    | 2.32                     | 0.48              |
| 6:D1:72:LYS:HE3    | 6:D1:73:LEU:N      | 2.28                     | 0.48              |
| 66:e3:19:GLY:O     | 81:A3:1903:G:O2'   | 2.27                     | 0.48              |
| 75:q3:35:LYS:O     | 75:q3:39:GLU:HG3   | 2.14                     | 0.48              |
| 81:A3:2748:G:N2    | 81:A3:2751:A:OP2   | 2.42                     | 0.48              |
| 3:h1:1621:C:OP1    | 14:L1:16:ARG:NH2   | 2.47                     | 0.48              |
| 3:h1:1642:C:O2     | 3:h1:1773:A:N6     | 2.46                     | 0.48              |
| 19:Q1:120:GLN:OE1  | 19:Q1:181:LEU:HD21 | 2.12                     | 0.48              |
| 30:b1:31:LYS:NZ    | 30:b1:35:GLU:OE1   | 2.45                     | 0.48              |
| 36:W2:56:C:C5      | 81:A3:2489:A:C4    | 3.02                     | 0.48              |
| 81:A3:721:G:N2     | 81:A3:724:G:OP2    | 2.41                     | 0.48              |
| 3:h1:1285:U:OP1    | 88:h1:2169:HOH:O   | 2.20                     | 0.48              |
| 69:h3:212:GLU:OE2  | 69:h3:213:ASP:OD1  | 2.31                     | 0.48              |
| 76:r3:79:ILE:HD12  | 76:r3:328:ILE:HD13 | 1.94                     | 0.48              |
| 19:Q1:171:SER:HG   | 19:Q1:173:ASP:CG   | 2.21                     | 0.48              |
| 29:a1:126:LEU:HD22 | 29:a1:137:CYS:SG   | 2.54                     | 0.48              |
| 30:b1:65:ASP:OD1   | 30:b1:66:GLU:N     | 2.46                     | 0.48              |
| 33:e1:23:ARG:NH1   | 33:e1:65:LEU:O     | 2.47                     | 0.48              |
| 42:H3:182:ALA:O    | 42:H3:183:GLN:HG2  | 2.12                     | 0.48              |
| 76:r3:277:HIS:ND1  | 81:A3:3140:U:OP1   | 2.42                     | 0.48              |
| 77:s3:19:MET:H     | 77:s3:19:MET:CE    | 2.27                     | 0.48              |
| 81:A3:2367:G:H22   | 81:A3:2399:G:H1'   | 1.78                     | 0.48              |
| 18:P1:150:LYS:CD   | 18:P1:150:LYS:H    | 2.27                     | 0.48              |
| 43:I3:70:ASN:O     | 43:I3:75:LYS:NZ    | 2.46                     | 0.48              |
| 81:A3:1161:A:OP2   | 88:A3:3725:HOH:O   | 2.19                     | 0.48              |
| 81:A3:1842:C:O2'   | 81:A3:1848:A:N1    | 2.44                     | 0.48              |
| 3:h1:81:U:H4'      | 3:h1:82:G:OP2      | 2.12                     | 0.48              |
| 29:a1:165:GLN:N    | 29:a1:166:PRO:HD2  | 2.29                     | 0.48              |
| 63:b3:229:VAL:O    | 63:b3:230:PHE:HB2  | 2.14                     | 0.48              |
| 75:q3:100:LYS:NZ   | 88:q3:403:HOH:O    | 2.44                     | 0.48              |
| 77:s3:364:HIS:CE1  | 81:A3:549:U:HO2'   | 2.25                     | 0.48              |
| 7:E1:136:ALA:HA    | 7:E1:139:ILE:HD12  | 1.96                     | 0.47              |
| 28:Z1:56:GLU:HA    | 28:Z1:56:GLU:OE1   | 2.13                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 65:d3:66:ARG:NH1   | 81:A3:3011:G:OP1  | 2.47                     | 0.47              |
| 69:h3:94:ASN:OD1   | 69:h3:96:ALA:N    | 2.47                     | 0.47              |
| 2:k1:226:GLU:OE1   | 2:k1:227:LYS:N    | 2.47                     | 0.47              |
| 3:h1:888:G:H2'     | 3:h1:889:U:C6     | 2.49                     | 0.47              |
| 8:F1:171:ILE:HG23  | 8:F1:196:GLU:OE2  | 2.14                     | 0.47              |
| 72:m3:81:ILE:HG22  | 72:m3:82:GLU:H    | 1.80                     | 0.47              |
| 81:A3:674:OMC:HM22 | 81:A3:675:OMU:O4' | 2.14                     | 0.47              |
| 58:X3:20:ASN:ND2   | 58:X3:42:ARG:O    | 2.46                     | 0.47              |
| 81:A3:3049:C:O2'   | 81:A3:3050:A:H5'  | 2.14                     | 0.47              |
| 3:h1:76:C:HO2'     | 3:h1:77:A:C1'     | 2.18                     | 0.47              |
| 25:W1:106:ARG:HA   | 25:W1:106:ARG:NE  | 2.29                     | 0.47              |
| 75:q3:14:LYS:NZ    | 77:s3:300:ASP:OD2 | 2.41                     | 0.47              |
| 3:h1:1787:PSU:O2   | 88:h1:2167:HOH:O  | 2.20                     | 0.47              |
| 28:Z1:205:ARG:HB3  | 28:Z1:205:ARG:NH1 | 2.29                     | 0.47              |
| 44:J3:105:VAL:CG1  | 44:J3:109:MET:HE3 | 2.44                     | 0.47              |
| 65:d3:42:ARG:NH2   | 81:A3:3181:A:OP1  | 2.45                     | 0.47              |
| 66:e3:74:LYS:NZ    | 81:A3:2297:U:OP2  | 2.45                     | 0.47              |
| 79:u3:128:LYS:O    | 79:u3:167:LYS:NZ  | 2.48                     | 0.47              |
| 2:k1:20:ASP:OD2    | 2:k1:22:GLN:N     | 2.48                     | 0.47              |
| 2:k1:202:ARG:NH1   | 2:k1:202:ARG:HB3  | 2.28                     | 0.47              |
| 3:h1:370:A:OP1     | 3:h1:762:PSU:O2'  | 2.18                     | 0.47              |
| 3:h1:962:U:OP1     | 13:K1:32:SER:OG   | 2.30                     | 0.47              |
| 3:h1:971:U:OP1     | 3:h1:1036:C:O2'   | 2.32                     | 0.47              |
| 25:W1:132:THR:O    | 25:W1:132:THR:CG2 | 2.62                     | 0.47              |
| 37:C3:56:G:N2      | 88:C3:311:HOH:O   | 2.47                     | 0.47              |
| 40:F3:73:ARG:NH1   | 88:A3:3643:HOH:O  | 2.43                     | 0.47              |
| 77:s3:272:ASP:OD1  | 77:s3:272:ASP:N   | 2.44                     | 0.47              |
| 81:A3:193:G:N1     | 81:A3:196:A:OP2   | 2.43                     | 0.47              |
| 81:A3:728:A:N1     | 81:A3:791:G:O2'   | 2.42                     | 0.47              |
| 81:A3:2312:A:N3    | 81:A3:2964:G:O2'  | 2.45                     | 0.47              |
| 36:W2:19:G:C6      | 81:A3:2458:U:C2   | 3.03                     | 0.47              |
| 3:h1:19:A:OP1      | 88:h1:2172:HOH:O  | 2.21                     | 0.47              |
| 3:h1:204:U:O2      | 18:P1:193:ARG:NH1 | 2.48                     | 0.47              |
| 19:Q1:20:THR:HG1   | 19:Q1:35:SER:HG   | 1.63                     | 0.47              |
| 34:f1:89:ARG:NH2   | 34:f1:120:ASP:OD2 | 2.42                     | 0.47              |
| 42:H3:95:TRP:CH2   | 42:H3:99:MET:HE3  | 2.50                     | 0.47              |
| 57:W3:60:LEU:HD13  | 57:W3:61:PRO:HD2  | 1.96                     | 0.47              |
| 69:h3:91:GLY:O     | 69:h3:94:ASN:ND2  | 2.48                     | 0.47              |
| 70:j3:42:ASP:OD1   | 70:j3:42:ASP:N    | 2.45                     | 0.47              |
| 77:s3:205:ILE:HD12 | 77:s3:205:ILE:O   | 2.15                     | 0.47              |
| 63:b3:155:LYS:HE2  | 63:b3:155:LYS:H   | 1.80                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 81:A3:1901:A:O2'   | 81:A3:3055:G:H4'    | 2.14                     | 0.47              |
| 81:A3:1931:U:O2'   | 81:A3:1933:G:N7     | 2.47                     | 0.47              |
| 3:h1:783:U:O2      | 3:h1:784:A:N6       | 2.49                     | 0.46              |
| 3:h1:1763:A:O2'    | 3:h1:1764:A:O4'     | 2.22                     | 0.46              |
| 81:A3:2276:G:O2'   | 81:A3:2314:G:O6     | 2.28                     | 0.46              |
| 37:C3:55:A:N7      | 88:C3:306:HOH:O     | 2.36                     | 0.46              |
| 81:A3:51:G:H4'     | 81:A3:822:G:H4'     | 1.97                     | 0.46              |
| 19:Q1:171:SER:OG   | 19:Q1:172:TRP:N     | 2.47                     | 0.46              |
| 23:U1:84:LEU:HD12  | 23:U1:95:PHE:HB3    | 1.97                     | 0.46              |
| 39:E3:103:ASN:OD1  | 39:E3:103:ASN:C     | 2.57                     | 0.46              |
| 40:F3:96:ARG:NH1   | 40:F3:104:GLU:OE1   | 2.47                     | 0.46              |
| 43:I3:10:GLN:NE2   | 88:I3:201:HOH:O     | 2.36                     | 0.46              |
| 74:o3:143:ASN:OD1  | 74:o3:145:THR:OG1   | 2.30                     | 0.46              |
| 81:A3:91:C:OP1     | 85:A3:3450:SPD:H22  | 2.15                     | 0.46              |
| 2:k1:221:LEU:O     | 2:k1:221:LEU:HD13   | 2.15                     | 0.46              |
| 3:h1:15:U:H2'      | 3:h1:16:G:O4'       | 2.15                     | 0.46              |
| 3:h1:17:C:H5'      | 86:h1:2017:SPM:HN11 | 1.80                     | 0.46              |
| 3:h1:318:C:OP1     | 88:h1:2173:HOH:O    | 2.21                     | 0.46              |
| 3:h1:1034:U:H4'    | 3:h1:1035:G:OP2     | 2.16                     | 0.46              |
| 18:P1:186:SER:OG   | 18:P1:193:ARG:O     | 2.30                     | 0.46              |
| 19:Q1:277:LYS:HE3  | 19:Q1:277:LYS:HA    | 1.97                     | 0.46              |
| 50:P3:22:VAL:HG11  | 50:P3:97:ILE:HD12   | 1.97                     | 0.46              |
| 81:A3:61:A:N3      | 81:A3:76:U:O2'      | 2.43                     | 0.46              |
| 81:A3:555:G:H2'    | 81:A3:556:C:C6      | 2.50                     | 0.46              |
| 1:A1:32:SER:HG     | 1:A1:81:THR:HG1     | 1.58                     | 0.46              |
| 3:h1:465:G:OP1     | 30:b1:2:VAL:N       | 2.48                     | 0.46              |
| 3:h1:1030:A:OP1    | 3:h1:1797:G:O2'     | 2.27                     | 0.46              |
| 3:h1:1775:G:OP1    | 88:h1:2171:HOH:O    | 2.20                     | 0.46              |
| 14:L1:28:VAL:HG23  | 14:L1:38:ILE:HG23   | 1.97                     | 0.46              |
| 37:C3:28:C:O2'     | 37:C3:54:A:N1       | 2.44                     | 0.46              |
| 52:R3:113:ALA:HB3  | 52:R3:120:ILE:HD11  | 1.97                     | 0.46              |
| 81:A3:1006:G:N2    | 81:A3:1007:U:O4     | 2.36                     | 0.46              |
| 2:k1:144:ARG:HG3   | 2:k1:144:ARG:HH11   | 1.80                     | 0.46              |
| 37:C3:73:U:OP2     | 37:C3:74:A:O2'      | 2.11                     | 0.46              |
| 48:N3:34:SER:OG    | 48:N3:36:GLU:OE1    | 2.33                     | 0.46              |
| 73:n3:34:ALA:O     | 73:n3:39:GLY:N      | 2.46                     | 0.46              |
| 78:t3:108:ILE:HD12 | 78:t3:108:ILE:O     | 2.15                     | 0.46              |
| 81:A3:1375:A:H2'   | 81:A3:1376:U:O4'    | 2.16                     | 0.46              |
| 81:A3:2457:G:O6    | 81:A3:2464:A:O2'    | 2.22                     | 0.46              |
| 81:A3:3059:U:H3'   | 81:A3:3060:C:H4'    | 1.97                     | 0.46              |
| 13:K1:39:CYS:SG    | 13:K1:65:LEU:HD21   | 2.55                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:Q1:262:ASP:O    | 19:Q1:266:LYS:N    | 2.43                     | 0.46              |
| 42:H3:116:ASP:OD2  | 42:H3:116:ASP:N    | 2.43                     | 0.46              |
| 72:m3:82:GLU:OE1   | 72:m3:83:ARG:NH2   | 2.49                     | 0.46              |
| 3:h1:1548:G:O2'    | 3:h1:1549:A:OP2    | 2.30                     | 0.46              |
| 88:h1:2922:HOH:O   | 27:Y1:145:SER:HB3  | 2.15                     | 0.46              |
| 4:l1:95:LEU:HD21   | 4:l1:103:LEU:HD12  | 1.98                     | 0.46              |
| 41:G3:142:LYS:NZ   | 81:A3:985:C:O2'    | 2.49                     | 0.46              |
| 81:A3:327:G:C2     | 81:A3:328:G:C8     | 3.04                     | 0.46              |
| 41:G3:27:LYS:NZ    | 81:A3:1368:G:O6    | 2.47                     | 0.46              |
| 41:G3:177:ARG:O    | 67:f3:51:GLY:N     | 2.46                     | 0.46              |
| 62:a3:75:SER:O     | 62:a3:79:VAL:HG23  | 2.16                     | 0.46              |
| 81:A3:2148:A:H1'   | 81:A3:2284:A2M:H61 | 1.81                     | 0.46              |
| 3:h1:16:G:H2'      | 3:h1:17:C:C6       | 2.51                     | 0.46              |
| 3:h1:139:U:H4'     | 3:h1:140:OMC:O5'   | 2.14                     | 0.46              |
| 54:T3:104:LYS:NZ   | 81:A3:2556:U:OP1   | 2.49                     | 0.46              |
| 60:p3:24:SER:O     | 60:p3:25:LYS:HB2   | 2.16                     | 0.46              |
| 77:s3:121:ASN:OD1  | 81:A3:685:G:O2'    | 2.32                     | 0.46              |
| 81:A3:2194:PSU:OP2 | 88:A3:3734:HOH:O   | 2.20                     | 0.46              |
| 3:h1:964:U:C2      | 3:h1:965:C:C5      | 3.04                     | 0.45              |
| 38:D3:49:THR:OG1   | 38:D3:149:GLN:O    | 2.35                     | 0.45              |
| 81:A3:410:U:H2'    | 81:A3:411:C:C6     | 2.51                     | 0.45              |
| 2:k1:152:GLU:N     | 2:k1:152:GLU:CD    | 2.73                     | 0.45              |
| 3:h1:17:C:OP1      | 86:h1:2017:SPM:N1  | 2.49                     | 0.45              |
| 3:h1:759:A:H2'     | 3:h1:760:A:O4'     | 2.16                     | 0.45              |
| 3:h1:1117:G:O2'    | 3:h1:1133:G:O6     | 2.33                     | 0.45              |
| 13:K1:44:ASN:OD1   | 13:K1:45:ILE:N     | 2.49                     | 0.45              |
| 19:Q1:263:LEU:H    | 19:Q1:263:LEU:HD12 | 1.82                     | 0.45              |
| 27:Y1:82:VAL:HG13  | 27:Y1:111:GLN:OE1  | 2.16                     | 0.45              |
| 81:A3:1206:G:H2'   | 81:A3:1207:A:C8    | 2.52                     | 0.45              |
| 81:A3:1545:A:H2'   | 81:A3:1546:A:C8    | 2.51                     | 0.45              |
| 81:A3:1754:A:OP1   | 88:A3:3736:HOH:O   | 2.21                     | 0.45              |
| 81:A3:2614:U:H2'   | 81:A3:2615:U:C6    | 2.51                     | 0.45              |
| 81:A3:2631:A:N1    | 81:A3:2653:UY1:N3  | 2.64                     | 0.45              |
| 81:A3:2846:U:H2'   | 81:A3:2846:U:O2    | 2.15                     | 0.45              |
| 81:A3:3053:U:C2    | 81:A3:3054:G:C8    | 3.04                     | 0.45              |
| 1:A1:104:ASP:OD2   | 1:A1:104:ASP:C     | 2.59                     | 0.45              |
| 2:k1:205:LYS:NZ    | 3:h1:126:U:OP1     | 2.49                     | 0.45              |
| 3:h1:24:U:O2'      | 3:h1:26:A:OP1      | 2.34                     | 0.45              |
| 19:Q1:153:VAL:HG13 | 19:Q1:170:GLY:O    | 2.16                     | 0.45              |
| 25:W1:115:LEU:O    | 25:W1:119:GLU:HG3  | 2.16                     | 0.45              |
| 28:Z1:89:LYS:HE2   | 28:Z1:89:LYS:HA    | 1.97                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 81:A3:369:A2M:O5'   | 81:A3:369:A2M:H8   | 2.17                     | 0.45              |
| 81:A3:900:C:O2'     | 81:A3:2327:A:N3    | 2.47                     | 0.45              |
| 81:A3:2223:A2M:HM'2 | 81:A3:2224:G:O4'   | 2.16                     | 0.45              |
| 3:h1:293:C:C2       | 3:h1:294:G:C8      | 3.04                     | 0.45              |
| 3:h1:1383:OMU:HM21  | 34:f1:17:PHE:HB3   | 1.98                     | 0.45              |
| 44:J3:29:THR:O      | 44:J3:32:ARG:NE    | 2.49                     | 0.45              |
| 44:J3:105:VAL:HG12  | 44:J3:109:MET:HE3  | 1.99                     | 0.45              |
| 44:J3:130:ARG:NH2   | 81:A3:1074:G:N3    | 2.64                     | 0.45              |
| 67:f3:76:ASP:OD1    | 67:f3:77:ASN:ND2   | 2.46                     | 0.45              |
| 81:A3:174:G:C4      | 81:A3:175:A:C8     | 3.05                     | 0.45              |
| 81:A3:286:A:H2'     | 81:A3:287:G:H8     | 1.81                     | 0.45              |
| 81:A3:369:A2M:HM'2  | 81:A3:370:A:O4'    | 2.16                     | 0.45              |
| 81:A3:2503:U:O2'    | 81:A3:2504:U:P     | 2.73                     | 0.45              |
| 81:A3:3091:C:H2'    | 81:A3:3092:U:O4'   | 2.16                     | 0.45              |
| 3:h1:275:C:HO2'     | 3:h1:276:G:H8      | 1.61                     | 0.45              |
| 3:h1:648:U:O2       | 3:h1:688:G:C6      | 2.69                     | 0.45              |
| 8:F1:46:THR:OG1     | 21:S1:45:ASP:OD2   | 2.32                     | 0.45              |
| 17:O1:37:LEU:HB3    | 17:O1:41:LEU:CD1   | 2.46                     | 0.45              |
| 81:A3:667:A:H2'     | 81:A3:668:A:C8     | 2.52                     | 0.45              |
| 81:A3:2658:U:H4'    | 81:A3:2659:A:O4'   | 2.17                     | 0.45              |
| 81:A3:3021:C:H2'    | 81:A3:3022:U:O4'   | 2.17                     | 0.45              |
| 3:h1:855:A:OP1      | 42:H3:176:ARG:NH2  | 2.46                     | 0.45              |
| 3:h1:981:A:H2'      | 3:h1:982:A:O4'     | 2.17                     | 0.45              |
| 13:K1:74:ARG:NH1    | 13:K1:74:ARG:HB2   | 2.32                     | 0.45              |
| 17:O1:131:VAL:O     | 17:O1:134:ALA:N    | 2.50                     | 0.45              |
| 29:a1:142:SER:OG    | 29:a1:152:SER:OG   | 2.26                     | 0.45              |
| 45:K3:58:ASP:OD1    | 45:K3:59:SER:N     | 2.50                     | 0.45              |
| 53:S3:15:ARG:NH1    | 81:A3:3173:C:OP1   | 2.49                     | 0.45              |
| 81:A3:2692:G:H2'    | 81:A3:2692:G:N3    | 2.31                     | 0.45              |
| 3:h1:814:U:O2       | 17:O1:112:GLN:NE2  | 2.50                     | 0.45              |
| 3:h1:965:C:H2'      | 3:h1:966:A:O4'     | 2.17                     | 0.45              |
| 14:L1:64:LEU:HD23   | 32:d1:134:ILE:HD11 | 1.99                     | 0.45              |
| 29:a1:110:TYR:CD1   | 29:a1:110:TYR:C    | 2.94                     | 0.45              |
| 62:a3:8:ALA:O       | 62:a3:11:VAL:HG22  | 2.17                     | 0.45              |
| 69:h3:212:GLU:OE2   | 69:h3:212:GLU:C    | 2.59                     | 0.45              |
| 81:A3:799:A:OP1     | 88:A3:3735:HOH:O   | 2.21                     | 0.45              |
| 81:A3:2422:A:H2'    | 81:A3:2423:C:C6    | 2.52                     | 0.45              |
| 24:V1:22:ARG:NH1    | 24:V1:36:LEU:O     | 2.48                     | 0.45              |
| 69:h3:83:LEU:N      | 69:h3:84:PRO:CD    | 2.80                     | 0.45              |
| 6:D1:100:LYS:H      | 6:D1:100:LYS:HD3   | 1.82                     | 0.45              |
| 32:d1:133:ARG:NH2   | 32:d1:139:VAL:O    | 2.50                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:P3:56:LEU:HD23 | 54:T3:89:GLU:HG3   | 1.99                     | 0.45              |
| 64:c3:206:GLU:OE1 | 64:c3:206:GLU:N    | 2.42                     | 0.45              |
| 70:j3:29:THR:HG21 | 70:j3:147:ILE:HD11 | 1.97                     | 0.45              |
| 81:A3:3123:U:H4'  | 81:A3:3124:A:OP1   | 2.17                     | 0.45              |
| 8:F1:226:GLY:O    | 8:F1:230:GLU:HG2   | 2.17                     | 0.45              |
| 13:K1:10:LEU:HD22 | 33:e1:51:GLU:OE1   | 2.16                     | 0.45              |
| 37:C3:27:A:N7     | 88:C3:307:HOH:O    | 2.36                     | 0.45              |
| 79:u3:44:ASP:HB3  | 79:u3:61:ASP:OD1   | 2.17                     | 0.45              |
| 81:A3:196:A:O2'   | 81:A3:197:G:OP2    | 2.22                     | 0.45              |
| 81:A3:549:U:H3'   | 81:A3:550:G:C5'    | 2.47                     | 0.45              |
| 2:k1:221:LEU:HD13 | 2:k1:221:LEU:C     | 2.42                     | 0.44              |
| 3:h1:1543:A:N3    | 3:h1:1543:A:H2'    | 2.31                     | 0.44              |
| 5:C1:66:ALA:HB1   | 5:C1:95:ALA:HB2    | 1.99                     | 0.44              |
| 25:W1:67:THR:HG21 | 25:W1:74:ILE:HD11  | 1.98                     | 0.44              |
| 28:Z1:44:ASP:OD2  | 28:Z1:44:ASP:C     | 2.59                     | 0.44              |
| 34:f1:36:ILE:HD13 | 34:f1:59:ILE:HD11  | 1.98                     | 0.44              |
| 56:V3:76:THR:HG21 | 82:B3:97:C:O3'     | 2.16                     | 0.44              |
| 63:b3:197:GLU:OE2 | 63:b3:197:GLU:C    | 2.60                     | 0.44              |
| 81:A3:173:G:C6    | 81:A3:240:G:C6     | 3.05                     | 0.44              |
| 81:A3:355:G:N2    | 81:A3:358:A:OP2    | 2.47                     | 0.44              |
| 81:A3:2680:G:H2'  | 81:A3:2680:G:N3    | 2.31                     | 0.44              |
| 3:h1:628:C:H2'    | 3:h1:629:U:C6      | 2.52                     | 0.44              |
| 3:h1:1007:U:OP1   | 88:h1:2170:HOH:O   | 2.20                     | 0.44              |
| 14:L1:23:VAL:HG21 | 14:L1:64:LEU:HD22  | 1.98                     | 0.44              |
| 18:P1:29:LEU:HD12 | 18:P1:29:LEU:C     | 2.42                     | 0.44              |
| 19:Q1:113:ALA:HB3 | 19:Q1:122:VAL:HG12 | 2.00                     | 0.44              |
| 28:Z1:14:ASP:OD2  | 28:Z1:177:LEU:HD21 | 2.18                     | 0.44              |
| 28:Z1:147:PHE:O   | 28:Z1:165:ASN:ND2  | 2.44                     | 0.44              |
| 31:c1:48:THR:OG1  | 31:c1:74:GLU:OE1   | 2.30                     | 0.44              |
| 67:f3:85:GLU:O    | 67:f3:88:ASP:OD2   | 2.35                     | 0.44              |
| 70:j3:36:LEU:CD1  | 70:j3:92:ILE:HG21  | 2.47                     | 0.44              |
| 72:m3:15:ARG:NH1  | 81:A3:213:G:OP1    | 2.45                     | 0.44              |
| 3:h1:337:A:OP2    | 18:P1:55:LYS:NZ    | 2.50                     | 0.44              |
| 27:Y1:27:VAL:HG11 | 27:Y1:35:MET:HE1   | 1.98                     | 0.44              |
| 29:a1:181:ARG:HB3 | 29:a1:181:ARG:CZ   | 2.47                     | 0.44              |
| 36:i2:18:G:O2'    | 36:i2:60:C:N3      | 2.50                     | 0.44              |
| 36:i2:58:A:O2'    | 36:i2:60:C:OP2     | 2.24                     | 0.44              |
| 40:F3:171:TYR:CD1 | 40:F3:171:TYR:C    | 2.96                     | 0.44              |
| 81:A3:649:C:N4    | 81:A3:650:G:O6     | 2.50                     | 0.44              |
| 81:A3:3308:A:OP2  | 81:A3:3381:U:O2'   | 2.17                     | 0.44              |
| 82:B3:162:G:C2'   | 82:B3:163:C:H5'    | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:h1:1110:G:O2'    | 3:h1:1111:G:H5'    | 2.18                     | 0.44              |
| 3:h1:1781:4AC:O7   | 3:h1:1781:4AC:H5   | 2.17                     | 0.44              |
| 3:h1:1801:G:N2     | 12:J1:76:SER:OG    | 2.46                     | 0.44              |
| 6:D1:113:GLU:OE2   | 6:D1:113:GLU:O     | 2.34                     | 0.44              |
| 10:H1:119:VAL:HG21 | 10:H1:127:ALA:HB1  | 2.00                     | 0.44              |
| 34:f1:35:LEU:HD12  | 34:f1:35:LEU:C     | 2.42                     | 0.44              |
| 81:A3:404:A:C2     | 82:B3:20:A:H1'     | 2.53                     | 0.44              |
| 81:A3:473:G:H2'    | 81:A3:474:G:C8     | 2.52                     | 0.44              |
| 81:A3:1168:G:H2'   | 81:A3:1169:G:O4'   | 2.18                     | 0.44              |
| 81:A3:2152:A:H2'   | 81:A3:2153:A:C8    | 2.53                     | 0.44              |
| 17:O1:142:ARG:HB3  | 17:O1:150:ILE:HG22 | 1.98                     | 0.44              |
| 57:W3:67:GLN:OE1   | 57:W3:69:LEU:HD21  | 2.17                     | 0.44              |
| 72:m3:55:VAL:HG13  | 72:m3:103:VAL:HB   | 1.98                     | 0.44              |
| 81:A3:544:G:C6     | 81:A3:545:C:N4     | 2.86                     | 0.44              |
| 81:A3:666:C:H2'    | 81:A3:667:A:C8     | 2.52                     | 0.44              |
| 81:A3:2629:A:OP2   | 88:A3:3739:HOH:O   | 2.21                     | 0.44              |
| 3:h1:812:C:C2      | 3:h1:813:A:C8      | 3.06                     | 0.44              |
| 3:h1:889:U:O2      | 21:S1:136:THR:OG1  | 2.34                     | 0.44              |
| 3:h1:1446:C:H2'    | 3:h1:1447:OMU:H6   | 1.99                     | 0.44              |
| 3:h1:1461:C:OP1    | 3:h1:1462:C:O2'    | 2.23                     | 0.44              |
| 14:L1:14:MET:HG3   | 14:L1:39:MET:HE2   | 1.99                     | 0.44              |
| 28:Z1:21:ALA:HB2   | 28:Z1:173:VAL:HG21 | 2.00                     | 0.44              |
| 30:b1:64:LEU:O     | 30:b1:71:ARG:NH1   | 2.48                     | 0.44              |
| 34:f1:112:ILE:HA   | 34:f1:115:ILE:HG22 | 2.00                     | 0.44              |
| 45:K3:36:ILE:HG22  | 45:K3:64:ARG:HG3   | 1.99                     | 0.44              |
| 50:P3:32:TYR:CZ    | 50:P3:36:LEU:HD11  | 2.53                     | 0.44              |
| 54:T3:50:ARG:NH2   | 81:A3:1743:C:O2    | 2.50                     | 0.44              |
| 75:q3:67:ARG:NH2   | 81:A3:521:G:OP1    | 2.50                     | 0.44              |
| 81:A3:6:C:H2'      | 81:A3:7:C:C6       | 2.52                     | 0.44              |
| 81:A3:1147:A:O4'   | 81:A3:2639:A:N6    | 2.50                     | 0.44              |
| 81:A3:1449:U:OP2   | 88:A3:3740:HOH:O   | 2.21                     | 0.44              |
| 81:A3:1624:A:H2'   | 81:A3:1625:C:O4'   | 2.18                     | 0.44              |
| 81:A3:2482:G:HO2'  | 81:A3:2483:A:P     | 2.41                     | 0.44              |
| 81:A3:866:G:C2'    | 81:A3:867:G:O5'    | 2.66                     | 0.44              |
| 81:A3:1718:G:O2'   | 81:A3:1735:G:N2    | 2.49                     | 0.44              |
| 3:h1:864:U:H2'     | 3:h1:865:A:O4'     | 2.18                     | 0.44              |
| 3:h1:1118:U:H4'    | 60:p3:10:MET:HE2   | 1.99                     | 0.44              |
| 19:Q1:100:ARG:HA   | 19:Q1:100:ARG:NE   | 2.32                     | 0.44              |
| 40:F3:48:ALA:HB1   | 40:F3:53:TYR:HB3   | 2.00                     | 0.44              |
| 63:b3:227:GLU:OE1  | 63:b3:227:GLU:HA   | 2.16                     | 0.44              |
| 1:A1:19:MET:HE1    | 3:h1:792:U:C4      | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:h1:647:A:N1      | 3:h1:690:C:N4      | 2.66                     | 0.44              |
| 3:h1:1049:G:OP2    | 88:h1:2174:HOH:O   | 2.21                     | 0.44              |
| 3:h1:1106:PSU:OP2  | 88:h1:2176:HOH:O   | 2.21                     | 0.44              |
| 3:h1:1511:C:H2'    | 3:h1:1512:A:O4'    | 2.18                     | 0.44              |
| 17:O1:162:ASN:OD1  | 17:O1:162:ASN:N    | 2.50                     | 0.44              |
| 19:Q1:66:PHE:C     | 19:Q1:83:SER:HG    | 2.25                     | 0.44              |
| 53:S3:50:LEU:HD21  | 53:S3:79:PRO:HD3   | 2.00                     | 0.44              |
| 81:A3:540:A:HO2'   | 81:A3:541:U:C5'    | 2.20                     | 0.44              |
| 81:A3:2242:G:O6    | 88:A3:3728:HOH:O   | 2.19                     | 0.44              |
| 81:A3:2826:G:C6    | 81:A3:2827:G:N7    | 2.85                     | 0.44              |
| 3:h1:295:C:C2      | 3:h1:296:A:C8      | 3.06                     | 0.43              |
| 22:T1:21:ARG:NH2   | 88:T1:301:HOH:O    | 2.39                     | 0.43              |
| 29:a1:194:ASP:OD1  | 29:a1:195:TRP:N    | 2.51                     | 0.43              |
| 3:h1:81:U:O2'      | 3:h1:82:G:OP1      | 2.34                     | 0.43              |
| 3:h1:1504:U:C2     | 3:h1:1505:G:C8     | 3.06                     | 0.43              |
| 19:Q1:31:MET:SD    | 19:Q1:31:MET:C     | 3.01                     | 0.43              |
| 62:a3:23:ARG:NH2   | 88:a3:202:HOH:O    | 2.51                     | 0.43              |
| 3:h1:1177:C:O2'    | 3:h1:1199:A:N6     | 2.50                     | 0.43              |
| 6:D1:35:LEU:HD21   | 6:D1:50:ILE:HG22   | 2.00                     | 0.43              |
| 81:A3:546:C:C2     | 81:A3:547:C:C5     | 3.07                     | 0.43              |
| 81:A3:1143:C:H2'   | 81:A3:1144:A2M:H8  | 2.00                     | 0.43              |
| 81:A3:1185:G:H2'   | 81:A3:1186:C:C6    | 2.53                     | 0.43              |
| 81:A3:1830:C:C2    | 81:A3:1831:G:C8    | 3.06                     | 0.43              |
| 3:h1:127:G:H3'     | 3:h1:128:G:H5'     | 2.01                     | 0.43              |
| 3:h1:193:G:O2'     | 3:h1:194:A:OP2     | 2.31                     | 0.43              |
| 3:h1:503:C:O2'     | 3:h1:504:U:O5'     | 2.32                     | 0.43              |
| 3:h1:1382:U:O2     | 3:h1:1384:C:N4     | 2.49                     | 0.43              |
| 5:C1:30:ALA:O      | 5:C1:34:VAL:HG12   | 2.19                     | 0.43              |
| 6:D1:20:TYR:OH     | 29:a1:214:HIS:O    | 2.20                     | 0.43              |
| 25:W1:138:VAL:HG22 | 25:W1:138:VAL:O    | 2.19                     | 0.43              |
| 40:F3:46:ASP:OD1   | 40:F3:46:ASP:N     | 2.51                     | 0.43              |
| 61:Z3:2:VAL:N      | 61:Z3:90:HIS:O     | 2.52                     | 0.43              |
| 62:a3:26:ILE:CD1   | 74:o3:180:LEU:HD11 | 2.49                     | 0.43              |
| 71:k3:71:GLN:HG2   | 71:k3:72:TYR:N     | 2.33                     | 0.43              |
| 71:k3:141:ASP:OD1  | 71:k3:141:ASP:N    | 2.51                     | 0.43              |
| 72:m3:87:GLU:OE2   | 72:m3:87:GLU:HA    | 2.18                     | 0.43              |
| 81:A3:3015:U:H2'   | 81:A3:3016:U:C6    | 2.53                     | 0.43              |
| 81:A3:3115:A:N1    | 81:A3:3124:A:C8    | 2.87                     | 0.43              |
| 3:h1:194:A:HO2'    | 3:h1:195:A:H8      | 1.65                     | 0.43              |
| 3:h1:983:G:H4'     | 3:h1:1784:A:H4'    | 1.99                     | 0.43              |
| 81:A3:187:U:O2'    | 88:A3:3616:HOH:O   | 2.02                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 81:A3:777:U:C2      | 81:A3:778:G:C8     | 3.06                     | 0.43              |
| 81:A3:2542:C:H6     | 81:A3:2542:C:O5'   | 2.02                     | 0.43              |
| 82:B3:127:C:H2'     | 82:B3:128:C:N1     | 2.33                     | 0.43              |
| 23:U1:110:ASP:OD1   | 23:U1:110:ASP:N    | 2.52                     | 0.43              |
| 53:S3:89:LYS:NZ     | 81:A3:1176:G:OP1   | 2.39                     | 0.43              |
| 67:f3:54:GLY:O      | 88:f3:302:HOH:O    | 2.22                     | 0.43              |
| 81:A3:1191:C:C2     | 81:A3:1193:G:C8    | 3.06                     | 0.43              |
| 81:A3:3137:G:C4     | 81:A3:3138:G:C8    | 3.07                     | 0.43              |
| 2:k1:18:ILE:HG22    | 2:k1:20:ASP:H      | 1.84                     | 0.43              |
| 3:h1:188:U:O4       | 18:P1:151:SER:OG   | 2.36                     | 0.43              |
| 3:h1:1737:U:H2'     | 3:h1:1738:G:O4'    | 2.18                     | 0.43              |
| 18:P1:169:PRO:O     | 18:P1:173:GLU:HG3  | 2.18                     | 0.43              |
| 43:I3:173:ARG:NH2   | 65:d3:17:ARG:O     | 2.50                     | 0.43              |
| 47:M3:61:LYS:NZ     | 81:A3:1816:C:OP1   | 2.45                     | 0.43              |
| 47:M3:67:ARG:NH1    | 81:A3:1818:G:O6    | 2.45                     | 0.43              |
| 75:q3:235:ASN:O     | 75:q3:239:ARG:HG2  | 2.19                     | 0.43              |
| 76:r3:139:THR:O     | 76:r3:142:GLY:N    | 2.51                     | 0.43              |
| 3:h1:569:C:H4'      | 15:M1:5:HIS:O      | 2.18                     | 0.43              |
| 5:C1:134:LEU:O      | 5:C1:134:LEU:HD13  | 2.19                     | 0.43              |
| 36:W2:7:A:N6        | 36:W2:49:G:O6      | 2.51                     | 0.43              |
| 42:H3:180:ARG:O     | 42:H3:183:GLN:HB3  | 2.19                     | 0.43              |
| 81:A3:2948:G:O2'    | 81:A3:2951:OMC:OP2 | 2.33                     | 0.43              |
| 81:A3:3210:U:O2'    | 88:A3:3709:HOH:O   | 2.16                     | 0.43              |
| 2:k1:130:GLU:OE2    | 2:k1:131:LYS:O     | 2.37                     | 0.43              |
| 2:k1:185:THR:OG1    | 2:k1:188:THR:HG23  | 2.19                     | 0.43              |
| 43:I3:175:ASN:OD1   | 81:A3:3182:G:N2    | 2.40                     | 0.43              |
| 69:h3:119:TYR:OH    | 69:h3:138:ARG:O    | 2.36                     | 0.43              |
| 81:A3:1411:G:C6     | 81:A3:1423:G:C5    | 3.07                     | 0.43              |
| 81:A3:1745:A:H2'    | 81:A3:1746:G:O4'   | 2.19                     | 0.43              |
| 81:A3:2804:A2M:HM'2 | 81:A3:2804:A2M:H1' | 1.84                     | 0.43              |
| 5:C1:48:LEU:HD23    | 16:N1:102:VAL:HG21 | 2.01                     | 0.43              |
| 17:O1:80:LEU:HD22   | 17:O1:95:PHE:CZ    | 2.54                     | 0.43              |
| 25:W1:30:ALA:O      | 25:W1:34:GLU:HG3   | 2.19                     | 0.43              |
| 77:s3:369:GLU:OE1   | 77:s3:369:GLU:N    | 2.36                     | 0.43              |
| 81:A3:280:G:O6      | 81:A3:301:G:H1'    | 2.19                     | 0.43              |
| 81:A3:897:G:H2'     | 81:A3:898:U:C6     | 2.54                     | 0.43              |
| 81:A3:962:A:H4'     | 81:A3:978:G:N2     | 2.33                     | 0.43              |
| 81:A3:2273:A:H2'    | 81:A3:2274:A:C8    | 2.54                     | 0.43              |
| 81:A3:2457:G:H2'    | 81:A3:2460:G:O6    | 2.19                     | 0.43              |
| 81:A3:2715:U:OP2    | 88:A3:3744:HOH:O   | 2.22                     | 0.43              |
| 3:h1:399:U:H2'      | 3:h1:400:G:O4'     | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:h1:478:A:OP1     | 30:b1:147:SER:OG   | 2.25                     | 0.42              |
| 3:h1:927:A:H2'     | 3:h1:928:G:C8      | 2.55                     | 0.42              |
| 3:h1:1476:A:H2     | 3:h1:1479:G:N3     | 2.16                     | 0.42              |
| 3:h1:1530:A:H2'    | 3:h1:1531:A:C8     | 2.54                     | 0.42              |
| 36:W2:67:C:H2'     | 36:W2:68:A:C8      | 2.54                     | 0.42              |
| 47:M3:76:ASN:OD1   | 47:M3:77:TYR:N     | 2.52                     | 0.42              |
| 57:W3:35:LYS:NZ    | 81:A3:1756:G:O6    | 2.48                     | 0.42              |
| 81:A3:1728:A:N1    | 81:A3:1794:C:O2'   | 2.43                     | 0.42              |
| 81:A3:2148:A:H1'   | 81:A3:2284:A2M:N6  | 2.34                     | 0.42              |
| 3:h1:569:C:H2'     | 3:h1:570:A:O4'     | 2.19                     | 0.42              |
| 3:h1:932:A:C8      | 21:S1:136:THR:O    | 2.72                     | 0.42              |
| 3:h1:1780:C:H2'    | 3:h1:1781:4AC:H6   | 2.01                     | 0.42              |
| 20:R1:37:LYS:HE2   | 20:R1:37:LYS:HB3   | 1.91                     | 0.42              |
| 28:Z1:17:MET:HE1   | 28:Z1:176:TRP:CE3  | 2.54                     | 0.42              |
| 31:c1:175:VAL:HG11 | 31:c1:220:PHE:HA   | 2.01                     | 0.42              |
| 41:G3:176:ALA:O    | 41:G3:183:ARG:HB2  | 2.18                     | 0.42              |
| 81:A3:2884:C:H2'   | 81:A3:2885:U:C6    | 2.53                     | 0.42              |
| 3:h1:766:A:OP1     | 30:b1:81:ARG:NH2   | 2.41                     | 0.42              |
| 3:h1:1149:G:H2'    | 3:h1:1150:A:C8     | 2.55                     | 0.42              |
| 8:F1:120:LEU:HD21  | 8:F1:122:GLU:HG3   | 2.01                     | 0.42              |
| 19:Q1:69:ASP:C     | 19:Q1:69:ASP:OD2   | 2.61                     | 0.42              |
| 25:W1:87:ASP:OD1   | 25:W1:88:LEU:N     | 2.52                     | 0.42              |
| 25:W1:99:ARG:NH2   | 25:W1:143:SER:OG   | 2.51                     | 0.42              |
| 81:A3:148:A:C4     | 81:A3:149:G:C8     | 3.07                     | 0.42              |
| 81:A3:2141:U:C6    | 81:A3:2145:U:C4    | 3.06                     | 0.42              |
| 82:B3:10:U:H2'     | 82:B3:11:C:C6      | 2.54                     | 0.42              |
| 3:h1:204:U:O2      | 18:P1:193:ARG:NH2  | 2.53                     | 0.42              |
| 3:h1:782:C:O2'     | 3:h1:783:U:O4'     | 2.36                     | 0.42              |
| 79:u3:89:LYS:HB3   | 79:u3:191:VAL:HG22 | 2.02                     | 0.42              |
| 81:A3:1234:G:HO2'  | 81:A3:1235:A:P     | 2.41                     | 0.42              |
| 82:B3:72:U:H2'     | 82:B3:73:G:O4'     | 2.20                     | 0.42              |
| 3:h1:202:C:C2      | 3:h1:203:A:C8      | 3.07                     | 0.42              |
| 3:h1:891:U:O2      | 3:h1:991:C:O2'     | 2.36                     | 0.42              |
| 3:h1:1607:G:OP2    | 7:E1:92:HIS:NE2    | 2.42                     | 0.42              |
| 5:C1:72:PRO:HA     | 5:C1:75:VAL:HG22   | 2.01                     | 0.42              |
| 33:e1:10:ALA:O     | 33:e1:14:MET:HG3   | 2.19                     | 0.42              |
| 34:f1:110:LYS:NZ   | 34:f1:114:ASP:OD2  | 2.40                     | 0.42              |
| 43:I3:143:GLN:HG3  | 79:u3:4:ILE:HD12   | 2.01                     | 0.42              |
| 81:A3:92:G:OP1     | 85:A3:3450:SPD:N1  | 2.51                     | 0.42              |
| 81:A3:184:A:O2'    | 81:A3:185:A:O4'    | 2.36                     | 0.42              |
| 3:h1:1190:PSU:OP2  | 88:h1:2177:HOH:O   | 2.21                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:h1:1601:U:OP2    | 3:h1:1602:C:N4     | 2.44                     | 0.42              |
| 14:L1:8:ALA:HB1    | 14:L1:28:VAL:HB    | 2.02                     | 0.42              |
| 36:i2:18:G:N2      | 36:i2:58:A:O4'     | 2.53                     | 0.42              |
| 81:A3:7:C:H2'      | 81:A3:8:C:O4'      | 2.19                     | 0.42              |
| 81:A3:1119:U:H2'   | 81:A3:1120:C:C6    | 2.55                     | 0.42              |
| 81:A3:1648:G:OP1   | 81:A3:1826:U:O2'   | 2.36                     | 0.42              |
| 81:A3:1847:A:H1'   | 81:A3:1854:U:O4'   | 2.20                     | 0.42              |
| 81:A3:1906:A:O2'   | 81:A3:1912:G:N7    | 2.52                     | 0.42              |
| 3:h1:1738:G:HO2'   | 3:h1:1739:A:H8     | 1.64                     | 0.42              |
| 20:R1:27:LEU:HD21  | 20:R1:115:VAL:HG22 | 2.01                     | 0.42              |
| 44:J3:70:ARG:NH2   | 69:h3:40:ASP:OD1   | 2.53                     | 0.42              |
| 77:s3:109:LYS:HG2  | 77:s3:111:TRP:CZ2  | 2.54                     | 0.42              |
| 79:u3:49:LYS:HB2   | 79:u3:49:LYS:HE2   | 1.86                     | 0.42              |
| 81:A3:227:G:OP1    | 81:A3:701:G:N1     | 2.33                     | 0.42              |
| 81:A3:315:A:OP1    | 88:A3:3738:HOH:O   | 2.21                     | 0.42              |
| 81:A3:965:U:OP1    | 88:A3:3747:HOH:O   | 2.22                     | 0.42              |
| 3:h1:130:A:N6      | 3:h1:268:G:OP1     | 2.51                     | 0.42              |
| 17:O1:127:LEU:O    | 17:O1:130:VAL:HG12 | 2.19                     | 0.42              |
| 23:U1:101:ASN:OD1  | 78:t3:120:PRO:HD2  | 2.19                     | 0.42              |
| 55:U3:46:LEU:HD11  | 64:c3:165:LEU:HA   | 2.02                     | 0.42              |
| 57:W3:56:LEU:O     | 57:W3:60:LEU:HD23  | 2.20                     | 0.42              |
| 76:r3:230:GLU:OE1  | 88:r3:501:HOH:O    | 2.22                     | 0.42              |
| 81:A3:2540:G:O6    | 81:A3:2549:C:N4    | 2.53                     | 0.42              |
| 2:k1:53:MET:HG3    | 2:k1:114:VAL:HG13  | 2.01                     | 0.42              |
| 3:h1:777:C:O2'     | 3:h1:791:G:N2      | 2.53                     | 0.42              |
| 3:h1:1283:4AC:H5   | 3:h1:1283:4AC:O7   | 2.20                     | 0.42              |
| 5:C1:71:GLN:HB2    | 5:C1:74:TYR:HB3    | 2.01                     | 0.42              |
| 8:F1:33:LYS:NZ     | 8:F1:42:ASN:OD1    | 2.49                     | 0.42              |
| 22:T1:130:LEU:HD11 | 22:T1:134:LYS:HE3  | 2.01                     | 0.42              |
| 25:W1:132:THR:O    | 25:W1:132:THR:HG22 | 2.20                     | 0.42              |
| 81:A3:50:A:N6      | 88:A3:4021:HOH:O   | 2.40                     | 0.42              |
| 81:A3:1178:U:OP1   | 88:A3:3746:HOH:O   | 2.22                     | 0.42              |
| 81:A3:1697:U:O3'   | 81:A3:1778:U:O2'   | 2.37                     | 0.42              |
| 3:h1:1683:U:H2'    | 3:h1:1684:C:O4'    | 2.20                     | 0.42              |
| 19:Q1:165:PRO:HB2  | 19:Q1:181:LEU:HD23 | 2.01                     | 0.42              |
| 20:R1:27:LEU:CD2   | 20:R1:115:VAL:HG22 | 2.50                     | 0.42              |
| 64:c3:206:GLU:O    | 64:c3:210:ILE:HG13 | 2.20                     | 0.42              |
| 67:f3:118:GLN:N    | 67:f3:118:GLN:CD   | 2.78                     | 0.42              |
| 76:r3:326:LEU:HB3  | 76:r3:328:ILE:HD11 | 2.01                     | 0.42              |
| 81:A3:1695:U:H2'   | 81:A3:1696:G:C8    | 2.54                     | 0.42              |
| 81:A3:1822:G:H2'   | 81:A3:1823:C:C6    | 2.55                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 81:A3:2177:G:O4'  | 81:A3:2179:U:C6    | 2.73                     | 0.42              |
| 82:B3:19:G:O2'    | 82:B3:20:A:OP2     | 2.35                     | 0.42              |
| 2:k1:160:ASN:OD1  | 2:k1:163:ARG:NH2   | 2.48                     | 0.41              |
| 3:h1:1059:G:O2'   | 3:h1:1060:C:OP1    | 2.34                     | 0.41              |
| 19:Q1:15:HIS:NE2  | 19:Q1:34:THR:OG1   | 2.46                     | 0.41              |
| 25:W1:110:ASP:O   | 25:W1:114:ARG:HG2  | 2.20                     | 0.41              |
| 31:c1:193:VAL:HB  | 31:c1:194:PRO:HD3  | 2.01                     | 0.41              |
| 36:i2:74:C:H5'    | 81:A3:2974:A:H1'   | 2.02                     | 0.41              |
| 55:U3:32:ARG:O    | 81:A3:263:C:N4     | 2.53                     | 0.41              |
| 75:q3:17:LYS:O    | 75:q3:21:GLU:HG3   | 2.20                     | 0.41              |
| 81:A3:760:G:C8    | 81:A3:761:A:C8     | 3.08                     | 0.41              |
| 81:A3:2543:A:HO2' | 81:A3:2544:C:P     | 2.34                     | 0.41              |
| 81:A3:2992:U:H2'  | 81:A3:2993:G:O4'   | 2.20                     | 0.41              |
| 3:h1:512:G:H2'    | 3:h1:513:G:C1'     | 2.50                     | 0.41              |
| 3:h1:970:A:OP2    | 25:W1:124:ARG:NH2  | 2.43                     | 0.41              |
| 3:h1:1105:G:OP1   | 88:h1:2178:HOH:O   | 2.22                     | 0.41              |
| 3:h1:1789:MA6:C9  | 3:h1:1790:MA6:H93  | 2.48                     | 0.41              |
| 23:U1:63:GLU:HA   | 23:U1:66:SER:OG    | 2.20                     | 0.41              |
| 23:U1:65:ASP:O    | 23:U1:69:VAL:HG12  | 2.20                     | 0.41              |
| 67:f3:21:ARG:NH1  | 81:A3:651:U:OP1    | 2.53                     | 0.41              |
| 81:A3:196:A:C4    | 81:A3:198:G:C8     | 3.08                     | 0.41              |
| 81:A3:802:C:H2'   | 81:A3:803:C:C6     | 2.55                     | 0.41              |
| 81:A3:2221:G:H2'  | 81:A3:2222:A:H8    | 1.85                     | 0.41              |
| 81:A3:2408:C:O2   | 81:A3:2822:A:N1    | 2.53                     | 0.41              |
| 81:A3:2450:G:O6   | 81:A3:2451:A:N6    | 2.53                     | 0.41              |
| 81:A3:2514:U:H2'  | 81:A3:2515:U:O4'   | 2.19                     | 0.41              |
| 81:A3:2885:U:H2'  | 81:A3:2886:OMU:O4' | 2.20                     | 0.41              |
| 81:A3:3086:C:H2'  | 81:A3:3087:G:O4'   | 2.20                     | 0.41              |
| 3:h1:616:G:H4'    | 3:h1:617:C:OP1     | 2.20                     | 0.41              |
| 3:h1:976:A:H2'    | 3:h1:977:A2M:H8    | 2.02                     | 0.41              |
| 3:h1:1171:U:O2'   | 88:h1:2155:HOH:O   | 2.17                     | 0.41              |
| 3:h1:1488:A:H2'   | 3:h1:1489:A:C8     | 2.55                     | 0.41              |
| 17:O1:29:ASP:OD2  | 17:O1:29:ASP:N     | 2.52                     | 0.41              |
| 19:Q1:69:ASP:CG   | 19:Q1:112:VAL:HG12 | 2.44                     | 0.41              |
| 33:e1:11:LEU:HD12 | 33:e1:74:VAL:HG23  | 2.01                     | 0.41              |
| 37:C3:88:U:H2'    | 37:C3:89:G:O4'     | 2.20                     | 0.41              |
| 52:R3:97:ILE:HG21 | 52:R3:106:ARG:HG2  | 2.03                     | 0.41              |
| 76:r3:259:HIS:HA  | 76:r3:260:PRO:C    | 2.46                     | 0.41              |
| 81:A3:424:G:N2    | 88:A3:4045:HOH:O   | 2.41                     | 0.41              |
| 81:A3:722:A:O2'   | 88:A3:3737:HOH:O   | 2.21                     | 0.41              |
| 81:A3:959:C:O2'   | 81:A3:981:G:OP1    | 2.28                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 81:A3:2238:C:C2   | 81:A3:2239:OMG:C8  | 3.09                     | 0.41              |
| 3:h1:114:U:O2'    | 3:h1:116:G:H2'     | 2.21                     | 0.41              |
| 3:h1:187:C:H2'    | 3:h1:188:U:O4'     | 2.20                     | 0.41              |
| 3:h1:523:A:H2'    | 3:h1:524:A:O4'     | 2.21                     | 0.41              |
| 3:h1:971:U:H2'    | 3:h1:972:C:O4'     | 2.20                     | 0.41              |
| 3:h1:1316:A:O2'   | 3:h1:1318:U:OP1    | 2.37                     | 0.41              |
| 3:h1:1487:C:O2'   | 34:f1:79:GLY:O     | 2.35                     | 0.41              |
| 29:a1:77:GLN:NE2  | 29:a1:84:GLU:OE2   | 2.53                     | 0.41              |
| 40:F3:124:ASP:OD1 | 40:F3:127:TYR:N    | 2.47                     | 0.41              |
| 52:R3:83:LEU:HD21 | 52:R3:113:ALA:HB2  | 2.03                     | 0.41              |
| 66:e3:13:LYS:HD2  | 66:e3:128:LEU:HD11 | 2.02                     | 0.41              |
| 67:f3:38:MET:HE1  | 85:A3:3450:SPD:H32 | 2.02                     | 0.41              |
| 76:r3:78:ILE:HG13 | 76:r3:327:LEU:HD12 | 2.01                     | 0.41              |
| 81:A3:720:G:H1'   | 81:A3:764:G:O2'    | 2.20                     | 0.41              |
| 81:A3:910:G:H1'   | 81:A3:1594:A:N6    | 2.35                     | 0.41              |
| 81:A3:2547:C:H2'  | 81:A3:2548:C:O4'   | 2.21                     | 0.41              |
| 81:A3:2851:G:C6   | 81:A3:2852:C:C5    | 3.08                     | 0.41              |
| 81:A3:2885:U:H2'  | 81:A3:2886:OMU:C6  | 2.50                     | 0.41              |
| 81:A3:3022:U:H2'  | 81:A3:3035:A:H61   | 1.85                     | 0.41              |
| 3:h1:210:A:H2'    | 3:h1:211:G:O4'     | 2.19                     | 0.41              |
| 3:h1:515:A:OP1    | 30:b1:172:GLY:N    | 2.41                     | 0.41              |
| 3:h1:1278:A:C2    | 3:h1:1443:G:C4     | 3.09                     | 0.41              |
| 6:D1:81:ARG:C     | 6:D1:82:MET:HE2    | 2.45                     | 0.41              |
| 27:Y1:47:ARG:HB3  | 27:Y1:48:PRO:HD3   | 2.03                     | 0.41              |
| 40:F3:33:LEU:HD21 | 64:c3:56:ILE:HD13  | 2.01                     | 0.41              |
| 47:M3:114:LYS:O   | 47:M3:118:GLU:HG3  | 2.19                     | 0.41              |
| 74:o3:122:ASP:OD1 | 74:o3:122:ASP:C    | 2.64                     | 0.41              |
| 81:A3:660:A2M:H2' | 81:A3:661:C:C6     | 2.55                     | 0.41              |
| 81:A3:1139:U:H2'  | 81:A3:1140:A:O4'   | 2.20                     | 0.41              |
| 81:A3:2416:A:H2'  | 81:A3:2417:G:H8    | 1.85                     | 0.41              |
| 2:k1:226:GLU:C    | 2:k1:226:GLU:CD    | 2.88                     | 0.41              |
| 3:h1:1261:U:OP1   | 4:l1:28:MET:N      | 2.54                     | 0.41              |
| 3:h1:1414:G:N1    | 3:h1:1417:G:OP2    | 2.54                     | 0.41              |
| 3:h1:1597:C:H2'   | 3:h1:1598:G:H8     | 1.86                     | 0.41              |
| 22:T1:18:ARG:O    | 88:T1:303:HOH:O    | 2.22                     | 0.41              |
| 26:X1:48:GLU:OE1  | 26:X1:48:GLU:N     | 2.39                     | 0.41              |
| 62:a3:34:HIS:O    | 62:a3:48:LYS:NZ    | 2.54                     | 0.41              |
| 67:f3:27:LYS:NZ   | 81:A3:811:A:OP1    | 2.48                     | 0.41              |
| 67:f3:118:GLN:CD  | 67:f3:118:GLN:H    | 2.28                     | 0.41              |
| 70:j3:48:LEU:HB3  | 70:j3:89:THR:HG23  | 2.03                     | 0.41              |
| 74:o3:14:SER:O    | 88:o3:401:HOH:O    | 2.22                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 81:A3:473:G:H2'    | 81:A3:474:G:H8     | 1.85                     | 0.41              |
| 81:A3:2458:U:O5'   | 81:A3:2459:A:OP2   | 2.38                     | 0.41              |
| 81:A3:2726:U:H2'   | 81:A3:2727:U:C6    | 2.56                     | 0.41              |
| 81:A3:2885:U:H2'   | 81:A3:2886:OMU:H6  | 2.01                     | 0.41              |
| 1:A1:49:ARG:NH2    | 3:h1:452:C:OP1     | 2.41                     | 0.41              |
| 3:h1:981:A:O2'     | 3:h1:1795:C:O2     | 2.37                     | 0.41              |
| 8:F1:227:LYS:HA    | 8:F1:230:GLU:HG3   | 2.02                     | 0.41              |
| 17:O1:77:HIS:O     | 17:O1:81:VAL:HG12  | 2.20                     | 0.41              |
| 19:Q1:27:ASP:OD2   | 19:Q1:29:SER:N     | 2.53                     | 0.41              |
| 19:Q1:130:ILE:HB   | 19:Q1:143:ILE:HG13 | 2.03                     | 0.41              |
| 19:Q1:240:ALA:HB3  | 19:Q1:253:ALA:HB3  | 2.03                     | 0.41              |
| 81:A3:107:A:H4'    | 81:A3:108:G:OP1    | 2.21                     | 0.41              |
| 81:A3:827:A2M:HM'3 | 81:A3:930:A:C4     | 2.55                     | 0.41              |
| 81:A3:1345:C:C2    | 81:A3:1346:C:C5    | 3.08                     | 0.41              |
| 3:h1:818:A:N3      | 3:h1:818:A:H2'     | 2.35                     | 0.41              |
| 3:h1:1553:A:H2'    | 3:h1:1554:U:O4'    | 2.20                     | 0.41              |
| 57:W3:29:LYS:HE3   | 57:W3:29:LYS:HB3   | 1.93                     | 0.41              |
| 66:e3:12:ASN:ND2   | 81:A3:3040:U:O2    | 2.47                     | 0.41              |
| 81:A3:676:G:O2'    | 81:A3:677:A:H5'    | 2.21                     | 0.41              |
| 81:A3:1011:G:H2'   | 81:A3:1012:C:C6    | 2.56                     | 0.41              |
| 81:A3:1698:U:O2'   | 81:A3:1699:U:H5'   | 2.20                     | 0.41              |
| 81:A3:2638:A:H4'   | 81:A3:2639:A:O5'   | 2.21                     | 0.41              |
| 81:A3:3077:C:C2    | 81:A3:3078:C:C5    | 3.09                     | 0.41              |
| 1:A1:181:VAL:HG11  | 1:A1:195:ILE:HD11  | 2.02                     | 0.41              |
| 3:h1:12:U:H2'      | 3:h1:13:C:C6       | 2.55                     | 0.41              |
| 3:h1:626:A:O2'     | 88:h1:2149:HOH:O   | 2.15                     | 0.41              |
| 3:h1:1543:A:O5'    | 3:h1:1578:G:N2     | 2.48                     | 0.41              |
| 3:h1:1571:C:H2'    | 3:h1:1572:U:O4'    | 2.20                     | 0.41              |
| 3:h1:1763:A:N6     | 22:T1:63:SER:HG    | 2.19                     | 0.41              |
| 4:l1:38:ILE:HD11   | 4:l1:64:VAL:HG11   | 2.03                     | 0.41              |
| 6:D1:69:ILE:HG22   | 6:D1:71:LEU:CD1    | 2.51                     | 0.41              |
| 12:J1:67:LEU:HD11  | 21:S1:130:ASP:OD2  | 2.21                     | 0.41              |
| 18:P1:150:LYS:H    | 18:P1:150:LYS:HD3  | 1.86                     | 0.41              |
| 27:Y1:114:VAL:HA   | 27:Y1:118:MET:HE2  | 2.03                     | 0.41              |
| 42:H3:160:GLU:OE2  | 42:H3:160:GLU:HA   | 2.21                     | 0.41              |
| 48:N3:137:LYS:NZ   | 81:A3:489:C:OP2    | 2.54                     | 0.41              |
| 73:n3:33:VAL:O     | 73:n3:37:THR:HG23  | 2.21                     | 0.41              |
| 81:A3:409:G:H2'    | 81:A3:410:U:C6     | 2.56                     | 0.41              |
| 81:A3:419:A:H2'    | 81:A3:420:A:O4'    | 2.21                     | 0.41              |
| 81:A3:569:U:O2'    | 81:A3:570:G:H5'    | 2.20                     | 0.41              |
| 81:A3:1615:U:O4    | 88:A3:3743:HOH:O   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 81:A3:1678:G:C2   | 81:A3:1679:G:C8   | 3.09                     | 0.41              |
| 81:A3:2378:G:O2'  | 81:A3:2380:G:OP2  | 2.36                     | 0.41              |
| 81:A3:2638:A:H4'  | 81:A3:2639:A:N3   | 2.35                     | 0.41              |
| 81:A3:2841:A:C2   | 81:A3:2854:A:C4   | 3.09                     | 0.41              |
| 81:A3:2842:G:O6   | 81:A3:2848:A:O2'  | 2.34                     | 0.41              |
| 81:A3:2850:A:C4   | 81:A3:2851:G:C8   | 3.09                     | 0.41              |
| 81:A3:3002:G:H2'  | 81:A3:3003:U:C6   | 2.56                     | 0.41              |
| 3:h1:28:A2M:OP1   | 88:h1:2181:HOH:O  | 2.22                     | 0.41              |
| 28:Z1:72:LYS:HE2  | 28:Z1:95:GLY:O    | 2.21                     | 0.41              |
| 28:Z1:144:THR:O   | 28:Z1:158:ASP:HB2 | 2.21                     | 0.41              |
| 36:W2:19:G:C6     | 81:A3:2489:A:N1   | 2.86                     | 0.41              |
| 63:b3:97:ARG:NH2  | 81:A3:3259:A:OP1  | 2.49                     | 0.41              |
| 81:A3:983:A:H2'   | 81:A3:984:G:O4'   | 2.21                     | 0.41              |
| 81:A3:1121:C:H2'  | 81:A3:1122:A:O4'  | 2.21                     | 0.41              |
| 81:A3:1340:C:H2'  | 81:A3:1341:U:O4'  | 2.21                     | 0.41              |
| 81:A3:2372:G:H2'  | 81:A3:2373:G:C8   | 2.56                     | 0.41              |
| 1:A1:182:MET:HB2  | 1:A1:228:LEU:HD11 | 2.03                     | 0.40              |
| 3:h1:129:U:H3'    | 3:h1:130:A:H5'    | 2.02                     | 0.40              |
| 3:h1:1230:A:C6    | 5:C1:104:LEU:HD22 | 2.56                     | 0.40              |
| 17:O1:15:GLU:C    | 17:O1:15:GLU:OE2  | 2.64                     | 0.40              |
| 19:Q1:49:ASP:OD1  | 19:Q1:49:ASP:N    | 2.54                     | 0.40              |
| 34:f1:76:VAL:HG21 | 34:f1:88:ILE:HD11 | 2.02                     | 0.40              |
| 58:X3:13:LEU:HD22 | 81:A3:1504:G:H2'  | 2.03                     | 0.40              |
| 64:c3:41:LYS:NZ   | 81:A3:1583:C:OP1  | 2.41                     | 0.40              |
| 75:q3:100:LYS:O   | 75:q3:104:GLN:HG3 | 2.20                     | 0.40              |
| 81:A3:81:C:H2'    | 81:A3:82:U:O4'    | 2.21                     | 0.40              |
| 81:A3:290:C:H2'   | 81:A3:291:A:O4'   | 2.21                     | 0.40              |
| 81:A3:796:A:H4'   | 81:A3:797:G:O5'   | 2.20                     | 0.40              |
| 81:A3:2699:A:H2'  | 81:A3:2700:A:C8   | 2.56                     | 0.40              |
| 3:h1:154:A:H2'    | 3:h1:155:A:O4'    | 2.22                     | 0.40              |
| 3:h1:533:C:C2     | 3:h1:534:C:C6     | 3.09                     | 0.40              |
| 3:h1:804:U:H2'    | 3:h1:805:G:H8     | 1.87                     | 0.40              |
| 3:h1:1044:G:H2'   | 3:h1:1045:G:C8    | 2.56                     | 0.40              |
| 3:h1:1601:U:O2'   | 88:h1:2165:HOH:O  | 2.19                     | 0.40              |
| 5:C1:78:VAL:HG21  | 5:C1:121:CYS:SG   | 2.62                     | 0.40              |
| 25:W1:62:GLN:O    | 25:W1:65:SER:OG   | 2.31                     | 0.40              |
| 32:d1:41:GLU:C    | 32:d1:41:GLU:CD   | 2.88                     | 0.40              |
| 33:e1:70:ASN:N    | 33:e1:130:TYR:O   | 2.54                     | 0.40              |
| 64:c3:26:GLU:OE2  | 64:c3:28:ARG:NH2  | 2.54                     | 0.40              |
| 67:f3:36:GLY:HA3  | 67:f3:40:HIS:CE1  | 2.56                     | 0.40              |
| 77:s3:146:ARG:NH2 | 81:A3:1397:C:OP1  | 2.54                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:u3:55:LYS:HA    | 79:u3:55:LYS:HE2   | 2.03                     | 0.40              |
| 81:A3:24:A:C8      | 81:A3:327:G:C8     | 3.08                     | 0.40              |
| 81:A3:99:C:OP2     | 88:A3:3749:HOH:O   | 2.22                     | 0.40              |
| 81:A3:641:A:H2'    | 81:A3:642:U:C6     | 2.56                     | 0.40              |
| 81:A3:986:U:H2'    | 81:A3:987:C:O4'    | 2.22                     | 0.40              |
| 81:A3:1665:G:H2'   | 81:A3:1666:G:N3    | 2.37                     | 0.40              |
| 81:A3:2410:C:H2'   | 81:A3:2411:U:H6    | 1.86                     | 0.40              |
| 81:A3:2460:G:N1    | 81:A3:2463:U:OP1   | 2.50                     | 0.40              |
| 81:A3:2698:G:OP2   | 81:A3:2698:G:N2    | 2.35                     | 0.40              |
| 3:h1:1166:A:N3     | 3:h1:1619:U:O2'    | 2.50                     | 0.40              |
| 3:h1:1585:U:H2'    | 3:h1:1586:C:C6     | 2.56                     | 0.40              |
| 3:h1:1784:A:H2'    | 3:h1:1785:G:C8     | 2.56                     | 0.40              |
| 15:M1:30:PRO:HB2   | 15:M1:34:ALA:HB3   | 2.03                     | 0.40              |
| 17:O1:15:GLU:OE2   | 17:O1:16:PRO:O     | 2.39                     | 0.40              |
| 17:O1:119:LEU:C    | 17:O1:119:LEU:HD23 | 2.46                     | 0.40              |
| 23:U1:66:SER:HA    | 23:U1:69:VAL:HG12  | 2.03                     | 0.40              |
| 75:q3:34:LYS:HB2   | 75:q3:34:LYS:HE2   | 1.87                     | 0.40              |
| 77:s3:322:ASN:HB3  | 77:s3:325:LYS:HD2  | 2.03                     | 0.40              |
| 81:A3:402:U:H2'    | 81:A3:403:G:O4'    | 2.22                     | 0.40              |
| 81:A3:941:C:OP2    | 81:A3:942:U:O2'    | 2.34                     | 0.40              |
| 81:A3:2479:G:O6    | 81:A3:2480:G:O6    | 2.39                     | 0.40              |
| 3:h1:17:C:H2'      | 3:h1:18:C:C6       | 2.57                     | 0.40              |
| 3:h1:540:G:OP1     | 30:b1:177:LYS:NZ   | 2.48                     | 0.40              |
| 3:h1:1561:A:OP1    | 27:Y1:54:ARG:NE    | 2.44                     | 0.40              |
| 3:h1:1644:G:H2'    | 3:h1:1645:OMC:O4'  | 2.21                     | 0.40              |
| 33:e1:105:THR:O    | 33:e1:105:THR:HG23 | 2.20                     | 0.40              |
| 36:W2:5:G:H22      | 36:W2:68:A:H2      | 1.69                     | 0.40              |
| 44:J3:136:LYS:HD3  | 75:q3:80:GLU:OE2   | 2.22                     | 0.40              |
| 76:r3:243:ARG:NH1  | 88:r3:506:HOH:O    | 2.55                     | 0.40              |
| 81:A3:369:A2M:HM'3 | 81:A3:369:A2M:H1'  | 1.84                     | 0.40              |
| 81:A3:399:OMG:H4'  | 81:A3:400:C:O5'    | 2.20                     | 0.40              |
| 81:A3:1426:C:H2'   | 81:A3:1427:G:O4'   | 2.21                     | 0.40              |
| 3:h1:184:C:OP1     | 18:P1:161:ARG:NH2  | 2.47                     | 0.40              |
| 3:h1:450:A:N1      | 3:h1:465:G:O2'     | 2.49                     | 0.40              |
| 3:h1:901:A:C2      | 3:h1:918:A:C5      | 3.09                     | 0.40              |
| 3:h1:1612:C:C5     | 85:h1:2016:SPD:H32 | 2.57                     | 0.40              |
| 3:h1:1801:G:H4'    | 3:h1:1802:A:OP1    | 2.21                     | 0.40              |
| 72:m3:59:ARG:NH1   | 81:A3:197:G:OP1    | 2.52                     | 0.40              |
| 81:A3:218:A:C2     | 81:A3:221:C:C5     | 3.08                     | 0.40              |
| 81:A3:1217:G:C6    | 81:A3:1312:G:N2    | 2.90                     | 0.40              |
| 81:A3:2964:G:H2'   | 81:A3:2965:U:C6    | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | A1    | 257/264 (97%) | 254 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | k1    | 228/249 (92%) | 228 (100%) | 0       | 0        | 100         | 100 |
| 4   | l1    | 89/208 (43%)  | 87 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 5   | C1    | 115/144 (80%) | 114 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 6   | D1    | 117/149 (78%) | 115 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 7   | E1    | 134/143 (94%) | 132 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 8   | F1    | 214/261 (82%) | 213 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 9   | G1    | 81/83 (98%)   | 80 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 10  | H1    | 125/133 (94%) | 123 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 11  | I1    | 72/107 (67%)  | 70 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 12  | J1    | 96/127 (76%)  | 96 (100%)  | 0       | 0        | 100         | 100 |
| 13  | K1    | 82/86 (95%)   | 81 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 14  | L1    | 59/65 (91%)   | 58 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 15  | M1    | 48/62 (77%)   | 45 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 16  | N1    | 67/156 (43%)  | 66 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 17  | O1    | 186/191 (97%) | 182 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 18  | P1    | 182/224 (81%) | 180 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 19  | Q1    | 305/328 (93%) | 297 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 20  | R1    | 100/122 (82%) | 98 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 21  | S1    | 130/150 (87%) | 129 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 22  | T1    | 139/142 (98%) | 136 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 23  | U1    | 140/152 (92%) | 136 (97%)  | 4 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 24  | V1    | 53/56 (95%)   | 53 (100%)  | 0       | 0        | 100         | 100 |
| 25  | W1    | 147/151 (97%) | 146 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 26  | X1    | 143/159 (90%) | 141 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 27  | Y1    | 129/152 (85%) | 126 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 28  | Z1    | 200/336 (60%) | 197 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 29  | a1    | 209/248 (84%) | 201 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 30  | b1    | 181/197 (92%) | 176 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 31  | c1    | 215/280 (77%) | 210 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 32  | d1    | 192/210 (91%) | 184 (96%)  | 7 (4%)  | 1 (0%)   | 24          | 27  |
| 33  | e1    | 127/130 (98%) | 126 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 34  | f1    | 139/147 (95%) | 138 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 38  | D3    | 198/206 (96%) | 195 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 39  | E3    | 128/134 (96%) | 126 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 40  | F3    | 201/204 (98%) | 199 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 41  | G3    | 184/187 (98%) | 182 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 42  | H3    | 180/214 (84%) | 179 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 43  | I3    | 175/178 (98%) | 174 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 44  | J3    | 161/164 (98%) | 160 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 45  | K3    | 97/127 (76%)  | 93 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 46  | L3    | 60/164 (37%)  | 57 (95%)   | 3 (5%)  | 0        | 100         | 100 |
| 47  | M3    | 132/135 (98%) | 131 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 48  | N3    | 140/143 (98%) | 136 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 49  | O3    | 47/61 (77%)   | 46 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 50  | P3    | 95/113 (84%)  | 94 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 51  | Q3    | 106/120 (88%) | 106 (100%) | 0       | 0        | 100         | 100 |
| 52  | R3    | 124/133 (93%) | 123 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 53  | S3    | 109/112 (97%) | 108 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 54  | T3    | 112/120 (93%) | 111 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 55  | U3    | 96/110 (87%)  | 96 (100%)  | 0       | 0        | 100         | 100 |
| 56  | V3    | 84/95 (88%)   | 82 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 57  | W3    | 66/69 (96%)   | 66 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 58  | X3    | 48/51 (94%)       | 47 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 59  | Y3    | 49/128 (38%)      | 49 (100%)   | 0        | 0        | 100         | 100 |
| 60  | p3    | 23/25 (92%)       | 23 (100%)   | 0        | 0        | 100         | 100 |
| 61  | Z3    | 96/105 (91%)      | 95 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 62  | a3    | 89/92 (97%)       | 84 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 63  | b3    | 204/230 (89%)     | 201 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 64  | c3    | 231/258 (90%)     | 228 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 65  | d3    | 203/206 (98%)     | 199 (98%)   | 4 (2%)   | 0        | 100         | 100 |
| 66  | e3    | 129/140 (92%)     | 125 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 67  | f3    | 145/148 (98%)     | 137 (94%)   | 7 (5%)   | 1 (1%)   | 18          | 19  |
| 68  | g3    | 205/221 (93%)     | 202 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 69  | h3    | 286/301 (95%)     | 278 (97%)   | 8 (3%)   | 0        | 100         | 100 |
| 70  | j3    | 152/175 (87%)     | 150 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 71  | k3    | 115/154 (75%)     | 113 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 72  | m3    | 124/146 (85%)     | 120 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 73  | n3    | 120/123 (98%)     | 117 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 74  | o3    | 243/260 (94%)     | 234 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 75  | q3    | 236/242 (98%)     | 231 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 76  | r3    | 384/389 (99%)     | 380 (99%)   | 4 (1%)   | 0        | 100         | 100 |
| 77  | s3    | 396/405 (98%)     | 390 (98%)   | 6 (2%)   | 0        | 100         | 100 |
| 78  | t3    | 170/181 (94%)     | 168 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 79  | u3    | 189/194 (97%)     | 188 (100%)  | 1 (0%)   | 0        | 100         | 100 |
| All | All   | 11033/12575 (88%) | 10841 (98%) | 190 (2%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | d1    | 85  | HIS  |
| 67  | f3    | 15  | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A1    | 225/228 (99%) | 225 (100%) | 0        | 100         | 100 |
| 2   | k1    | 199/213 (93%) | 199 (100%) | 0        | 100         | 100 |
| 4   | l1    | 85/169 (50%)  | 85 (100%)  | 0        | 100         | 100 |
| 5   | C1    | 94/112 (84%)  | 94 (100%)  | 0        | 100         | 100 |
| 6   | D1    | 109/124 (88%) | 109 (100%) | 0        | 100         | 100 |
| 7   | E1    | 111/114 (97%) | 111 (100%) | 0        | 100         | 100 |
| 8   | F1    | 195/228 (86%) | 195 (100%) | 0        | 100         | 100 |
| 9   | G1    | 70/70 (100%)  | 70 (100%)  | 0        | 100         | 100 |
| 10  | H1    | 108/113 (96%) | 107 (99%)  | 1 (1%)   | 70          | 84  |
| 11  | I1    | 64/89 (72%)   | 64 (100%)  | 0        | 100         | 100 |
| 12  | J1    | 87/109 (80%)  | 87 (100%)  | 0        | 100         | 100 |
| 13  | K1    | 76/78 (97%)   | 76 (100%)  | 0        | 100         | 100 |
| 14  | L1    | 54/57 (95%)   | 54 (100%)  | 0        | 100         | 100 |
| 15  | M1    | 41/49 (84%)   | 41 (100%)  | 0        | 100         | 100 |
| 16  | N1    | 60/134 (45%)  | 60 (100%)  | 0        | 100         | 100 |
| 17  | O1    | 169/171 (99%) | 167 (99%)  | 2 (1%)   | 63          | 78  |
| 18  | P1    | 158/178 (89%) | 158 (100%) | 0        | 100         | 100 |
| 19  | Q1    | 266/279 (95%) | 264 (99%)  | 2 (1%)   | 73          | 85  |
| 20  | R1    | 93/108 (86%)  | 93 (100%)  | 0        | 100         | 100 |
| 21  | S1    | 103/120 (86%) | 102 (99%)  | 1 (1%)   | 68          | 81  |
| 22  | T1    | 113/114 (99%) | 112 (99%)  | 1 (1%)   | 70          | 84  |
| 23  | U1    | 122/131 (93%) | 122 (100%) | 0        | 100         | 100 |
| 24  | V1    | 46/47 (98%)   | 46 (100%)  | 0        | 100         | 100 |
| 25  | W1    | 130/131 (99%) | 130 (100%) | 0        | 100         | 100 |
| 26  | X1    | 124/131 (95%) | 124 (100%) | 0        | 100         | 100 |
| 27  | Y1    | 115/130 (88%) | 115 (100%) | 0        | 100         | 100 |
| 28  | Z1    | 171/256 (67%) | 171 (100%) | 0        | 100         | 100 |
| 29  | a1    | 179/215 (83%) | 178 (99%)  | 1 (1%)   | 78          | 89  |
| 30  | b1    | 161/171 (94%) | 161 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 31  | c1    | 184/226 (81%) | 183 (100%) | 1 (0%)   | 81          | 90  |
| 32  | d1    | 165/175 (94%) | 165 (100%) | 0        | 100         | 100 |
| 33  | e1    | 111/112 (99%) | 111 (100%) | 0        | 100         | 100 |
| 34  | f1    | 116/120 (97%) | 116 (100%) | 0        | 100         | 100 |
| 38  | D3    | 165/171 (96%) | 164 (99%)  | 1 (1%)   | 78          | 89  |
| 39  | E3    | 114/117 (97%) | 113 (99%)  | 1 (1%)   | 70          | 84  |
| 40  | F3    | 176/177 (99%) | 175 (99%)  | 1 (1%)   | 78          | 89  |
| 41  | G3    | 154/155 (99%) | 154 (100%) | 0        | 100         | 100 |
| 42  | H3    | 160/182 (88%) | 160 (100%) | 0        | 100         | 100 |
| 43  | I3    | 163/164 (99%) | 161 (99%)  | 2 (1%)   | 63          | 78  |
| 44  | J3    | 140/141 (99%) | 139 (99%)  | 1 (1%)   | 76          | 87  |
| 45  | K3    | 91/109 (84%)  | 91 (100%)  | 0        | 100         | 100 |
| 46  | L3    | 57/133 (43%)  | 56 (98%)   | 1 (2%)   | 51          | 68  |
| 47  | M3    | 117/118 (99%) | 117 (100%) | 0        | 100         | 100 |
| 48  | N3    | 123/124 (99%) | 123 (100%) | 0        | 100         | 100 |
| 49  | O3    | 43/53 (81%)   | 43 (100%)  | 0        | 100         | 100 |
| 50  | P3    | 85/98 (87%)   | 85 (100%)  | 0        | 100         | 100 |
| 51  | Q3    | 95/106 (90%)  | 95 (100%)  | 0        | 100         | 100 |
| 52  | R3    | 114/121 (94%) | 114 (100%) | 0        | 100         | 100 |
| 53  | S3    | 98/99 (99%)   | 97 (99%)   | 1 (1%)   | 68          | 81  |
| 54  | T3    | 100/104 (96%) | 98 (98%)   | 2 (2%)   | 48          | 64  |
| 55  | U3    | 83/90 (92%)   | 83 (100%)  | 0        | 100         | 100 |
| 56  | V3    | 72/77 (94%)   | 71 (99%)   | 1 (1%)   | 59          | 75  |
| 57  | W3    | 64/65 (98%)   | 62 (97%)   | 2 (3%)   | 35          | 48  |
| 58  | X3    | 47/48 (98%)   | 47 (100%)  | 0        | 100         | 100 |
| 59  | Y3    | 46/114 (40%)  | 46 (100%)  | 0        | 100         | 100 |
| 60  | p3    | 24/24 (100%)  | 24 (100%)  | 0        | 100         | 100 |
| 61  | Z3    | 86/92 (94%)   | 86 (100%)  | 0        | 100         | 100 |
| 62  | a3    | 73/74 (99%)   | 73 (100%)  | 0        | 100         | 100 |
| 63  | b3    | 175/194 (90%) | 175 (100%) | 0        | 100         | 100 |
| 64  | c3    | 202/221 (91%) | 202 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 65  | d3    | 173/174 (99%)    | 171 (99%)   | 2 (1%)   | 63          | 78  |
| 66  | e3    | 103/109 (94%)    | 103 (100%)  | 0        | 100         | 100 |
| 67  | f3    | 119/120 (99%)    | 119 (100%)  | 0        | 100         | 100 |
| 68  | g3    | 173/181 (96%)    | 171 (99%)   | 2 (1%)   | 63          | 78  |
| 69  | h3    | 244/254 (96%)    | 243 (100%)  | 1 (0%)   | 84          | 92  |
| 70  | j3    | 135/154 (88%)    | 134 (99%)   | 1 (1%)   | 76          | 87  |
| 71  | k3    | 106/134 (79%)    | 106 (100%)  | 0        | 100         | 100 |
| 72  | m3    | 115/131 (88%)    | 113 (98%)   | 2 (2%)   | 53          | 69  |
| 73  | n3    | 109/110 (99%)    | 109 (100%)  | 0        | 100         | 100 |
| 74  | o3    | 190/197 (96%)    | 189 (100%)  | 1 (0%)   | 81          | 90  |
| 75  | q3    | 207/209 (99%)    | 207 (100%)  | 0        | 100         | 100 |
| 76  | r3    | 330/332 (99%)    | 328 (99%)   | 2 (1%)   | 78          | 89  |
| 77  | s3    | 326/329 (99%)    | 325 (100%)  | 1 (0%)   | 86          | 93  |
| 78  | t3    | 149/157 (95%)    | 148 (99%)   | 1 (1%)   | 76          | 87  |
| 79  | u3    | 167/170 (98%)    | 165 (99%)   | 2 (1%)   | 63          | 78  |
| All | All   | 9617/10634 (90%) | 9580 (100%) | 37 (0%)  | 81          | 92  |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | H1    | 23  | GLN  |
| 17  | O1    | 29  | ASP  |
| 17  | O1    | 31  | GLU  |
| 19  | Q1    | 257 | SER  |
| 19  | Q1    | 326 | ILE  |
| 21  | S1    | 81  | SER  |
| 22  | T1    | 104 | PHE  |
| 29  | a1    | 38  | SER  |
| 31  | c1    | 168 | VAL  |
| 38  | D3    | 38  | GLN  |
| 39  | E3    | 7   | VAL  |
| 40  | F3    | 99  | ARG  |
| 43  | I3    | 10  | GLN  |
| 43  | I3    | 65  | GLU  |
| 44  | J3    | 96  | VAL  |
| 46  | L3    | 36  | SER  |
| 53  | S3    | 112 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | T3    | 56  | HIS  |
| 54  | T3    | 85  | SER  |
| 56  | V3    | 83  | GLU  |
| 57  | W3    | 52  | LYS  |
| 57  | W3    | 67  | GLN  |
| 65  | d3    | 3   | SER  |
| 65  | d3    | 194 | LEU  |
| 68  | g3    | 50  | VAL  |
| 68  | g3    | 186 | SER  |
| 69  | h3    | 209 | THR  |
| 70  | j3    | 45  | LYS  |
| 72  | m3    | 36  | SER  |
| 72  | m3    | 55  | VAL  |
| 74  | o3    | 208 | GLU  |
| 76  | r3    | 114 | LEU  |
| 76  | r3    | 377 | THR  |
| 77  | s3    | 158 | SER  |
| 78  | t3    | 32  | LEU  |
| 79  | u3    | 42  | ASN  |
| 79  | u3    | 142 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 67  | GLN  |
| 1   | A1    | 98  | ASN  |
| 1   | A1    | 112 | HIS  |
| 4   | I1    | 44  | GLN  |
| 5   | C1    | 58  | HIS  |
| 5   | C1    | 138 | GLN  |
| 7   | E1    | 86  | ASN  |
| 8   | F1    | 63  | HIS  |
| 8   | F1    | 124 | HIS  |
| 9   | G1    | 62  | GLN  |
| 10  | H1    | 16  | ASN  |
| 12  | J1    | 13  | HIS  |
| 12  | J1    | 72  | GLN  |
| 18  | P1    | 95  | GLN  |
| 18  | P1    | 116 | GLN  |
| 19  | Q1    | 134 | ASN  |
| 24  | V1    | 3   | HIS  |
| 26  | X1    | 33  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | X1    | 82  | ASN  |
| 27  | Y1    | 144 | HIS  |
| 28  | Z1    | 16  | GLN  |
| 28  | Z1    | 132 | GLN  |
| 28  | Z1    | 193 | HIS  |
| 31  | c1    | 99  | GLN  |
| 31  | c1    | 104 | GLN  |
| 32  | d1    | 26  | ASN  |
| 32  | d1    | 107 | HIS  |
| 33  | e1    | 8   | ASN  |
| 33  | e1    | 42  | GLN  |
| 34  | f1    | 65  | HIS  |
| 38  | D3    | 149 | GLN  |
| 40  | F3    | 156 | HIS  |
| 41  | G3    | 134 | ASN  |
| 43  | I3    | 23  | HIS  |
| 48  | N3    | 78  | GLN  |
| 48  | N3    | 86  | ASN  |
| 53  | S3    | 6   | GLN  |
| 53  | S3    | 27  | ASN  |
| 61  | Z3    | 59  | HIS  |
| 61  | Z3    | 90  | HIS  |
| 63  | b3    | 37  | ASN  |
| 64  | c3    | 151 | HIS  |
| 64  | c3    | 239 | GLN  |
| 65  | d3    | 18  | HIS  |
| 65  | d3    | 178 | GLN  |
| 66  | e3    | 27  | ASN  |
| 67  | f3    | 40  | HIS  |
| 68  | g3    | 92  | HIS  |
| 69  | h3    | 188 | GLN  |
| 70  | j3    | 56  | GLN  |
| 70  | j3    | 122 | GLN  |
| 72  | m3    | 18  | HIS  |
| 74  | o3    | 168 | GLN  |
| 76  | r3    | 25  | HIS  |
| 76  | r3    | 317 | HIS  |
| 77  | s3    | 350 | GLN  |
| 78  | t3    | 17  | GLN  |
| 78  | t3    | 153 | GLN  |
| 78  | t3    | 175 | ASN  |
| 79  | u3    | 37  | ASN  |

## 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 3   | h1    | 1617/1808 (89%) | 223 (13%)         | 0               |
| 35  | B1    | 11/12 (91%)     | 1 (9%)            | 0               |
| 36  | W2    | 75/76 (98%)     | 10 (13%)          | 0               |
| 36  | i2    | 75/76 (98%)     | 8 (10%)           | 0               |
| 37  | C3    | 118/119 (99%)   | 8 (6%)            | 0               |
| 81  | A3    | 3191/3390 (94%) | 417 (13%)         | 19 (0%)         |
| 82  | B3    | 162/163 (99%)   | 26 (16%)          | 0               |
| All | All   | 5249/5644 (93%) | 693 (13%)         | 19 (0%)         |

All (693) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | h1    | 2   | A    |
| 3   | h1    | 4   | C    |
| 3   | h1    | 17  | C    |
| 3   | h1    | 25  | C    |
| 3   | h1    | 26  | A    |
| 3   | h1    | 34  | G    |
| 3   | h1    | 38  | OMC  |
| 3   | h1    | 42  | G    |
| 3   | h1    | 43  | A    |
| 3   | h1    | 45  | U    |
| 3   | h1    | 47  | A    |
| 3   | h1    | 56  | U    |
| 3   | h1    | 68  | A    |
| 3   | h1    | 82  | G    |
| 3   | h1    | 84  | G    |
| 3   | h1    | 105 | A    |
| 3   | h1    | 115 | A    |
| 3   | h1    | 117 | U    |
| 3   | h1    | 123 | OMU  |
| 3   | h1    | 128 | G    |
| 3   | h1    | 129 | U    |
| 3   | h1    | 130 | A    |
| 3   | h1    | 132 | C    |
| 3   | h1    | 133 | U    |
| 3   | h1    | 135 | C    |
| 3   | h1    | 136 | U    |
| 3   | h1    | 139 | U    |
| 3   | h1    | 140 | OMC  |
| 3   | h1    | 144 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | h1    | 150 | U    |
| 3   | h1    | 151 | A    |
| 3   | h1    | 158 | C    |
| 3   | h1    | 164 | C    |
| 3   | h1    | 174 | C    |
| 3   | h1    | 186 | A    |
| 3   | h1    | 189 | U    |
| 3   | h1    | 190 | C    |
| 3   | h1    | 191 | U    |
| 3   | h1    | 192 | G    |
| 3   | h1    | 193 | G    |
| 3   | h1    | 194 | A    |
| 3   | h1    | 213 | U    |
| 3   | h1    | 214 | A    |
| 3   | h1    | 252 | U    |
| 3   | h1    | 253 | C    |
| 3   | h1    | 260 | A    |
| 3   | h1    | 274 | A    |
| 3   | h1    | 277 | G    |
| 3   | h1    | 278 | C    |
| 3   | h1    | 291 | G    |
| 3   | h1    | 303 | A    |
| 3   | h1    | 318 | C    |
| 3   | h1    | 320 | A    |
| 3   | h1    | 324 | U    |
| 3   | h1    | 326 | G    |
| 3   | h1    | 341 | G    |
| 3   | h1    | 342 | C    |
| 3   | h1    | 365 | C    |
| 3   | h1    | 382 | A    |
| 3   | h1    | 384 | U    |
| 3   | h1    | 392 | OMG  |
| 3   | h1    | 394 | G    |
| 3   | h1    | 404 | A    |
| 3   | h1    | 406 | C    |
| 3   | h1    | 415 | C    |
| 3   | h1    | 420 | A    |
| 3   | h1    | 427 | G    |
| 3   | h1    | 428 | C    |
| 3   | h1    | 429 | A    |
| 3   | h1    | 430 | G    |
| 3   | h1    | 438 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | h1    | 443 | U    |
| 3   | h1    | 448 | C    |
| 3   | h1    | 449 | A    |
| 3   | h1    | 472 | A    |
| 3   | h1    | 481 | A    |
| 3   | h1    | 489 | C    |
| 3   | h1    | 490 | G    |
| 3   | h1    | 504 | U    |
| 3   | h1    | 505 | G    |
| 3   | h1    | 510 | U    |
| 3   | h1    | 513 | G    |
| 3   | h1    | 518 | A    |
| 3   | h1    | 522 | C    |
| 3   | h1    | 541 | A    |
| 3   | h1    | 544 | A2M  |
| 3   | h1    | 545 | U    |
| 3   | h1    | 552 | G    |
| 3   | h1    | 558 | A    |
| 3   | h1    | 560 | G    |
| 3   | h1    | 568 | C    |
| 3   | h1    | 581 | OMU  |
| 3   | h1    | 582 | A    |
| 3   | h1    | 584 | PSU  |
| 3   | h1    | 585 | U    |
| 3   | h1    | 597 | A    |
| 3   | h1    | 598 | OMG  |
| 3   | h1    | 609 | A    |
| 3   | h1    | 614 | OMU  |
| 3   | h1    | 620 | U    |
| 3   | h1    | 622 | A2M  |
| 3   | h1    | 623 | A    |
| 3   | h1    | 625 | A    |
| 3   | h1    | 626 | A    |
| 3   | h1    | 642 | U    |
| 3   | h1    | 647 | A    |
| 3   | h1    | 759 | A    |
| 3   | h1    | 769 | G    |
| 3   | h1    | 770 | C    |
| 3   | h1    | 775 | A    |
| 3   | h1    | 782 | C    |
| 3   | h1    | 783 | U    |
| 3   | h1    | 785 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | h1    | 786  | G    |
| 3   | h1    | 790  | U    |
| 3   | h1    | 793  | A    |
| 3   | h1    | 816  | A    |
| 3   | h1    | 832  | A    |
| 3   | h1    | 834  | U    |
| 3   | h1    | 866  | A    |
| 3   | h1    | 931  | G    |
| 3   | h1    | 936  | A    |
| 3   | h1    | 938  | U    |
| 3   | h1    | 954  | A    |
| 3   | h1    | 963  | U    |
| 3   | h1    | 991  | C    |
| 3   | h1    | 1006 | A    |
| 3   | h1    | 1007 | U    |
| 3   | h1    | 1008 | A    |
| 3   | h1    | 1029 | A    |
| 3   | h1    | 1031 | C    |
| 3   | h1    | 1042 | A    |
| 3   | h1    | 1059 | G    |
| 3   | h1    | 1060 | C    |
| 3   | h1    | 1085 | U    |
| 3   | h1    | 1090 | A    |
| 3   | h1    | 1095 | A    |
| 3   | h1    | 1100 | U    |
| 3   | h1    | 1141 | A    |
| 3   | h1    | 1153 | G    |
| 3   | h1    | 1161 | C    |
| 3   | h1    | 1166 | A    |
| 3   | h1    | 1170 | G    |
| 3   | h1    | 1188 | U    |
| 3   | h1    | 1197 | A    |
| 3   | h1    | 1199 | A    |
| 3   | h1    | 1202 | G    |
| 3   | h1    | 1203 | G    |
| 3   | h1    | 1204 | G    |
| 3   | h1    | 1205 | A    |
| 3   | h1    | 1220 | A    |
| 3   | h1    | 1221 | G    |
| 3   | h1    | 1234 | OMU  |
| 3   | h1    | 1246 | G    |
| 3   | h1    | 1247 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | h1    | 1248 | G    |
| 3   | h1    | 1249 | C    |
| 3   | h1    | 1255 | C    |
| 3   | h1    | 1272 | OMU  |
| 3   | h1    | 1274 | OMG  |
| 3   | h1    | 1302 | G    |
| 3   | h1    | 1317 | U    |
| 3   | h1    | 1318 | U    |
| 3   | h1    | 1324 | A    |
| 3   | h1    | 1328 | A    |
| 3   | h1    | 1364 | U    |
| 3   | h1    | 1365 | A    |
| 3   | h1    | 1366 | U    |
| 3   | h1    | 1375 | G    |
| 3   | h1    | 1395 | U    |
| 3   | h1    | 1396 | A    |
| 3   | h1    | 1403 | U    |
| 3   | h1    | 1404 | U    |
| 3   | h1    | 1418 | U    |
| 3   | h1    | 1420 | U    |
| 3   | h1    | 1432 | A    |
| 3   | h1    | 1433 | OMG  |
| 3   | h1    | 1437 | U    |
| 3   | h1    | 1440 | G    |
| 3   | h1    | 1451 | A    |
| 3   | h1    | 1464 | C    |
| 3   | h1    | 1465 | A    |
| 3   | h1    | 1476 | A    |
| 3   | h1    | 1493 | G    |
| 3   | h1    | 1495 | U    |
| 3   | h1    | 1500 | G    |
| 3   | h1    | 1503 | U    |
| 3   | h1    | 1518 | G    |
| 3   | h1    | 1523 | A    |
| 3   | h1    | 1524 | PSU  |
| 3   | h1    | 1528 | U    |
| 3   | h1    | 1530 | A    |
| 3   | h1    | 1543 | A    |
| 3   | h1    | 1548 | G    |
| 3   | h1    | 1563 | U    |
| 3   | h1    | 1565 | G    |
| 3   | h1    | 1579 | A2M  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | h1    | 1596 | G    |
| 3   | h1    | 1607 | G    |
| 3   | h1    | 1617 | A    |
| 3   | h1    | 1637 | A    |
| 3   | h1    | 1640 | C    |
| 3   | h1    | 1646 | C    |
| 3   | h1    | 1657 | A    |
| 3   | h1    | 1663 | U    |
| 3   | h1    | 1664 | G    |
| 3   | h1    | 1686 | G    |
| 3   | h1    | 1763 | A    |
| 3   | h1    | 1765 | G    |
| 3   | h1    | 1774 | A    |
| 3   | h1    | 1775 | G    |
| 3   | h1    | 1777 | U    |
| 3   | h1    | 1787 | PSU  |
| 3   | h1    | 1788 | G    |
| 3   | h1    | 1790 | MA6  |
| 3   | h1    | 1791 | C    |
| 3   | h1    | 1800 | G    |
| 3   | h1    | 1801 | G    |
| 3   | h1    | 1802 | A    |
| 3   | h1    | 1803 | U    |
| 3   | h1    | 1804 | C    |
| 3   | h1    | 1807 | U    |
| 3   | h1    | 1808 | G    |
| 35  | B1    | 19   | U    |
| 36  | i2    | 16   | U    |
| 36  | i2    | 17   | U    |
| 36  | i2    | 21   | A    |
| 36  | i2    | 35   | A    |
| 36  | i2    | 36   | A    |
| 36  | i2    | 73   | A    |
| 36  | i2    | 74   | C    |
| 36  | i2    | 76   | A    |
| 36  | W2    | 10   | G    |
| 36  | W2    | 17   | U    |
| 36  | W2    | 19   | G    |
| 36  | W2    | 20   | G    |
| 36  | W2    | 21   | A    |
| 36  | W2    | 38   | A    |
| 36  | W2    | 47   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | W2    | 56  | C    |
| 36  | W2    | 63  | C    |
| 36  | W2    | 76  | A    |
| 37  | C3    | 7   | G    |
| 37  | C3    | 25  | G    |
| 37  | C3    | 33  | U    |
| 37  | C3    | 38  | U    |
| 37  | C3    | 53  | U    |
| 37  | C3    | 54  | A    |
| 37  | C3    | 64  | G    |
| 37  | C3    | 110 | G    |
| 81  | A3    | 11  | G    |
| 81  | A3    | 12  | U    |
| 81  | A3    | 14  | A    |
| 81  | A3    | 24  | A    |
| 81  | A3    | 38  | A    |
| 81  | A3    | 41  | A    |
| 81  | A3    | 47  | A    |
| 81  | A3    | 58  | A    |
| 81  | A3    | 64  | A    |
| 81  | A3    | 90  | G    |
| 81  | A3    | 97  | A    |
| 81  | A3    | 107 | A    |
| 81  | A3    | 108 | G    |
| 81  | A3    | 109 | C    |
| 81  | A3    | 114 | C    |
| 81  | A3    | 120 | A    |
| 81  | A3    | 131 | U    |
| 81  | A3    | 132 | C    |
| 81  | A3    | 133 | C    |
| 81  | A3    | 134 | G    |
| 81  | A3    | 140 | C    |
| 81  | A3    | 154 | G    |
| 81  | A3    | 155 | A    |
| 81  | A3    | 163 | C    |
| 81  | A3    | 167 | A    |
| 81  | A3    | 168 | G    |
| 81  | A3    | 184 | A    |
| 81  | A3    | 187 | U    |
| 81  | A3    | 188 | C    |
| 81  | A3    | 194 | G    |
| 81  | A3    | 197 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | A3    | 207 | G    |
| 81  | A3    | 215 | G    |
| 81  | A3    | 216 | A    |
| 81  | A3    | 245 | A    |
| 81  | A3    | 247 | C    |
| 81  | A3    | 248 | A    |
| 81  | A3    | 258 | G    |
| 81  | A3    | 262 | A    |
| 81  | A3    | 266 | G    |
| 81  | A3    | 283 | U    |
| 81  | A3    | 292 | A    |
| 81  | A3    | 296 | OMG  |
| 81  | A3    | 302 | U    |
| 81  | A3    | 320 | A    |
| 81  | A3    | 326 | G    |
| 81  | A3    | 347 | C    |
| 81  | A3    | 373 | G    |
| 81  | A3    | 396 | A    |
| 81  | A3    | 398 | U    |
| 81  | A3    | 399 | OMG  |
| 81  | A3    | 400 | C    |
| 81  | A3    | 417 | G    |
| 81  | A3    | 418 | G    |
| 81  | A3    | 419 | A    |
| 81  | A3    | 436 | C    |
| 81  | A3    | 439 | U    |
| 81  | A3    | 449 | U    |
| 81  | A3    | 453 | A    |
| 81  | A3    | 454 | U    |
| 81  | A3    | 467 | C    |
| 81  | A3    | 468 | G    |
| 81  | A3    | 523 | C    |
| 81  | A3    | 525 | A    |
| 81  | A3    | 538 | C    |
| 81  | A3    | 539 | G    |
| 81  | A3    | 540 | A    |
| 81  | A3    | 541 | U    |
| 81  | A3    | 544 | G    |
| 81  | A3    | 547 | C    |
| 81  | A3    | 550 | G    |
| 81  | A3    | 552 | A    |
| 81  | A3    | 571 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | A3    | 574 | U    |
| 81  | A3    | 577 | G    |
| 81  | A3    | 582 | G    |
| 81  | A3    | 591 | C    |
| 81  | A3    | 592 | G    |
| 81  | A3    | 602 | G    |
| 81  | A3    | 607 | C    |
| 81  | A3    | 610 | C    |
| 81  | A3    | 620 | A    |
| 81  | A3    | 636 | U    |
| 81  | A3    | 637 | C    |
| 81  | A3    | 660 | A2M  |
| 81  | A3    | 661 | C    |
| 81  | A3    | 671 | A    |
| 81  | A3    | 688 | A    |
| 81  | A3    | 693 | A    |
| 81  | A3    | 698 | C    |
| 81  | A3    | 701 | G    |
| 81  | A3    | 718 | A    |
| 81  | A3    | 725 | C    |
| 81  | A3    | 728 | A    |
| 81  | A3    | 729 | U    |
| 81  | A3    | 730 | U    |
| 81  | A3    | 731 | G    |
| 81  | A3    | 743 | C    |
| 81  | A3    | 747 | G    |
| 81  | A3    | 753 | C    |
| 81  | A3    | 775 | U    |
| 81  | A3    | 777 | U    |
| 81  | A3    | 781 | A    |
| 81  | A3    | 790 | A    |
| 81  | A3    | 791 | G    |
| 81  | A3    | 795 | G    |
| 81  | A3    | 797 | G    |
| 81  | A3    | 816 | A    |
| 81  | A3    | 827 | A2M  |
| 81  | A3    | 840 | G    |
| 81  | A3    | 867 | G    |
| 81  | A3    | 871 | C    |
| 81  | A3    | 884 | U    |
| 81  | A3    | 889 | U    |
| 81  | A3    | 906 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 917  | G    |
| 81  | A3    | 918  | OMG  |
| 81  | A3    | 924  | A    |
| 81  | A3    | 926  | G    |
| 81  | A3    | 927  | A    |
| 81  | A3    | 933  | C    |
| 81  | A3    | 946  | A2M  |
| 81  | A3    | 947  | G    |
| 81  | A3    | 954  | C    |
| 81  | A3    | 969  | C    |
| 81  | A3    | 970  | PSU  |
| 81  | A3    | 984  | G    |
| 81  | A3    | 987  | C    |
| 81  | A3    | 991  | U    |
| 81  | A3    | 992  | G    |
| 81  | A3    | 1003 | C    |
| 81  | A3    | 1006 | G    |
| 81  | A3    | 1013 | C    |
| 81  | A3    | 1014 | A    |
| 81  | A3    | 1022 | G    |
| 81  | A3    | 1028 | U    |
| 81  | A3    | 1036 | G    |
| 81  | A3    | 1041 | G    |
| 81  | A3    | 1048 | A    |
| 81  | A3    | 1059 | A    |
| 81  | A3    | 1076 | A    |
| 81  | A3    | 1077 | C    |
| 81  | A3    | 1087 | G    |
| 81  | A3    | 1093 | U    |
| 81  | A3    | 1094 | U    |
| 81  | A3    | 1106 | C    |
| 81  | A3    | 1107 | G    |
| 81  | A3    | 1108 | G    |
| 81  | A3    | 1109 | A    |
| 81  | A3    | 1114 | A    |
| 81  | A3    | 1115 | G    |
| 81  | A3    | 1128 | G    |
| 81  | A3    | 1142 | G    |
| 81  | A3    | 1170 | A    |
| 81  | A3    | 1191 | C    |
| 81  | A3    | 1192 | U    |
| 81  | A3    | 1193 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 1195 | G    |
| 81  | A3    | 1201 | A    |
| 81  | A3    | 1202 | C    |
| 81  | A3    | 1205 | A    |
| 81  | A3    | 1213 | C    |
| 81  | A3    | 1217 | G    |
| 81  | A3    | 1218 | G    |
| 81  | A3    | 1221 | G    |
| 81  | A3    | 1239 | C    |
| 81  | A3    | 1295 | C    |
| 81  | A3    | 1297 | G    |
| 81  | A3    | 1299 | A    |
| 81  | A3    | 1321 | U    |
| 81  | A3    | 1328 | U    |
| 81  | A3    | 1329 | A    |
| 81  | A3    | 1335 | G    |
| 81  | A3    | 1343 | C    |
| 81  | A3    | 1360 | A    |
| 81  | A3    | 1361 | A    |
| 81  | A3    | 1362 | G    |
| 81  | A3    | 1363 | U    |
| 81  | A3    | 1364 | G    |
| 81  | A3    | 1365 | C    |
| 81  | A3    | 1366 | C    |
| 81  | A3    | 1410 | U    |
| 81  | A3    | 1430 | G    |
| 81  | A3    | 1445 | G    |
| 81  | A3    | 1448 | OMC  |
| 81  | A3    | 1457 | A    |
| 81  | A3    | 1463 | A    |
| 81  | A3    | 1492 | A    |
| 81  | A3    | 1494 | G    |
| 81  | A3    | 1513 | G    |
| 81  | A3    | 1538 | C    |
| 81  | A3    | 1566 | A    |
| 81  | A3    | 1571 | G    |
| 81  | A3    | 1577 | U    |
| 81  | A3    | 1578 | U    |
| 81  | A3    | 1585 | U    |
| 81  | A3    | 1587 | C    |
| 81  | A3    | 1588 | U    |
| 81  | A3    | 1592 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 1593 | A    |
| 81  | A3    | 1594 | A    |
| 81  | A3    | 1598 | A    |
| 81  | A3    | 1602 | G    |
| 81  | A3    | 1609 | A    |
| 81  | A3    | 1625 | C    |
| 81  | A3    | 1633 | U    |
| 81  | A3    | 1635 | G    |
| 81  | A3    | 1649 | G    |
| 81  | A3    | 1661 | C    |
| 81  | A3    | 1698 | U    |
| 81  | A3    | 1729 | G    |
| 81  | A3    | 1748 | G    |
| 81  | A3    | 1755 | A    |
| 81  | A3    | 1756 | G    |
| 81  | A3    | 1770 | G    |
| 81  | A3    | 1771 | C    |
| 81  | A3    | 1772 | G    |
| 81  | A3    | 1774 | G    |
| 81  | A3    | 1775 | G    |
| 81  | A3    | 1802 | G    |
| 81  | A3    | 1803 | A    |
| 81  | A3    | 1821 | U    |
| 81  | A3    | 1827 | C    |
| 81  | A3    | 1828 | C    |
| 81  | A3    | 1852 | OMC  |
| 81  | A3    | 1853 | A    |
| 81  | A3    | 1855 | C    |
| 81  | A3    | 1856 | A    |
| 81  | A3    | 1872 | C    |
| 81  | A3    | 1873 | A    |
| 81  | A3    | 1884 | G    |
| 81  | A3    | 1885 | A    |
| 81  | A3    | 1886 | U    |
| 81  | A3    | 1912 | G    |
| 81  | A3    | 1949 | C    |
| 81  | A3    | 2096 | A    |
| 81  | A3    | 2100 | G    |
| 81  | A3    | 2116 | U    |
| 81  | A3    | 2118 | C    |
| 81  | A3    | 2126 | OMG  |
| 81  | A3    | 2135 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 2144 | U    |
| 81  | A3    | 2162 | A    |
| 81  | A3    | 2208 | U    |
| 81  | A3    | 2213 | G    |
| 81  | A3    | 2244 | U    |
| 81  | A3    | 2245 | A    |
| 81  | A3    | 2259 | A2M  |
| 81  | A3    | 2265 | A    |
| 81  | A3    | 2273 | A    |
| 81  | A3    | 2276 | G    |
| 81  | A3    | 2283 | A    |
| 81  | A3    | 2285 | U    |
| 81  | A3    | 2286 | G    |
| 81  | A3    | 2291 | OMG  |
| 81  | A3    | 2310 | G    |
| 81  | A3    | 2313 | U    |
| 81  | A3    | 2316 | A    |
| 81  | A3    | 2317 | PSU  |
| 81  | A3    | 2318 | G    |
| 81  | A3    | 2337 | U    |
| 81  | A3    | 2338 | G    |
| 81  | A3    | 2339 | U    |
| 81  | A3    | 2368 | OMC  |
| 81  | A3    | 2376 | A    |
| 81  | A3    | 2377 | C    |
| 81  | A3    | 2378 | G    |
| 81  | A3    | 2388 | G    |
| 81  | A3    | 2396 | G    |
| 81  | A3    | 2397 | G    |
| 81  | A3    | 2400 | A    |
| 81  | A3    | 2405 | A    |
| 81  | A3    | 2406 | G    |
| 81  | A3    | 2407 | A    |
| 81  | A3    | 2414 | U    |
| 81  | A3    | 2415 | G    |
| 81  | A3    | 2438 | G    |
| 81  | A3    | 2448 | U    |
| 81  | A3    | 2457 | G    |
| 81  | A3    | 2459 | A    |
| 81  | A3    | 2462 | A    |
| 81  | A3    | 2463 | U    |
| 81  | A3    | 2464 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 2465 | A    |
| 81  | A3    | 2466 | G    |
| 81  | A3    | 2468 | G    |
| 81  | A3    | 2469 | G    |
| 81  | A3    | 2470 | G    |
| 81  | A3    | 2471 | A    |
| 81  | A3    | 2483 | A    |
| 81  | A3    | 2486 | G    |
| 81  | A3    | 2488 | G    |
| 81  | A3    | 2489 | A    |
| 81  | A3    | 2492 | U    |
| 81  | A3    | 2495 | C    |
| 81  | A3    | 2496 | A    |
| 81  | A3    | 2497 | C    |
| 81  | A3    | 2499 | A    |
| 81  | A3    | 2502 | U    |
| 81  | A3    | 2503 | U    |
| 81  | A3    | 2504 | U    |
| 81  | A3    | 2505 | A    |
| 81  | A3    | 2506 | A    |
| 81  | A3    | 2519 | U    |
| 81  | A3    | 2520 | A    |
| 81  | A3    | 2529 | A    |
| 81  | A3    | 2544 | C    |
| 81  | A3    | 2545 | U    |
| 81  | A3    | 2546 | G    |
| 81  | A3    | 2556 | U    |
| 81  | A3    | 2573 | U    |
| 81  | A3    | 2574 | U    |
| 81  | A3    | 2575 | G    |
| 81  | A3    | 2576 | C    |
| 81  | A3    | 2588 | G    |
| 81  | A3    | 2596 | A    |
| 81  | A3    | 2609 | G    |
| 81  | A3    | 2610 | G    |
| 81  | A3    | 2617 | G    |
| 81  | A3    | 2629 | A    |
| 81  | A3    | 2640 | A    |
| 81  | A3    | 2655 | U    |
| 81  | A3    | 2659 | A    |
| 81  | A3    | 2660 | A    |
| 81  | A3    | 2677 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 2680 | G    |
| 81  | A3    | 2692 | G    |
| 81  | A3    | 2694 | A    |
| 81  | A3    | 2699 | A    |
| 81  | A3    | 2706 | A    |
| 81  | A3    | 2707 | A    |
| 81  | A3    | 2717 | G    |
| 81  | A3    | 2722 | U    |
| 81  | A3    | 2731 | G    |
| 81  | A3    | 2732 | OMU  |
| 81  | A3    | 2756 | G    |
| 81  | A3    | 2758 | C    |
| 81  | A3    | 2780 | G    |
| 81  | A3    | 2781 | G    |
| 81  | A3    | 2799 | G    |
| 81  | A3    | 2802 | A    |
| 81  | A3    | 2803 | G    |
| 81  | A3    | 2804 | A2M  |
| 81  | A3    | 2813 | C    |
| 81  | A3    | 2817 | G    |
| 81  | A3    | 2820 | A    |
| 81  | A3    | 2845 | U    |
| 81  | A3    | 2846 | U    |
| 81  | A3    | 2847 | C    |
| 81  | A3    | 2848 | A    |
| 81  | A3    | 2870 | C    |
| 81  | A3    | 2874 | G    |
| 81  | A3    | 2875 | A    |
| 81  | A3    | 2890 | A    |
| 81  | A3    | 2892 | C    |
| 81  | A3    | 2902 | C    |
| 81  | A3    | 2914 | A2M  |
| 81  | A3    | 2938 | U    |
| 81  | A3    | 2939 | A    |
| 81  | A3    | 2948 | G    |
| 81  | A3    | 2950 | G    |
| 81  | A3    | 2954 | G    |
| 81  | A3    | 2956 | UR3  |
| 81  | A3    | 2975 | G    |
| 81  | A3    | 2983 | U    |
| 81  | A3    | 2986 | C    |
| 81  | A3    | 2993 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 3000 | G    |
| 81  | A3    | 3014 | A    |
| 81  | A3    | 3030 | G    |
| 81  | A3    | 3060 | C    |
| 81  | A3    | 3061 | G    |
| 81  | A3    | 3080 | G    |
| 81  | A3    | 3081 | U    |
| 81  | A3    | 3094 | C    |
| 81  | A3    | 3103 | G    |
| 81  | A3    | 3118 | G    |
| 81  | A3    | 3124 | A    |
| 81  | A3    | 3132 | A    |
| 81  | A3    | 3133 | U    |
| 81  | A3    | 3144 | A    |
| 81  | A3    | 3154 | G    |
| 81  | A3    | 3170 | U    |
| 81  | A3    | 3171 | G    |
| 81  | A3    | 3172 | C    |
| 81  | A3    | 3179 | G    |
| 81  | A3    | 3185 | G    |
| 81  | A3    | 3191 | U    |
| 81  | A3    | 3194 | G    |
| 81  | A3    | 3201 | A    |
| 81  | A3    | 3208 | C    |
| 81  | A3    | 3209 | G    |
| 81  | A3    | 3211 | G    |
| 81  | A3    | 3236 | A    |
| 81  | A3    | 3240 | G    |
| 81  | A3    | 3254 | C    |
| 81  | A3    | 3257 | G    |
| 81  | A3    | 3268 | U    |
| 81  | A3    | 3272 | U    |
| 81  | A3    | 3278 | G    |
| 81  | A3    | 3279 | G    |
| 81  | A3    | 3296 | C    |
| 81  | A3    | 3308 | A    |
| 81  | A3    | 3311 | C    |
| 81  | A3    | 3312 | G    |
| 81  | A3    | 3337 | G    |
| 81  | A3    | 3342 | C    |
| 81  | A3    | 3343 | U    |
| 81  | A3    | 3344 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 3346 | C    |
| 81  | A3    | 3359 | C    |
| 81  | A3    | 3361 | G    |
| 81  | A3    | 3370 | C    |
| 81  | A3    | 3374 | U    |
| 81  | A3    | 3383 | C    |
| 81  | A3    | 3384 | G    |
| 81  | A3    | 3390 | U    |
| 82  | B3    | 2    | A    |
| 82  | B3    | 26   | C    |
| 82  | B3    | 37   | U    |
| 82  | B3    | 38   | C    |
| 82  | B3    | 62   | A    |
| 82  | B3    | 65   | C    |
| 82  | B3    | 66   | U    |
| 82  | B3    | 78   | OMG  |
| 82  | B3    | 83   | A    |
| 82  | B3    | 84   | U    |
| 82  | B3    | 85   | U    |
| 82  | B3    | 87   | C    |
| 82  | B3    | 88   | G    |
| 82  | B3    | 89   | U    |
| 82  | B3    | 90   | G    |
| 82  | B3    | 93   | C    |
| 82  | B3    | 94   | C    |
| 82  | B3    | 96   | PSU  |
| 82  | B3    | 98   | G    |
| 82  | B3    | 107  | A    |
| 82  | B3    | 109  | C    |
| 82  | B3    | 128  | C    |
| 82  | B3    | 130  | U    |
| 82  | B3    | 131  | U    |
| 82  | B3    | 133  | G    |
| 82  | B3    | 156  | C    |

All (19) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | A3    | 11  | G    |
| 81  | A3    | 398 | U    |
| 81  | A3    | 399 | OMG  |
| 81  | A3    | 540 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 81  | A3    | 601  | C    |
| 81  | A3    | 692  | A    |
| 81  | A3    | 866  | G    |
| 81  | A3    | 883  | C    |
| 81  | A3    | 926  | G    |
| 81  | A3    | 990  | G    |
| 81  | A3    | 1027 | A    |
| 81  | A3    | 1634 | U    |
| 81  | A3    | 1852 | OMC  |
| 81  | A3    | 2468 | G    |
| 81  | A3    | 2482 | G    |
| 81  | A3    | 2496 | A    |
| 81  | A3    | 2503 | U    |
| 81  | A3    | 2543 | A    |
| 81  | A3    | 3123 | U    |

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

216 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 | $\# Z  > 2$ |
| 81  | PSU  | A3    | 902  | 84,83,81 | 18,21,22     | 4.65 | 8 (44%)     | 22,30,33    | 1.81 | 5 (22%)     |
| 81  | A2M  | A3    | 2284 | 81       | 22,25,26     | 3.89 | 9 (40%)     | 31,36,39    | 3.17 | 14 (45%)    |
| 81  | PSU  | A3    | 2257 | 81       | 18,21,22     | 4.64 | 8 (44%)     | 22,30,33    | 1.85 | 5 (22%)     |
| 3   | PSU  | h1    | 1190 | 3        | 18,21,22     | 4.65 | 8 (44%)     | 22,30,33    | 1.83 | 5 (22%)     |
| 81  | OMG  | A3    | 2818 | 81       | 23,26,27     | 2.55 | 9 (39%)     | 33,38,41    | 2.17 | 12 (36%)    |
| 81  | A2M  | A3    | 369  | 81       | 22,25,26     | 3.93 | 8 (36%)     | 31,36,39    | 3.02 | 13 (41%)    |
| 81  | PSU  | A3    | 1135 | 81       | 18,21,22     | 4.64 | 8 (44%)     | 22,30,33    | 1.86 | 5 (22%)     |
| 81  | OMG  | A3    | 296  | 81       | 23,26,27     | 2.57 | 8 (34%)     | 33,38,41    | 2.21 | 11 (33%)    |
| 81  | A2M  | A3    | 2259 | 81       | 22,25,26     | 3.97 | 9 (40%)     | 31,36,39    | 3.07 | 14 (45%)    |
| 81  | UY1  | A3    | 2653 | 81       | 19,22,23     | 4.20 | 7 (36%)     | 22,31,34    | 1.87 | 5 (22%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 81  | PSU  | A3    | 2868 | 81    | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.90 | 6 (27%)  |
| 3   | PSU  | h1    | 310  | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 81  | A2M  | A3    | 2329 | 81    | 22,25,26     | 3.94 | 8 (36%)  | 31,36,39    | 3.00 | 11 (35%) |
| 3   | 4AC  | h1    | 1283 | 3     | 21,24,25     | 3.25 | 11 (52%) | 29,34,37    | 0.98 | 2 (6%)   |
| 3   | OMC  | h1    | 473  | 3     | 19,22,23     | 3.30 | 8 (42%)  | 26,31,34    | 0.72 | 0        |
| 3   | PSU  | h1    | 1304 | 3     | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | OMC  | A3    | 2200 | 84,81 | 19,22,23     | 3.29 | 8 (42%)  | 26,31,34    | 0.80 | 0        |
| 3   | PSU  | h1    | 1634 | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 81  | OMU  | A3    | 3304 | 81    | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.64 | 4 (15%)  |
| 3   | B8N  | h1    | 1194 | 3     | 24,29,30     | 3.04 | 7 (29%)  | 29,42,45    | 1.73 | 6 (20%)  |
| 81  | PSU  | A3    | 150  | 84,81 | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 81  | A2M  | A3    | 2643 | 81    | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 2.96 | 12 (38%) |
| 81  | A2M  | A3    | 946  | 81    | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 3.07 | 14 (45%) |
| 81  | OMU  | A3    | 1068 | 81    | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.70 | 5 (19%)  |
| 81  | A2M  | A3    | 2223 | 81    | 22,25,26     | 3.95 | 9 (40%)  | 31,36,39    | 2.96 | 11 (35%) |
| 3   | OMG  | h1    | 246  | 84,3  | 23,26,27     | 2.59 | 8 (34%)  | 33,38,41    | 2.27 | 10 (30%) |
| 81  | PSU  | A3    | 2263 | 81    | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 3   | OMG  | h1    | 598  | 3     | 23,26,27     | 2.57 | 8 (34%)  | 33,38,41    | 2.25 | 10 (30%) |
| 3   | PSU  | h1    | 103  | 84,3  | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 81  | PSU  | A3    | 2267 | 81    | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | OMC  | A3    | 2340 | 81    | 19,22,23     | 3.28 | 8 (42%)  | 26,31,34    | 0.68 | 0        |
| 81  | A2M  | A3    | 1144 | 81    | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 3.00 | 13 (41%) |
| 3   | UY1  | h1    | 603  | 3     | 19,22,23     | 4.17 | 7 (36%)  | 22,31,34    | 1.84 | 5 (22%)  |
| 81  | OMU  | A3    | 2738 | 81    | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.67 | 5 (19%)  |
| 3   | PSU  | h1    | 1308 | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.78 | 5 (22%)  |
| 3   | PSU  | h1    | 584  | 3     | 18,21,22     | 4.75 | 9 (50%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 3   | OMU  | h1    | 886  | 3     | 19,22,23     | 3.22 | 8 (42%)  | 26,31,34    | 1.80 | 5 (19%)  |
| 3   | PSU  | h1    | 339  | 84,3  | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.80 | 6 (27%)  |
| 81  | PSU  | A3    | 228  | 81    | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | OMG  | A3    | 2920 | 81    | 23,26,27     | 2.55 | 8 (34%)  | 33,38,41    | 2.21 | 11 (33%) |
| 3   | PSU  | h1    | 306  | 3     | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.76 | 5 (22%)  |
| 3   | A2M  | h1    | 440  | 3     | 22,25,26     | 3.94 | 8 (36%)  | 31,36,39    | 3.04 | 12 (38%) |
| 81  | OMG  | A3    | 1857 | 81    | 23,26,27     | 2.54 | 8 (34%)  | 33,38,41    | 2.19 | 11 (33%) |
| 3   | PSU  | h1    | 121  | 3,83  | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 81  | A2M  | A3    | 886  | 81    | 22,25,26     | 3.93 | 9 (40%)  | 31,36,39    | 2.96 | 13 (41%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 82  | PSU  | B3    | 96   | 82,84 | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.75 | 5 (22%)  |
| 81  | OMC  | A3    | 674  | 81    | 19,22,23     | 3.25 | 8 (42%)  | 26,31,34    | 0.68 | 0        |
| 81  | PSU  | A3    | 976  | 84,81 | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | A2M  | A3    | 1460 | 81    | 22,25,26     | 3.93 | 9 (40%)  | 31,36,39    | 2.99 | 12 (38%) |
| 81  | PSU  | A3    | 2214 | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 81  | 5MC  | A3    | 2281 | 81    | 18,22,23     | 4.01 | 7 (38%)  | 26,32,35    | 1.04 | 2 (7%)   |
| 81  | PSU  | A3    | 2958 | 81    | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 3   | PSU  | h1    | 258  | 3     | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 81  | PSU  | A3    | 1482 | 81    | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.76 | 5 (22%)  |
| 81  | PSU  | A3    | 1134 | 81    | 18,21,22     | 4.60 | 8 (44%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 81  | OMG  | A3    | 2622 | 36,81 | 23,26,27     | 2.57 | 8 (34%)  | 33,38,41    | 2.22 | 10 (30%) |
| 3   | A2M  | h1    | 544  | 3     | 22,25,26     | 3.91 | 9 (40%)  | 31,36,39    | 2.98 | 13 (41%) |
| 3   | OMU  | h1    | 1234 | 3     | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.65 | 4 (15%)  |
| 81  | PSU  | A3    | 717  | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 81  | PSU  | A3    | 2137 | 84,81 | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.92 | 5 (22%)  |
| 3   | OMU  | h1    | 1447 | 3     | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.61 | 4 (15%)  |
| 81  | PSU  | A3    | 1685 | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.87 | 6 (27%)  |
| 3   | PSU  | h1    | 95   | 3     | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 3   | PSU  | h1    | 753  | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 3   | PSU  | h1    | 1615 | 3     | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 81  | OMU  | A3    | 48   | 81    | 19,22,23     | 3.19 | 8 (42%)  | 26,31,34    | 1.63 | 4 (15%)  |
| 81  | OMC  | A3    | 2839 | 81    | 19,22,23     | 3.28 | 8 (42%)  | 26,31,34    | 0.78 | 0        |
| 3   | PSU  | h1    | 1210 | 3     | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 3   | PSU  | h1    | 605  | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 81  | PSU  | A3    | 510  | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 81  | OMG  | A3    | 2127 | 81    | 23,26,27     | 2.54 | 9 (39%)  | 33,38,41    | 2.18 | 13 (39%) |
| 81  | PSU  | A3    | 2857 | 81    | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 81  | PSU  | A3    | 2829 | 81    | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.90 | 6 (27%)  |
| 81  | OMG  | A3    | 2394 | 81    | 23,26,27     | 2.54 | 9 (39%)  | 33,38,41    | 2.15 | 12 (36%) |
| 3   | PSU  | h1    | 1002 | 3     | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | OMG  | A3    | 2794 | 81    | 23,26,27     | 2.55 | 8 (34%)  | 33,38,41    | 2.14 | 11 (33%) |
| 81  | PSU  | A3    | 2419 | 81    | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 81  | PSU  | A3    | 2883 | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.85 | 6 (27%)  |
| 3   | OMC  | h1    | 38   | 3     | 19,22,23     | 3.32 | 8 (42%)  | 26,31,34    | 0.71 | 0        |
| 3   | A2M  | h1    | 468  | 3     | 22,25,26     | 3.95 | 8 (36%)  | 31,36,39    | 3.01 | 12 (38%) |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 81  | 1MA  | A3    | 656  | 81       | 21,25,26     | 2.77 | 5 (23%)  | 31,37,40    | 1.73 | 7 (22%)  |
| 81  | OMG  | A3    | 918  | 84,81    | 23,26,27     | 2.57 | 8 (34%)  | 33,38,41    | 2.26 | 10 (30%) |
| 3   | OMU  | h1    | 373  | 3        | 19,22,23     | 3.22 | 8 (42%)  | 26,31,34    | 1.66 | 4 (15%)  |
| 81  | OMU  | A3    | 1894 | 81       | 19,22,23     | 3.23 | 8 (42%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 3   | PSU  | h1    | 1567 | 3        | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | A2M  | A3    | 827  | 84,83,81 | 22,25,26     | 3.96 | 9 (40%)  | 31,36,39    | 3.04 | 12 (38%) |
| 81  | OMC  | A3    | 1862 | 81       | 19,22,23     | 3.26 | 8 (42%)  | 26,31,34    | 0.68 | 0        |
| 81  | PSU  | A3    | 2947 | 84,81    | 18,21,22     | 4.64 | 9 (50%)  | 22,30,33    | 1.85 | 6 (27%)  |
| 3   | A2M  | h1    | 1579 | 3        | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 3.04 | 13 (41%) |
| 81  | OMU  | A3    | 2720 | 81       | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.64 | 4 (15%)  |
| 81  | PSU  | A3    | 2194 | 84,81    | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 81  | OMG  | A3    | 2654 | 81       | 23,26,27     | 2.53 | 9 (39%)  | 33,38,41    | 2.13 | 13 (39%) |
| 82  | OMG  | B3    | 78   | 82       | 23,26,27     | 2.56 | 8 (34%)  | 33,38,41    | 2.23 | 10 (30%) |
| 81  | PSU  | A3    | 464  | 81       | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.80 | 6 (27%)  |
| 81  | PSU  | A3    | 2897 | 81       | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 81  | OMG  | A3    | 2126 | 81       | 23,26,27     | 2.54 | 8 (34%)  | 33,38,41    | 2.20 | 11 (33%) |
| 81  | PSU  | A3    | 966  | 81       | 18,21,22     | 4.61 | 8 (44%)  | 22,30,33    | 1.74 | 5 (22%)  |
| 81  | PSU  | A3    | 2139 | 81       | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 3   | PSU  | h1    | 1178 | 3        | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | OMC  | A3    | 2685 | 81       | 19,22,23     | 3.28 | 8 (42%)  | 26,31,34    | 0.73 | 0        |
| 81  | OMG  | A3    | 2796 | 81       | 23,26,27     | 2.56 | 8 (34%)  | 33,38,41    | 2.20 | 11 (33%) |
| 81  | UR3  | A3    | 2956 | 81       | 19,22,23     | 2.79 | 8 (42%)  | 26,32,35    | 1.31 | 2 (7%)   |
| 3   | OMU  | h1    | 614  | 3        | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.65 | 5 (19%)  |
| 3   | OMU  | h1    | 581  | 84,3     | 19,22,23     | 3.23 | 8 (42%)  | 26,31,34    | 1.67 | 4 (15%)  |
| 81  | OMG  | A3    | 399  | 81       | 23,26,27     | 2.60 | 8 (34%)  | 33,38,41    | 2.32 | 10 (30%) |
| 81  | OMC  | A3    | 1480 | 81       | 19,22,23     | 3.30 | 8 (42%)  | 26,31,34    | 0.73 | 0        |
| 81  | OMG  | A3    | 2925 | 81       | 23,26,27     | 2.57 | 8 (34%)  | 33,38,41    | 2.25 | 10 (30%) |
| 81  | PSU  | A3    | 895  | 81       | 18,21,22     | 4.61 | 8 (44%)  | 22,30,33    | 1.78 | 5 (22%)  |
| 81  | PSU  | A3    | 34   | 81       | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 3   | A2M  | h1    | 1758 | 3        | 22,25,26     | 3.94 | 10 (45%) | 31,36,39    | 2.97 | 12 (38%) |
| 81  | OMU  | A3    | 3289 | 81       | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.63 | 4 (15%)  |
| 81  | PSU  | A3    | 684  | 81       | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 3   | PSU  | h1    | 1184 | 3        | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 3   | 6MZ  | h1    | 1771 | 84,3,83  | 22,25,26     | 2.75 | 5 (22%)  | 30,36,39    | 2.45 | 11 (36%) |
| 3   | PSU  | h1    | 1787 | 3        | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | A2M  | h1    | 28   | 3,83  | 22,25,26     | 3.93 | 8 (36%)  | 31,36,39    | 3.00 | 12 (38%) |
| 3   | OMU  | h1    | 1272 | 3     | 19,22,23     | 3.23 | 8 (42%)  | 26,31,34    | 1.66 | 4 (15%)  |
| 81  | OMG  | A3    | 2398 | 81    | 23,26,27     | 2.53 | 9 (39%)  | 33,38,41    | 2.17 | 13 (39%) |
| 3   | PSU  | h1    | 1120 | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.77 | 5 (22%)  |
| 3   | PSU  | h1    | 809  | 3     | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | OMU  | A3    | 2732 | 81    | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.61 | 4 (15%)  |
| 81  | OMC  | A3    | 2882 | 81    | 19,22,23     | 3.27 | 8 (42%)  | 26,31,34    | 0.75 | 0        |
| 81  | A2M  | A3    | 2949 | 81    | 22,25,26     | 3.95 | 9 (40%)  | 31,36,39    | 3.04 | 15 (48%) |
| 81  | OMU  | A3    | 675  | 81    | 19,22,23     | 3.22 | 8 (42%)  | 26,31,34    | 1.69 | 5 (19%)  |
| 81  | PSU  | A3    | 970  | 81    | 18,21,22     | 4.66 | 9 (50%)  | 22,30,33    | 1.89 | 5 (22%)  |
| 81  | PSU  | A3    | 2261 | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | PSU  | A3    | 2317 | 84,81 | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.90 | 5 (22%)  |
| 3   | PSU  | h1    | 1485 | 3     | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | PSU  | A3    | 2321 | 83,81 | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 3   | PSU  | h1    | 961  | 84,3  | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 3   | A2M  | h1    | 424  | 3     | 22,25,26     | 3.95 | 9 (40%)  | 31,36,39    | 3.02 | 14 (45%) |
| 3   | PSU  | h1    | 451  | 84,3  | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.87 | 6 (27%)  |
| 3   | OMU  | h1    | 1383 | 3,83  | 19,22,23     | 3.23 | 8 (42%)  | 26,31,34    | 1.67 | 4 (15%)  |
| 81  | OMC  | A3    | 2296 | 81    | 19,22,23     | 3.29 | 8 (42%)  | 26,31,34    | 0.74 | 0        |
| 82  | PSU  | B3    | 21   | 82,81 | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.78 | 5 (22%)  |
| 81  | PSU  | A3    | 829  | 81    | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 3   | PSU  | h1    | 1217 | 3     | 18,21,22     | 4.68 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 82  | PSU  | B3    | 77   | 82    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.86 | 5 (22%)  |
| 3   | MA6  | h1    | 1790 | 3     | 23,26,27     | 1.24 | 3 (13%)  | 34,38,41    | 2.86 | 14 (41%) |
| 3   | PSU  | h1    | 635  | 3     | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 3   | A2M  | h1    | 1329 | 3     | 22,25,26     | 3.95 | 9 (40%)  | 31,36,39    | 3.02 | 13 (41%) |
| 81  | OMU  | A3    | 2886 | 81    | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.63 | 4 (15%)  |
| 81  | OMG  | A3    | 2239 | 81    | 23,26,27     | 2.59 | 8 (34%)  | 33,38,41    | 2.24 | 10 (30%) |
| 3   | PSU  | h1    | 763  | 3     | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 3   | MA6  | h1    | 1789 | 3     | 23,26,27     | 1.24 | 3 (13%)  | 34,38,41    | 2.82 | 14 (41%) |
| 81  | PSU  | A3    | 2435 | 81    | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.90 | 6 (27%)  |
| 3   | OMC  | h1    | 1218 | 3     | 19,22,23     | 3.31 | 8 (42%)  | 26,31,34    | 0.71 | 0        |
| 3   | PSU  | h1    | 1106 | 3     | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | PSU  | A3    | 1016 | 84,81 | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 3   | PSU  | h1    | 762  | 3     | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 81  | OMG  | A3    | 2412 | 84,81 | 23,26,27     | 2.56 | 8 (34%)  | 33,38,41    | 2.25 | 11 (33%) |
| 81  | A2M  | A3    | 2804 | 81    | 22,25,26     | 3.90 | 8 (36%)  | 31,36,39    | 3.20 | 15 (48%) |
| 81  | PSU  | A3    | 1002 | 81    | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 81  | OMG  | A3    | 815  | 81    | 23,26,27     | 2.57 | 8 (34%)  | 33,38,41    | 2.27 | 11 (33%) |
| 81  | OMC  | A3    | 2368 | 81    | 19,22,23     | 3.27 | 8 (42%)  | 26,31,34    | 0.69 | 0        |
| 81  | A2M  | A3    | 660  | 81    | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 3.12 | 14 (45%) |
| 81  | PSU  | A3    | 786  | 81    | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.73 | 5 (22%)  |
| 81  | OMG  | A3    | 1461 | 81    | 23,26,27     | 2.55 | 8 (34%)  | 33,38,41    | 2.26 | 12 (36%) |
| 81  | OMU  | A3    | 2413 | 84,81 | 19,22,23     | 3.17 | 8 (42%)  | 26,31,34    | 1.59 | 4 (15%)  |
| 81  | PSU  | A3    | 1056 | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 81  | PSU  | A3    | 311  | 84,81 | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.73 | 5 (22%)  |
| 3   | PSU  | h1    | 362  | 3     | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 81  | OMC  | A3    | 1852 | 81    | 19,22,23     | 3.31 | 8 (42%)  | 26,31,34    | 0.74 | 0        |
| 3   | PSU  | h1    | 470  | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 3   | OMG  | h1    | 392  | 3     | 23,26,27     | 2.59 | 8 (34%)  | 33,38,41    | 2.24 | 10 (30%) |
| 81  | OMU  | A3    | 804  | 81    | 19,22,23     | 3.22 | 8 (42%)  | 26,31,34    | 1.69 | 5 (19%)  |
| 81  | A2M  | A3    | 2324 | 81    | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 3.01 | 13 (41%) |
| 81  | OMU  | A3    | 2424 | 81    | 19,22,23     | 3.22 | 8 (42%)  | 26,31,34    | 1.68 | 5 (19%)  |
| 81  | A2M  | A3    | 817  | 81    | 22,25,26     | 3.91 | 9 (40%)  | 31,36,39    | 3.05 | 14 (45%) |
| 81  | OMG  | A3    | 2291 | 81    | 23,26,27     | 2.56 | 8 (34%)  | 33,38,41    | 2.24 | 10 (30%) |
| 81  | OMC  | A3    | 1448 | 81    | 19,22,23     | 3.29 | 8 (42%)  | 26,31,34    | 0.87 | 1 (3%)   |
| 3   | PSU  | h1    | 417  | 3     | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | A2M  | A3    | 2914 | 81    | 22,25,26     | 3.93 | 9 (40%)  | 31,36,39    | 3.07 | 12 (38%) |
| 3   | PSU  | h1    | 1535 | 3     | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 81  | OMU  | A3    | 144  | 81    | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.65 | 4 (15%)  |
| 81  | OMU  | A3    | 44   | 84,81 | 19,22,23     | 3.23 | 8 (42%)  | 26,31,34    | 1.63 | 4 (15%)  |
| 3   | PSU  | h1    | 606  | 3     | 18,21,22     | 4.61 | 8 (44%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 3   | PSU  | h1    | 607  | 3     | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.86 | 6 (27%)  |
| 3   | PSU  | h1    | 1524 | 3     | 18,21,22     | 4.69 | 8 (44%)  | 22,30,33    | 1.75 | 5 (22%)  |
| 3   | PSU  | h1    | 1027 | 3     | 18,21,22     | 4.68 | 9 (50%)  | 22,30,33    | 1.81 | 5 (22%)  |
| 3   | OMC  | h1    | 1645 | 3     | 19,22,23     | 3.30 | 8 (42%)  | 26,31,34    | 0.71 | 0        |
| 81  | PSU  | A3    | 277  | 81    | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | PSU  | A3    | 1064 | 81    | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 81  | PSU  | A3    | 2926 | 84,81 | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.88 | 5 (22%)  |
| 81  | OMU  | A3    | 2350 | 81    | 19,22,23     | 3.23 | 8 (42%)  | 26,31,34    | 1.67 | 5 (19%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMG  | h1    | 1274 | 3     | 23,26,27     | 2.58 | 8 (34%)  | 33,38,41    | 2.25 | 10 (30%) |
| 3   | A2M  | h1    | 622  | 3,83  | 22,25,26     | 3.91 | 9 (40%)  | 31,36,39    | 3.11 | 14 (45%) |
| 3   | 4AC  | h1    | 1781 | 3     | 21,24,25     | 3.26 | 11 (52%) | 29,34,37    | 1.04 | 3 (10%)  |
| 3   | OMU  | h1    | 123  | 3     | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.66 | 5 (19%)  |
| 81  | OMC  | A3    | 1849 | 81    | 19,22,23     | 3.25 | 8 (42%)  | 26,31,34    | 0.70 | 0        |
| 81  | PSU  | A3    | 1133 | 81    | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | OMU  | A3    | 1537 | 81    | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.63 | 4 (15%)  |
| 3   | A2M  | h1    | 977  | 3     | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 2.94 | 12 (38%) |
| 3   | A2M  | h1    | 800  | 3     | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 2.98 | 12 (38%) |
| 82  | A2M  | B3    | 46   | 82    | 22,25,26     | 3.93 | 9 (40%)  | 31,36,39    | 3.01 | 14 (45%) |
| 81  | A2M  | A3    | 1378 | 81    | 22,25,26     | 3.93 | 9 (40%)  | 31,36,39    | 2.96 | 12 (38%) |
| 3   | OMC  | h1    | 140  | 3     | 19,22,23     | 3.31 | 8 (42%)  | 26,31,34    | 0.72 | 0        |
| 3   | PSU  | h1    | 950  | 3     | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 81  | PSU  | A3    | 3113 | 81    | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.77 | 5 (22%)  |
| 81  | PSU  | A3    | 2978 | 81    | 18,21,22     | 4.65 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 3   | OMC  | h1    | 418  | 3     | 19,22,23     | 3.30 | 8 (42%)  | 26,31,34    | 0.89 | 1 (3%)   |
| 81  | 5MC  | A3    | 2873 | 84,81 | 18,22,23     | 4.02 | 7 (38%)  | 26,32,35    | 1.09 | 1 (3%)   |
| 81  | OMC  | A3    | 2962 | 81    | 19,22,23     | 3.25 | 8 (42%)  | 26,31,34    | 0.77 | 0        |
| 3   | OMG  | h1    | 1433 | 3,83  | 23,26,27     | 2.55 | 8 (34%)  | 33,38,41    | 2.19 | 11 (33%) |
| 81  | A2M  | A3    | 2129 | 81    | 22,25,26     | 3.96 | 9 (40%)  | 31,36,39    | 3.01 | 12 (38%) |
| 3   | OMU  | h1    | 1012 | 3     | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.67 | 4 (15%)  |
| 81  | PSU  | A3    | 1474 | 81    | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | PSU  | A3    | 2747 | 81    | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 81  | OMC  | A3    | 40   | 81    | 19,22,23     | 3.27 | 8 (42%)  | 26,31,34    | 0.89 | 1 (3%)   |
| 3   | A2M  | h1    | 162  | 3     | 22,25,26     | 3.95 | 9 (40%)  | 31,36,39    | 3.01 | 13 (41%) |
| 81  | PSU  | A3    | 2269 | 81    | 18,21,22     | 4.68 | 8 (44%)  | 22,30,33    | 1.78 | 5 (22%)  |
| 81  | OMC  | A3    | 2951 | 81    | 19,22,23     | 3.23 | 8 (42%)  | 26,31,34    | 0.78 | 0        |
| 3   | PSU  | h1    | 1293 | 3     | 18,21,22     | 4.66 | 8 (44%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 81  | PSU  | A3    | 42   | 84,81 | 18,21,22     | 4.64 | 8 (44%)  | 22,30,33    | 1.83 | 5 (22%)  |
| 81  | OMU  | A3    | 787  | 81    | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.65 | 5 (19%)  |
| 81  | OMU  | A3    | 2924 | 84,81 | 19,22,23     | 3.21 | 8 (42%)  | 26,31,34    | 1.68 | 4 (15%)  |

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   |
|-----|------|-------|------|----------|---------|------------|---------|
| 81  | PSU  | A3    | 902  | 84,83,81 | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | A2M  | A3    | 2284 | 81       | -       | 3/9/27/28  | 0/3/3/3 |
| 81  | PSU  | A3    | 2257 | 81       | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 1190 | 3        | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMG  | A3    | 2818 | 81       | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | A2M  | A3    | 369  | 81       | -       | 1/9/27/28  | 0/3/3/3 |
| 81  | PSU  | A3    | 1135 | 81       | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMG  | A3    | 296  | 81       | -       | 2/9/27/28  | 0/3/3/3 |
| 81  | A2M  | A3    | 2259 | 81       | -       | 2/9/27/28  | 0/3/3/3 |
| 81  | UY1  | A3    | 2653 | 81       | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | PSU  | A3    | 2868 | 81       | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 310  | 3        | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | A2M  | A3    | 2329 | 81       | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | 4AC  | h1    | 1283 | 3        | -       | 0/11/29/30 | 0/2/2/2 |
| 3   | OMC  | h1    | 473  | 3        | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 1304 | 3        | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMC  | A3    | 2200 | 84,81    | -       | 4/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 1634 | 3        | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMU  | A3    | 3304 | 81       | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | B8N  | h1    | 1194 | 3        | -       | 3/16/34/35 | 0/2/2/2 |
| 81  | PSU  | A3    | 150  | 84,81    | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | A2M  | A3    | 2643 | 81       | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | A2M  | A3    | 946  | 81       | -       | 2/9/27/28  | 0/3/3/3 |
| 81  | OMU  | A3    | 1068 | 81       | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | A2M  | A3    | 2223 | 81       | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | h1    | 246  | 84,3     | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | PSU  | A3    | 2263 | 81       | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | OMG  | h1    | 598  | 3        | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | PSU  | h1    | 103  | 84,3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 2267 | 81       | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMC  | A3    | 2340 | 81       | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | A2M  | A3    | 1144 | 81       | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | UY1  | h1    | 603  | 3        | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | OMU  | A3    | 2738 | 81       | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 1308 | 3        | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 584  | 3        | -       | 6/7/25/26  | 0/2/2/2 |
| 3   | OMU  | h1    | 886  | 3        | -       | 3/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 339  | 84,3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 228  | 81       | -       | 1/7/25/26  | 0/2/2/2 |
| 81  | OMG  | A3    | 2920 | 81       | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | h1    | 306  | 3        | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 3   | A2M  | h1    | 440  | 3     | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | OMG  | A3    | 1857 | 81    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | h1    | 121  | 3,83  | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | A2M  | A3    | 886  | 81    | -       | 0/9/27/28 | 0/3/3/3 |
| 82  | PSU  | B3    | 96   | 82,84 | -       | 2/7/25/26 | 0/2/2/2 |
| 81  | OMC  | A3    | 674  | 81    | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | PSU  | A3    | 976  | 84,81 | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | A2M  | A3    | 1460 | 81    | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | PSU  | A3    | 2214 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | 5MC  | A3    | 2281 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 2958 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 258  | 3     | -       | 1/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 1482 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 1134 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMG  | A3    | 2622 | 36,81 | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | A2M  | h1    | 544  | 3     | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | OMU  | h1    | 1234 | 3     | -       | 2/9/27/28 | 0/2/2/2 |
| 81  | PSU  | A3    | 717  | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 2137 | 84,81 | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | h1    | 1447 | 3     | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | PSU  | A3    | 1685 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 95   | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 753  | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 1615 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMU  | A3    | 48   | 81    | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | OMC  | A3    | 2839 | 81    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | h1    | 1210 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 605  | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 510  | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMG  | A3    | 2127 | 81    | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | PSU  | A3    | 2857 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 2829 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMG  | A3    | 2394 | 81    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | h1    | 1002 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMG  | A3    | 2794 | 81    | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | PSU  | A3    | 2419 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 2883 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | h1    | 38   | 3     | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | A2M  | h1    | 468  | 3     | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | 1MA  | A3    | 656  | 81    | -       | 2/7/25/26 | 0/3/3/3 |
| 81  | OMG  | A3    | 918  | 84,81 | -       | 2/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions  | Rings   |
|-----|------|-------|------|----------|---------|-----------|---------|
| 3   | OMU  | h1    | 373  | 3        | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | OMU  | A3    | 1894 | 81       | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | h1    | 1567 | 3        | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | A2M  | A3    | 827  | 84,83,81 | -       | 3/9/27/28 | 0/3/3/3 |
| 81  | OMC  | A3    | 1862 | 81       | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | PSU  | A3    | 2947 | 84,81    | -       | 2/7/25/26 | 0/2/2/2 |
| 3   | A2M  | h1    | 1579 | 3        | -       | 2/9/27/28 | 0/3/3/3 |
| 81  | OMU  | A3    | 2720 | 81       | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | PSU  | A3    | 2194 | 84,81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMG  | A3    | 2654 | 81       | -       | 0/9/27/28 | 0/3/3/3 |
| 82  | OMG  | B3    | 78   | 82       | -       | 2/9/27/28 | 0/3/3/3 |
| 81  | PSU  | A3    | 464  | 81       | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 2897 | 81       | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMG  | A3    | 2126 | 81       | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | PSU  | A3    | 966  | 81       | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 2139 | 81       | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 1178 | 3        | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMC  | A3    | 2685 | 81       | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | OMG  | A3    | 2796 | 81       | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | UR3  | A3    | 2956 | 81       | -       | 2/7/25/26 | 0/2/2/2 |
| 3   | OMU  | h1    | 614  | 3        | -       | 3/9/27/28 | 0/2/2/2 |
| 3   | OMU  | h1    | 581  | 84,3     | -       | 2/9/27/28 | 0/2/2/2 |
| 81  | OMG  | A3    | 399  | 81       | -       | 2/9/27/28 | 0/3/3/3 |
| 81  | OMC  | A3    | 1480 | 81       | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | OMG  | A3    | 2925 | 81       | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | PSU  | A3    | 895  | 81       | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 34   | 81       | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | h1    | 1758 | 3        | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | OMU  | A3    | 3289 | 81       | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | PSU  | A3    | 684  | 81       | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 1184 | 3        | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | 6MZ  | h1    | 1771 | 84,3,83  | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | h1    | 1787 | 3        | -       | 2/7/25/26 | 0/2/2/2 |
| 3   | A2M  | h1    | 28   | 3,83     | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMU  | h1    | 1272 | 3        | -       | 2/9/27/28 | 0/2/2/2 |
| 81  | OMG  | A3    | 2398 | 81       | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | h1    | 1120 | 3        | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | h1    | 809  | 3        | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMU  | A3    | 2732 | 81       | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | OMC  | A3    | 2882 | 81       | -       | 0/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 81  | A2M  | A3    | 2949 | 81    | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | OMU  | A3    | 675  | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | PSU  | A3    | 970  | 81    | -       | 1/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 2261 | 81    | -       | 1/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 2317 | 84,81 | -       | 3/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 1485 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 2321 | 83,81 | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 961  | 84,3  | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | h1    | 424  | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | h1    | 451  | 84,3  | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | h1    | 1383 | 3,83  | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | OMC  | A3    | 2296 | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 82  | PSU  | B3    | 21   | 82,81 | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 829  | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 1217 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 82  | PSU  | B3    | 77   | 82    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | MA6  | h1    | 1790 | 3     | -       | 4/11/29/30 | 0/3/3/3 |
| 3   | PSU  | h1    | 635  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | h1    | 1329 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | OMU  | A3    | 2886 | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | OMG  | A3    | 2239 | 81    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | h1    | 763  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | MA6  | h1    | 1789 | 3     | -       | 0/11/29/30 | 0/3/3/3 |
| 81  | PSU  | A3    | 2435 | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | h1    | 1218 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 1106 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 1016 | 84,81 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 762  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMG  | A3    | 2412 | 84,81 | -       | 1/9/27/28  | 0/3/3/3 |
| 81  | A2M  | A3    | 2804 | 81    | -       | 4/9/27/28  | 0/3/3/3 |
| 81  | PSU  | A3    | 1002 | 81    | -       | 2/7/25/26  | 0/2/2/2 |
| 81  | OMG  | A3    | 815  | 81    | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | OMC  | A3    | 2368 | 81    | -       | 3/9/27/28  | 0/2/2/2 |
| 81  | A2M  | A3    | 660  | 81    | -       | 2/9/27/28  | 0/3/3/3 |
| 81  | PSU  | A3    | 786  | 81    | -       | 3/7/25/26  | 0/2/2/2 |
| 81  | OMG  | A3    | 1461 | 81    | -       | 1/9/27/28  | 0/3/3/3 |
| 81  | OMU  | A3    | 2413 | 84,81 | -       | 2/9/27/28  | 0/2/2/2 |
| 81  | PSU  | A3    | 1056 | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 311  | 84,81 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 362  | 3     | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 81  | OMC  | A3    | 1852 | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 470  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | h1    | 392  | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 81  | OMU  | A3    | 804  | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | A2M  | A3    | 2324 | 81    | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | OMU  | A3    | 2424 | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | A2M  | A3    | 817  | 81    | -       | 1/9/27/28  | 0/3/3/3 |
| 81  | OMG  | A3    | 2291 | 81    | -       | 2/9/27/28  | 0/3/3/3 |
| 81  | OMC  | A3    | 1448 | 81    | -       | 3/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 417  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | A2M  | A3    | 2914 | 81    | -       | 5/9/27/28  | 0/3/3/3 |
| 3   | PSU  | h1    | 1535 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMU  | A3    | 144  | 81    | -       | 1/9/27/28  | 0/2/2/2 |
| 81  | OMU  | A3    | 44   | 84,81 | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 606  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 607  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 1524 | 3     | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | h1    | 1027 | 3     | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | OMC  | h1    | 1645 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | PSU  | A3    | 277  | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 1064 | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 2926 | 84,81 | -       | 3/7/25/26  | 0/2/2/2 |
| 81  | OMU  | A3    | 2350 | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMG  | h1    | 1274 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | h1    | 622  | 3,83  | -       | 4/9/27/28  | 0/3/3/3 |
| 3   | 4AC  | h1    | 1781 | 3     | -       | 0/11/29/30 | 0/2/2/2 |
| 3   | OMU  | h1    | 123  | 3     | -       | 2/9/27/28  | 0/2/2/2 |
| 81  | OMC  | A3    | 1849 | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 81  | PSU  | A3    | 1133 | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | OMU  | A3    | 1537 | 81    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | h1    | 977  | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | h1    | 800  | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 82  | A2M  | B3    | 46   | 82    | -       | 0/9/27/28  | 0/3/3/3 |
| 81  | A2M  | A3    | 1378 | 81    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMC  | h1    | 140  | 3     | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | PSU  | h1    | 950  | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 3113 | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | PSU  | A3    | 2978 | 81    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | h1    | 418  | 3     | -       | 2/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 81  | 5MC  | A3    | 2873 | 84,81 | -       | 4/7/25/26 | 0/2/2/2 |
| 81  | OMC  | A3    | 2962 | 81    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | OMG  | h1    | 1433 | 3,83  | -       | 1/9/27/28 | 0/3/3/3 |
| 81  | A2M  | A3    | 2129 | 81    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMU  | h1    | 1012 | 3     | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | PSU  | A3    | 1474 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 2747 | 81    | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMC  | A3    | 40   | 81    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | A2M  | h1    | 162  | 3     | -       | 0/9/27/28 | 0/3/3/3 |
| 81  | PSU  | A3    | 2269 | 81    | -       | 2/7/25/26 | 0/2/2/2 |
| 81  | OMC  | A3    | 2951 | 81    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | h1    | 1293 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | PSU  | A3    | 42   | 84,81 | -       | 0/7/25/26 | 0/2/2/2 |
| 81  | OMU  | A3    | 787  | 81    | -       | 0/9/27/28 | 0/2/2/2 |
| 81  | OMU  | A3    | 2924 | 84,81 | -       | 0/9/27/28 | 0/2/2/2 |

All (1749) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | h1    | 1524 | PSU  | C6-C5 | 12.36 | 1.49        | 1.35     |
| 3   | h1    | 584  | PSU  | C6-C5 | 12.34 | 1.49        | 1.35     |
| 81  | A3    | 2137 | PSU  | C6-C5 | 12.29 | 1.49        | 1.35     |
| 81  | A3    | 2269 | PSU  | C6-C5 | 12.27 | 1.49        | 1.35     |
| 3   | h1    | 1217 | PSU  | C6-C5 | 12.25 | 1.49        | 1.35     |
| 81  | A3    | 786  | PSU  | C6-C5 | 12.25 | 1.49        | 1.35     |
| 81  | A3    | 311  | PSU  | C6-C5 | 12.23 | 1.49        | 1.35     |
| 3   | h1    | 1027 | PSU  | C6-C5 | 12.23 | 1.49        | 1.35     |
| 3   | h1    | 451  | PSU  | C6-C5 | 12.22 | 1.49        | 1.35     |
| 3   | h1    | 1485 | PSU  | C6-C5 | 12.22 | 1.49        | 1.35     |
| 3   | h1    | 961  | PSU  | C6-C5 | 12.20 | 1.49        | 1.35     |
| 81  | A3    | 1685 | PSU  | C6-C5 | 12.20 | 1.49        | 1.35     |
| 81  | A3    | 902  | PSU  | C6-C5 | 12.19 | 1.49        | 1.35     |
| 81  | A3    | 1002 | PSU  | C6-C5 | 12.19 | 1.49        | 1.35     |
| 81  | A3    | 2883 | PSU  | C6-C5 | 12.19 | 1.49        | 1.35     |
| 81  | A3    | 3113 | PSU  | C6-C5 | 12.19 | 1.49        | 1.35     |
| 3   | h1    | 306  | PSU  | C6-C5 | 12.18 | 1.49        | 1.35     |
| 3   | h1    | 1567 | PSU  | C6-C5 | 12.18 | 1.49        | 1.35     |
| 3   | h1    | 1304 | PSU  | C6-C5 | 12.18 | 1.49        | 1.35     |
| 81  | A3    | 464  | PSU  | C6-C5 | 12.18 | 1.49        | 1.35     |
| 81  | A3    | 717  | PSU  | C6-C5 | 12.18 | 1.49        | 1.35     |
| 81  | A3    | 510  | PSU  | C6-C5 | 12.17 | 1.49        | 1.35     |
| 3   | h1    | 1535 | PSU  | C6-C5 | 12.17 | 1.49        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | h1    | 1184 | PSU  | C6-C5 | 12.17 | 1.49        | 1.35     |
| 3   | h1    | 258  | PSU  | C6-C5 | 12.17 | 1.49        | 1.35     |
| 3   | h1    | 95   | PSU  | C6-C5 | 12.17 | 1.49        | 1.35     |
| 3   | h1    | 121  | PSU  | C6-C5 | 12.16 | 1.49        | 1.35     |
| 81  | A3    | 976  | PSU  | C6-C5 | 12.16 | 1.49        | 1.35     |
| 81  | A3    | 2958 | PSU  | C6-C5 | 12.16 | 1.49        | 1.35     |
| 3   | h1    | 1106 | PSU  | C6-C5 | 12.16 | 1.49        | 1.35     |
| 3   | h1    | 1293 | PSU  | C6-C5 | 12.16 | 1.49        | 1.35     |
| 3   | h1    | 310  | PSU  | C6-C5 | 12.16 | 1.49        | 1.35     |
| 3   | h1    | 362  | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 3   | h1    | 950  | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 81  | A3    | 2317 | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 81  | A3    | 970  | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 81  | A3    | 2978 | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 3   | h1    | 1190 | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 81  | A3    | 2261 | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 81  | A3    | 2926 | PSU  | C6-C5 | 12.15 | 1.49        | 1.35     |
| 81  | A3    | 2214 | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 82  | B3    | 77   | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 81  | A3    | 150  | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 81  | A3    | 2139 | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 3   | h1    | 1634 | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 3   | h1    | 605  | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 81  | A3    | 1016 | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 3   | h1    | 1178 | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 81  | A3    | 2435 | PSU  | C6-C5 | 12.14 | 1.49        | 1.35     |
| 3   | h1    | 1120 | PSU  | C6-C5 | 12.13 | 1.49        | 1.35     |
| 3   | h1    | 1002 | PSU  | C6-C5 | 12.13 | 1.49        | 1.35     |
| 3   | h1    | 1787 | PSU  | C6-C5 | 12.13 | 1.49        | 1.35     |
| 3   | h1    | 470  | PSU  | C6-C5 | 12.13 | 1.49        | 1.35     |
| 3   | h1    | 763  | PSU  | C6-C5 | 12.13 | 1.49        | 1.35     |
| 81  | A3    | 228  | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 81  | A3    | 2419 | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 3   | h1    | 607  | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 81  | A3    | 2321 | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 3   | h1    | 417  | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 81  | A3    | 1056 | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 81  | A3    | 1474 | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 81  | A3    | 1064 | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 81  | A3    | 2947 | PSU  | C6-C5 | 12.12 | 1.49        | 1.35     |
| 81  | A3    | 2263 | PSU  | C6-C5 | 12.11 | 1.49        | 1.35     |
| 81  | A3    | 895  | PSU  | C6-C5 | 12.11 | 1.49        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | A3    | 2857 | PSU  | C6-C5   | 12.11 | 1.49        | 1.35     |
| 3   | h1    | 809  | PSU  | C6-C5   | 12.10 | 1.49        | 1.35     |
| 81  | A3    | 1133 | PSU  | C6-C5   | 12.10 | 1.49        | 1.35     |
| 81  | A3    | 2267 | PSU  | C6-C5   | 12.10 | 1.49        | 1.35     |
| 82  | B3    | 96   | PSU  | C6-C5   | 12.10 | 1.49        | 1.35     |
| 81  | A3    | 829  | PSU  | C6-C5   | 12.10 | 1.49        | 1.35     |
| 3   | h1    | 103  | PSU  | C6-C5   | 12.09 | 1.49        | 1.35     |
| 81  | A3    | 42   | PSU  | C6-C5   | 12.09 | 1.49        | 1.35     |
| 3   | h1    | 762  | PSU  | C6-C5   | 12.09 | 1.49        | 1.35     |
| 3   | h1    | 635  | PSU  | C6-C5   | 12.09 | 1.49        | 1.35     |
| 3   | h1    | 1615 | PSU  | C6-C5   | 12.09 | 1.49        | 1.35     |
| 81  | A3    | 684  | PSU  | C6-C5   | 12.09 | 1.49        | 1.35     |
| 81  | A3    | 1135 | PSU  | C6-C5   | 12.09 | 1.49        | 1.35     |
| 82  | B3    | 21   | PSU  | C6-C5   | 12.08 | 1.49        | 1.35     |
| 81  | A3    | 2897 | PSU  | C6-C5   | 12.08 | 1.49        | 1.35     |
| 3   | h1    | 339  | PSU  | C6-C5   | 12.07 | 1.49        | 1.35     |
| 3   | h1    | 753  | PSU  | C6-C5   | 12.07 | 1.49        | 1.35     |
| 81  | A3    | 966  | PSU  | C6-C5   | 12.07 | 1.49        | 1.35     |
| 81  | A3    | 2747 | PSU  | C6-C5   | 12.06 | 1.49        | 1.35     |
| 81  | A3    | 2868 | PSU  | C6-C5   | 12.06 | 1.49        | 1.35     |
| 3   | h1    | 1210 | PSU  | C6-C5   | 12.05 | 1.49        | 1.35     |
| 81  | A3    | 2257 | PSU  | C6-C5   | 12.05 | 1.49        | 1.35     |
| 81  | A3    | 2194 | PSU  | C6-C5   | 12.05 | 1.49        | 1.35     |
| 81  | A3    | 1134 | PSU  | C6-C5   | 12.02 | 1.49        | 1.35     |
| 81  | A3    | 34   | PSU  | C6-C5   | 12.01 | 1.49        | 1.35     |
| 81  | A3    | 277  | PSU  | C6-C5   | 12.01 | 1.49        | 1.35     |
| 3   | h1    | 1308 | PSU  | C6-C5   | 12.01 | 1.49        | 1.35     |
| 81  | A3    | 1482 | PSU  | C6-C5   | 12.00 | 1.49        | 1.35     |
| 81  | A3    | 2829 | PSU  | C6-C5   | 11.99 | 1.49        | 1.35     |
| 3   | h1    | 606  | PSU  | C6-C5   | 11.91 | 1.49        | 1.35     |
| 3   | h1    | 1771 | 6MZ  | C6-N6   | 11.50 | 1.46        | 1.34     |
| 81  | A3    | 2653 | UY1  | C6-C5   | 11.23 | 1.48        | 1.35     |
| 3   | h1    | 603  | UY1  | C6-C5   | 11.15 | 1.48        | 1.35     |
| 3   | h1    | 544  | A2M  | C3'-C4' | -9.90 | 1.27        | 1.53     |
| 81  | A3    | 817  | A2M  | C3'-C4' | -9.87 | 1.27        | 1.53     |
| 81  | A3    | 827  | A2M  | C3'-C4' | -9.86 | 1.27        | 1.53     |
| 81  | A3    | 946  | A2M  | C3'-C4' | -9.84 | 1.27        | 1.53     |
| 81  | A3    | 2259 | A2M  | C3'-C4' | -9.84 | 1.27        | 1.53     |
| 81  | A3    | 2914 | A2M  | C3'-C4' | -9.82 | 1.27        | 1.53     |
| 81  | A3    | 2129 | A2M  | C3'-C4' | -9.82 | 1.27        | 1.53     |
| 3   | h1    | 162  | A2M  | C3'-C4' | -9.81 | 1.27        | 1.53     |
| 81  | A3    | 1144 | A2M  | C2'-C1' | -9.80 | 1.27        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | h1    | 1579 | A2M  | C2'-C1' | -9.80 | 1.27        | 1.53     |
| 81  | A3    | 2329 | A2M  | C2'-C1' | -9.80 | 1.27        | 1.53     |
| 3   | h1    | 800  | A2M  | C3'-C4' | -9.80 | 1.28        | 1.53     |
| 3   | h1    | 468  | A2M  | C3'-C4' | -9.80 | 1.28        | 1.53     |
| 81  | A3    | 2324 | A2M  | C2'-C1' | -9.79 | 1.27        | 1.53     |
| 3   | h1    | 1329 | A2M  | C3'-C4' | -9.79 | 1.28        | 1.53     |
| 3   | h1    | 28   | A2M  | C3'-C4' | -9.79 | 1.28        | 1.53     |
| 81  | A3    | 2259 | A2M  | C2'-C1' | -9.79 | 1.27        | 1.53     |
| 81  | A3    | 1378 | A2M  | C3'-C4' | -9.78 | 1.28        | 1.53     |
| 3   | h1    | 1758 | A2M  | C3'-C4' | -9.76 | 1.28        | 1.53     |
| 81  | A3    | 2284 | A2M  | C2'-C1' | -9.76 | 1.28        | 1.53     |
| 3   | h1    | 424  | A2M  | C3'-C4' | -9.76 | 1.28        | 1.53     |
| 3   | h1    | 1758 | A2M  | C2'-C1' | -9.75 | 1.28        | 1.53     |
| 81  | A3    | 2643 | A2M  | C2'-C1' | -9.74 | 1.28        | 1.53     |
| 81  | A3    | 2223 | A2M  | C3'-C4' | -9.74 | 1.28        | 1.53     |
| 3   | h1    | 424  | A2M  | C2'-C1' | -9.74 | 1.28        | 1.53     |
| 81  | A3    | 2949 | A2M  | C2'-C1' | -9.74 | 1.28        | 1.53     |
| 81  | A3    | 2804 | A2M  | C3'-C4' | -9.73 | 1.28        | 1.53     |
| 3   | h1    | 468  | A2M  | C2'-C1' | -9.72 | 1.28        | 1.53     |
| 3   | h1    | 977  | A2M  | C3'-C4' | -9.72 | 1.28        | 1.53     |
| 3   | h1    | 622  | A2M  | C3'-C4' | -9.71 | 1.28        | 1.53     |
| 81  | A3    | 2223 | A2M  | C2'-C1' | -9.71 | 1.28        | 1.53     |
| 3   | h1    | 977  | A2M  | C2'-C1' | -9.71 | 1.28        | 1.53     |
| 81  | A3    | 2949 | A2M  | C3'-C4' | -9.71 | 1.28        | 1.53     |
| 81  | A3    | 1378 | A2M  | C2'-C1' | -9.70 | 1.28        | 1.53     |
| 81  | A3    | 2129 | A2M  | C2'-C1' | -9.70 | 1.28        | 1.53     |
| 81  | A3    | 2873 | 5MC  | C6-C5   | 9.69  | 1.50        | 1.34     |
| 81  | A3    | 886  | A2M  | C3'-C4' | -9.69 | 1.28        | 1.53     |
| 3   | h1    | 1329 | A2M  | C2'-C1' | -9.69 | 1.28        | 1.53     |
| 81  | A3    | 369  | A2M  | C2'-C1' | -9.68 | 1.28        | 1.53     |
| 81  | A3    | 660  | A2M  | C2'-C1' | -9.68 | 1.28        | 1.53     |
| 3   | h1    | 162  | A2M  | C2'-C1' | -9.68 | 1.28        | 1.53     |
| 3   | h1    | 440  | A2M  | C3'-C4' | -9.68 | 1.28        | 1.53     |
| 81  | A3    | 1460 | A2M  | C2'-C1' | -9.67 | 1.28        | 1.53     |
| 82  | B3    | 46   | A2M  | C3'-C4' | -9.67 | 1.28        | 1.53     |
| 81  | A3    | 2329 | A2M  | C3'-C4' | -9.66 | 1.28        | 1.53     |
| 81  | A3    | 42   | PSU  | C2-N1   | 9.65  | 1.49        | 1.36     |
| 81  | A3    | 660  | A2M  | C3'-C4' | -9.65 | 1.28        | 1.53     |
| 81  | A3    | 886  | A2M  | C2'-C1' | -9.65 | 1.28        | 1.53     |
| 81  | A3    | 2643 | A2M  | C3'-C4' | -9.64 | 1.28        | 1.53     |
| 3   | h1    | 584  | PSU  | C2-N1   | 9.64  | 1.49        | 1.36     |
| 81  | A3    | 2257 | PSU  | C2-N1   | 9.64  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | h1    | 1579 | A2M  | C3'-C4' | -9.64 | 1.28        | 1.53     |
| 82  | B3    | 46   | A2M  | C2'-C1' | -9.64 | 1.28        | 1.53     |
| 81  | A3    | 827  | A2M  | C2'-C1' | -9.63 | 1.28        | 1.53     |
| 81  | A3    | 1144 | A2M  | C3'-C4' | -9.63 | 1.28        | 1.53     |
| 81  | A3    | 2137 | PSU  | C2-N1   | 9.63  | 1.49        | 1.36     |
| 3   | h1    | 95   | PSU  | C2-N1   | 9.62  | 1.49        | 1.36     |
| 81  | A3    | 510  | PSU  | C2-N1   | 9.62  | 1.49        | 1.36     |
| 81  | A3    | 976  | PSU  | C2-N1   | 9.62  | 1.49        | 1.36     |
| 3   | h1    | 440  | A2M  | C2'-C1' | -9.61 | 1.28        | 1.53     |
| 81  | A3    | 946  | A2M  | C2'-C1' | -9.61 | 1.28        | 1.53     |
| 81  | A3    | 2653 | UY1  | C2-N1   | 9.61  | 1.49        | 1.36     |
| 81  | A3    | 1460 | A2M  | C3'-C4' | -9.61 | 1.28        | 1.53     |
| 3   | h1    | 1535 | PSU  | C2-N1   | 9.60  | 1.49        | 1.36     |
| 3   | h1    | 1293 | PSU  | C2-N1   | 9.59  | 1.49        | 1.36     |
| 3   | h1    | 121  | PSU  | C2-N1   | 9.59  | 1.49        | 1.36     |
| 81  | A3    | 2281 | 5MC  | C6-C5   | 9.59  | 1.50        | 1.34     |
| 3   | h1    | 28   | A2M  | C2'-C1' | -9.58 | 1.28        | 1.53     |
| 81  | A3    | 369  | A2M  | C3'-C4' | -9.58 | 1.28        | 1.53     |
| 3   | h1    | 1485 | PSU  | C2-N1   | 9.58  | 1.49        | 1.36     |
| 81  | A3    | 2321 | PSU  | C2-N1   | 9.58  | 1.49        | 1.36     |
| 3   | h1    | 961  | PSU  | C2-N1   | 9.58  | 1.49        | 1.36     |
| 81  | A3    | 1016 | PSU  | C2-N1   | 9.57  | 1.49        | 1.36     |
| 3   | h1    | 763  | PSU  | C2-N1   | 9.57  | 1.49        | 1.36     |
| 81  | A3    | 464  | PSU  | C2-N1   | 9.57  | 1.49        | 1.36     |
| 3   | h1    | 1002 | PSU  | C2-N1   | 9.57  | 1.49        | 1.36     |
| 81  | A3    | 970  | PSU  | C2-N1   | 9.57  | 1.49        | 1.36     |
| 82  | B3    | 77   | PSU  | C2-N1   | 9.56  | 1.49        | 1.36     |
| 81  | A3    | 2324 | A2M  | C3'-C4' | -9.55 | 1.28        | 1.53     |
| 81  | A3    | 2269 | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 3   | h1    | 1184 | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 3   | h1    | 1308 | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 3   | h1    | 1524 | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 81  | A3    | 2914 | A2M  | C2'-C1' | -9.55 | 1.28        | 1.53     |
| 3   | h1    | 258  | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 3   | h1    | 1217 | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 3   | h1    | 809  | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 81  | A3    | 34   | PSU  | C2-N1   | 9.55  | 1.49        | 1.36     |
| 81  | A3    | 717  | PSU  | C2-N1   | 9.54  | 1.49        | 1.36     |
| 81  | A3    | 2897 | PSU  | C2-N1   | 9.54  | 1.49        | 1.36     |
| 3   | h1    | 1027 | PSU  | C2-N1   | 9.54  | 1.49        | 1.36     |
| 81  | A3    | 684  | PSU  | C2-N1   | 9.54  | 1.49        | 1.36     |
| 81  | A3    | 228  | PSU  | C2-N1   | 9.54  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | h1    | 603  | UY1  | C2-N1   | 9.54  | 1.49        | 1.36     |
| 3   | h1    | 1106 | PSU  | C2-N1   | 9.54  | 1.49        | 1.36     |
| 3   | h1    | 306  | PSU  | C2-N1   | 9.53  | 1.49        | 1.36     |
| 81  | A3    | 2214 | PSU  | C2-N1   | 9.53  | 1.49        | 1.36     |
| 81  | A3    | 1135 | PSU  | C2-N1   | 9.53  | 1.49        | 1.36     |
| 81  | A3    | 2263 | PSU  | C2-N1   | 9.53  | 1.49        | 1.36     |
| 81  | A3    | 2317 | PSU  | C2-N1   | 9.53  | 1.49        | 1.36     |
| 82  | B3    | 96   | PSU  | C2-N1   | 9.53  | 1.49        | 1.36     |
| 3   | h1    | 622  | A2M  | C2'-C1' | -9.53 | 1.28        | 1.53     |
| 3   | h1    | 762  | PSU  | C2-N1   | 9.52  | 1.49        | 1.36     |
| 81  | A3    | 2857 | PSU  | C2-N1   | 9.52  | 1.49        | 1.36     |
| 3   | h1    | 1567 | PSU  | C2-N1   | 9.52  | 1.49        | 1.36     |
| 81  | A3    | 2194 | PSU  | C2-N1   | 9.52  | 1.49        | 1.36     |
| 3   | h1    | 753  | PSU  | C2-N1   | 9.52  | 1.49        | 1.36     |
| 3   | h1    | 339  | PSU  | C2-N1   | 9.52  | 1.49        | 1.36     |
| 81  | A3    | 1064 | PSU  | C2-N1   | 9.52  | 1.49        | 1.36     |
| 81  | A3    | 150  | PSU  | C2-N1   | 9.51  | 1.49        | 1.36     |
| 81  | A3    | 2978 | PSU  | C2-N1   | 9.51  | 1.49        | 1.36     |
| 81  | A3    | 1002 | PSU  | C2-N1   | 9.51  | 1.49        | 1.36     |
| 81  | A3    | 2261 | PSU  | C2-N1   | 9.51  | 1.49        | 1.36     |
| 3   | h1    | 417  | PSU  | C2-N1   | 9.50  | 1.49        | 1.36     |
| 3   | h1    | 470  | PSU  | C2-N1   | 9.50  | 1.49        | 1.36     |
| 3   | h1    | 1190 | PSU  | C2-N1   | 9.50  | 1.49        | 1.36     |
| 81  | A3    | 2435 | PSU  | C2-N1   | 9.50  | 1.49        | 1.36     |
| 3   | h1    | 800  | A2M  | C2'-C1' | -9.50 | 1.28        | 1.53     |
| 81  | A3    | 829  | PSU  | C2-N1   | 9.50  | 1.49        | 1.36     |
| 3   | h1    | 1304 | PSU  | C2-N1   | 9.50  | 1.49        | 1.36     |
| 81  | A3    | 1685 | PSU  | C2-N1   | 9.50  | 1.49        | 1.36     |
| 81  | A3    | 2868 | PSU  | C2-N1   | 9.49  | 1.49        | 1.36     |
| 3   | h1    | 451  | PSU  | C2-N1   | 9.49  | 1.49        | 1.36     |
| 3   | h1    | 1787 | PSU  | C2-N1   | 9.48  | 1.49        | 1.36     |
| 81  | A3    | 1474 | PSU  | C2-N1   | 9.48  | 1.49        | 1.36     |
| 3   | h1    | 103  | PSU  | C2-N1   | 9.48  | 1.49        | 1.36     |
| 81  | A3    | 2958 | PSU  | C2-N1   | 9.48  | 1.49        | 1.36     |
| 81  | A3    | 2284 | A2M  | C3'-C4' | -9.48 | 1.28        | 1.53     |
| 3   | h1    | 1615 | PSU  | C2-N1   | 9.48  | 1.49        | 1.36     |
| 3   | h1    | 605  | PSU  | C2-N1   | 9.48  | 1.49        | 1.36     |
| 81  | A3    | 1056 | PSU  | C2-N1   | 9.47  | 1.49        | 1.36     |
| 81  | A3    | 2926 | PSU  | C2-N1   | 9.47  | 1.49        | 1.36     |
| 81  | A3    | 2883 | PSU  | C2-N1   | 9.47  | 1.49        | 1.36     |
| 81  | A3    | 2267 | PSU  | C2-N1   | 9.47  | 1.49        | 1.36     |
| 81  | A3    | 277  | PSU  | C2-N1   | 9.47  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | A3    | 2829 | PSU  | C2-N1   | 9.47  | 1.49        | 1.36     |
| 81  | A3    | 1133 | PSU  | C2-N1   | 9.47  | 1.49        | 1.36     |
| 3   | h1    | 310  | PSU  | C2-N1   | 9.46  | 1.49        | 1.36     |
| 3   | h1    | 606  | PSU  | C2-N1   | 9.46  | 1.49        | 1.36     |
| 81  | A3    | 2419 | PSU  | C2-N1   | 9.46  | 1.49        | 1.36     |
| 81  | A3    | 1482 | PSU  | C2-N1   | 9.46  | 1.49        | 1.36     |
| 3   | h1    | 950  | PSU  | C2-N1   | 9.45  | 1.49        | 1.36     |
| 3   | h1    | 362  | PSU  | C2-N1   | 9.45  | 1.49        | 1.36     |
| 3   | h1    | 1210 | PSU  | C2-N1   | 9.45  | 1.49        | 1.36     |
| 81  | A3    | 895  | PSU  | C2-N1   | 9.44  | 1.49        | 1.36     |
| 81  | A3    | 2947 | PSU  | C2-N1   | 9.44  | 1.49        | 1.36     |
| 3   | h1    | 1120 | PSU  | C2-N1   | 9.44  | 1.49        | 1.36     |
| 81  | A3    | 3113 | PSU  | C2-N1   | 9.44  | 1.49        | 1.36     |
| 3   | h1    | 1178 | PSU  | C2-N1   | 9.44  | 1.49        | 1.36     |
| 3   | h1    | 607  | PSU  | C2-N1   | 9.44  | 1.49        | 1.36     |
| 3   | h1    | 1634 | PSU  | C2-N1   | 9.43  | 1.49        | 1.36     |
| 81  | A3    | 311  | PSU  | C2-N1   | 9.43  | 1.49        | 1.36     |
| 81  | A3    | 1134 | PSU  | C2-N1   | 9.43  | 1.49        | 1.36     |
| 81  | A3    | 902  | PSU  | C2-N1   | 9.43  | 1.49        | 1.36     |
| 81  | A3    | 966  | PSU  | C2-N1   | 9.41  | 1.49        | 1.36     |
| 3   | h1    | 635  | PSU  | C2-N1   | 9.40  | 1.49        | 1.36     |
| 81  | A3    | 2139 | PSU  | C2-N1   | 9.40  | 1.49        | 1.36     |
| 82  | B3    | 21   | PSU  | C2-N1   | 9.39  | 1.49        | 1.36     |
| 81  | A3    | 786  | PSU  | C2-N1   | 9.39  | 1.49        | 1.36     |
| 81  | A3    | 817  | A2M  | C2'-C1' | -9.36 | 1.29        | 1.53     |
| 81  | A3    | 2747 | PSU  | C2-N1   | 9.35  | 1.49        | 1.36     |
| 81  | A3    | 2804 | A2M  | C2'-C1' | -9.29 | 1.29        | 1.53     |
| 3   | h1    | 544  | A2M  | C2'-C1' | -9.25 | 1.29        | 1.53     |
| 3   | h1    | 417  | PSU  | C2-N3   | 8.34  | 1.51        | 1.37     |
| 3   | h1    | 339  | PSU  | C2-N3   | 8.33  | 1.51        | 1.37     |
| 81  | A3    | 464  | PSU  | C2-N3   | 8.29  | 1.51        | 1.37     |
| 81  | A3    | 2926 | PSU  | C2-N3   | 8.29  | 1.51        | 1.37     |
| 3   | h1    | 451  | PSU  | C2-N3   | 8.29  | 1.51        | 1.37     |
| 3   | h1    | 1567 | PSU  | C2-N3   | 8.28  | 1.51        | 1.37     |
| 3   | h1    | 961  | PSU  | C2-N3   | 8.28  | 1.51        | 1.37     |
| 3   | h1    | 584  | PSU  | C2-N3   | 8.27  | 1.51        | 1.37     |
| 3   | h1    | 1217 | PSU  | C2-N3   | 8.27  | 1.51        | 1.37     |
| 81  | A3    | 1135 | PSU  | C2-N3   | 8.27  | 1.51        | 1.37     |
| 81  | A3    | 228  | PSU  | C2-N3   | 8.27  | 1.51        | 1.37     |
| 3   | h1    | 607  | PSU  | C2-N3   | 8.27  | 1.51        | 1.37     |
| 81  | A3    | 717  | PSU  | C2-N3   | 8.27  | 1.51        | 1.37     |
| 3   | h1    | 1178 | PSU  | C2-N3   | 8.27  | 1.51        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | h1    | 258  | PSU  | C2-N3 | 8.27 | 1.51        | 1.37     |
| 3   | h1    | 1308 | PSU  | C2-N3 | 8.27 | 1.51        | 1.37     |
| 3   | h1    | 1210 | PSU  | C2-N3 | 8.27 | 1.51        | 1.37     |
| 3   | h1    | 809  | PSU  | C2-N3 | 8.27 | 1.51        | 1.37     |
| 3   | h1    | 1190 | PSU  | C2-N3 | 8.26 | 1.51        | 1.37     |
| 81  | A3    | 1685 | PSU  | C2-N3 | 8.26 | 1.51        | 1.37     |
| 3   | h1    | 1485 | PSU  | C2-N3 | 8.26 | 1.51        | 1.37     |
| 81  | A3    | 2267 | PSU  | C2-N3 | 8.25 | 1.51        | 1.37     |
| 81  | A3    | 2958 | PSU  | C2-N3 | 8.25 | 1.51        | 1.37     |
| 3   | h1    | 1787 | PSU  | C2-N3 | 8.25 | 1.51        | 1.37     |
| 3   | h1    | 121  | PSU  | C2-N3 | 8.25 | 1.51        | 1.37     |
| 3   | h1    | 762  | PSU  | C2-N3 | 8.25 | 1.51        | 1.37     |
| 3   | h1    | 763  | PSU  | C2-N3 | 8.25 | 1.51        | 1.37     |
| 81  | A3    | 150  | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 3   | h1    | 1524 | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 3   | h1    | 605  | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 3   | h1    | 103  | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 81  | A3    | 976  | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 82  | B3    | 77   | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 3   | h1    | 1535 | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 81  | A3    | 2317 | PSU  | C2-N3 | 8.24 | 1.51        | 1.37     |
| 81  | A3    | 2419 | PSU  | C2-N3 | 8.23 | 1.51        | 1.37     |
| 81  | A3    | 2139 | PSU  | C2-N3 | 8.23 | 1.51        | 1.37     |
| 82  | B3    | 96   | PSU  | C2-N3 | 8.23 | 1.51        | 1.37     |
| 3   | h1    | 1634 | PSU  | C2-N3 | 8.23 | 1.51        | 1.37     |
| 3   | h1    | 1120 | PSU  | C2-N3 | 8.23 | 1.51        | 1.37     |
| 81  | A3    | 902  | PSU  | C2-N3 | 8.23 | 1.51        | 1.37     |
| 81  | A3    | 2263 | PSU  | C2-N3 | 8.23 | 1.51        | 1.37     |
| 81  | A3    | 1002 | PSU  | C2-N3 | 8.22 | 1.51        | 1.37     |
| 81  | A3    | 1056 | PSU  | C2-N3 | 8.22 | 1.51        | 1.37     |
| 3   | h1    | 1615 | PSU  | C2-N3 | 8.22 | 1.51        | 1.37     |
| 3   | h1    | 470  | PSU  | C2-N3 | 8.22 | 1.51        | 1.37     |
| 3   | h1    | 95   | PSU  | C2-N3 | 8.22 | 1.51        | 1.37     |
| 81  | A3    | 970  | PSU  | C2-N3 | 8.22 | 1.51        | 1.37     |
| 81  | A3    | 2857 | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |
| 3   | h1    | 753  | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |
| 81  | A3    | 1474 | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |
| 3   | h1    | 1293 | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |
| 81  | A3    | 1482 | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |
| 3   | h1    | 606  | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |
| 81  | A3    | 277  | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |
| 81  | A3    | 2868 | PSU  | C2-N3 | 8.21 | 1.51        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | h1    | 635  | PSU  | C2-N3 | 8.21  | 1.51        | 1.37     |
| 81  | A3    | 2269 | PSU  | C2-N3 | 8.21  | 1.51        | 1.37     |
| 81  | A3    | 34   | PSU  | C2-N3 | 8.21  | 1.51        | 1.37     |
| 81  | A3    | 2214 | PSU  | C2-N3 | 8.21  | 1.51        | 1.37     |
| 3   | h1    | 310  | PSU  | C2-N3 | 8.20  | 1.51        | 1.37     |
| 81  | A3    | 1064 | PSU  | C2-N3 | 8.20  | 1.51        | 1.37     |
| 81  | A3    | 2261 | PSU  | C2-N3 | 8.20  | 1.51        | 1.37     |
| 81  | A3    | 2883 | PSU  | C2-N3 | 8.20  | 1.51        | 1.37     |
| 81  | A3    | 1016 | PSU  | C2-N3 | 8.20  | 1.51        | 1.37     |
| 81  | A3    | 2747 | PSU  | C2-N3 | 8.20  | 1.51        | 1.37     |
| 82  | B3    | 21   | PSU  | C2-N3 | 8.20  | 1.51        | 1.37     |
| 3   | h1    | 1002 | PSU  | C2-N3 | 8.19  | 1.51        | 1.37     |
| 81  | A3    | 2435 | PSU  | C2-N3 | 8.19  | 1.51        | 1.37     |
| 3   | h1    | 1304 | PSU  | C2-N3 | 8.19  | 1.51        | 1.37     |
| 3   | h1    | 950  | PSU  | C2-N3 | 8.19  | 1.51        | 1.37     |
| 81  | A3    | 2321 | PSU  | C2-N3 | 8.19  | 1.51        | 1.37     |
| 81  | A3    | 2897 | PSU  | C2-N3 | 8.18  | 1.51        | 1.37     |
| 81  | A3    | 2829 | PSU  | C2-N3 | 8.18  | 1.51        | 1.37     |
| 81  | A3    | 2257 | PSU  | C2-N3 | 8.18  | 1.51        | 1.37     |
| 81  | A3    | 311  | PSU  | C2-N3 | 8.18  | 1.51        | 1.37     |
| 81  | A3    | 786  | PSU  | C2-N3 | 8.18  | 1.51        | 1.37     |
| 3   | h1    | 1106 | PSU  | C2-N3 | 8.18  | 1.51        | 1.37     |
| 81  | A3    | 2947 | PSU  | C2-N3 | 8.17  | 1.51        | 1.37     |
| 81  | A3    | 2978 | PSU  | C2-N3 | 8.17  | 1.51        | 1.37     |
| 3   | h1    | 1184 | PSU  | C2-N3 | 8.16  | 1.51        | 1.37     |
| 81  | A3    | 684  | PSU  | C2-N3 | 8.16  | 1.51        | 1.37     |
| 3   | h1    | 1027 | PSU  | C2-N3 | 8.16  | 1.51        | 1.37     |
| 81  | A3    | 1133 | PSU  | C2-N3 | 8.15  | 1.51        | 1.37     |
| 3   | h1    | 306  | PSU  | C2-N3 | 8.15  | 1.51        | 1.37     |
| 81  | A3    | 829  | PSU  | C2-N3 | 8.14  | 1.51        | 1.37     |
| 81  | A3    | 1134 | PSU  | C2-N3 | 8.13  | 1.51        | 1.37     |
| 81  | A3    | 966  | PSU  | C2-N3 | 8.13  | 1.51        | 1.37     |
| 81  | A3    | 510  | PSU  | C2-N3 | 8.13  | 1.51        | 1.37     |
| 3   | h1    | 362  | PSU  | C2-N3 | 8.12  | 1.51        | 1.37     |
| 81  | A3    | 895  | PSU  | C2-N3 | 8.12  | 1.51        | 1.37     |
| 81  | A3    | 42   | PSU  | C2-N3 | 8.12  | 1.51        | 1.37     |
| 81  | A3    | 2194 | PSU  | C2-N3 | 8.11  | 1.51        | 1.37     |
| 81  | A3    | 3113 | PSU  | C2-N3 | 8.10  | 1.51        | 1.37     |
| 81  | A3    | 2137 | PSU  | C2-N3 | 8.01  | 1.51        | 1.37     |
| 3   | h1    | 1194 | B8N  | C4-N3 | -7.94 | 1.25        | 1.40     |
| 81  | A3    | 656  | 1MA  | C2-N3 | 7.89  | 1.45        | 1.30     |
| 3   | h1    | 1194 | B8N  | C6-N1 | 7.60  | 1.55        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | h1    | 603  | UY1  | C2-N3 | 7.44 | 1.50        | 1.37     |
| 81  | A3    | 2653 | UY1  | C2-N3 | 7.43 | 1.50        | 1.37     |
| 81  | A3    | 2956 | UR3  | C2-N1 | 7.23 | 1.48        | 1.38     |
| 81  | A3    | 2281 | 5MC  | C4-N3 | 7.21 | 1.46        | 1.34     |
| 81  | A3    | 2873 | 5MC  | C4-N3 | 7.10 | 1.46        | 1.34     |
| 3   | h1    | 140  | OMC  | C2-N3 | 7.05 | 1.50        | 1.36     |
| 3   | h1    | 373  | OMU  | C2-N3 | 7.03 | 1.50        | 1.38     |
| 3   | h1    | 1781 | 4AC  | C4-N3 | 7.03 | 1.45        | 1.32     |
| 3   | h1    | 1272 | OMU  | C2-N3 | 7.03 | 1.50        | 1.38     |
| 3   | h1    | 1447 | OMU  | C2-N3 | 7.03 | 1.50        | 1.38     |
| 81  | A3    | 44   | OMU  | C2-N3 | 7.02 | 1.50        | 1.38     |
| 81  | A3    | 804  | OMU  | C2-N3 | 7.02 | 1.50        | 1.38     |
| 3   | h1    | 581  | OMU  | C2-N3 | 7.01 | 1.50        | 1.38     |
| 3   | h1    | 123  | OMU  | C2-N3 | 7.01 | 1.50        | 1.38     |
| 3   | h1    | 1012 | OMU  | C2-N3 | 7.01 | 1.50        | 1.38     |
| 3   | h1    | 1383 | OMU  | C2-N3 | 7.01 | 1.50        | 1.38     |
| 3   | h1    | 38   | OMC  | C2-N3 | 7.01 | 1.50        | 1.36     |
| 81  | A3    | 1852 | OMC  | C2-N3 | 7.00 | 1.50        | 1.36     |
| 81  | A3    | 2281 | 5MC  | C2-N3 | 7.00 | 1.50        | 1.36     |
| 81  | A3    | 3289 | OMU  | C2-N3 | 7.00 | 1.50        | 1.38     |
| 81  | A3    | 2350 | OMU  | C2-N3 | 6.99 | 1.50        | 1.38     |
| 81  | A3    | 2720 | OMU  | C2-N3 | 6.99 | 1.50        | 1.38     |
| 81  | A3    | 2839 | OMC  | C2-N3 | 6.99 | 1.50        | 1.36     |
| 81  | A3    | 144  | OMU  | C2-N3 | 6.99 | 1.50        | 1.38     |
| 3   | h1    | 1218 | OMC  | C2-N3 | 6.99 | 1.50        | 1.36     |
| 81  | A3    | 2886 | OMU  | C2-N3 | 6.98 | 1.50        | 1.38     |
| 81  | A3    | 2685 | OMC  | C2-N3 | 6.98 | 1.50        | 1.36     |
| 81  | A3    | 2924 | OMU  | C2-N3 | 6.98 | 1.50        | 1.38     |
| 3   | h1    | 418  | OMC  | C2-N3 | 6.97 | 1.50        | 1.36     |
| 3   | h1    | 473  | OMC  | C2-N3 | 6.97 | 1.50        | 1.36     |
| 81  | A3    | 2296 | OMC  | C2-N3 | 6.97 | 1.50        | 1.36     |
| 81  | A3    | 2424 | OMU  | C2-N3 | 6.96 | 1.50        | 1.38     |
| 3   | h1    | 886  | OMU  | C2-N3 | 6.95 | 1.50        | 1.38     |
| 81  | A3    | 1894 | OMU  | C2-N3 | 6.95 | 1.50        | 1.38     |
| 81  | A3    | 675  | OMU  | C2-N3 | 6.94 | 1.50        | 1.38     |
| 3   | h1    | 1645 | OMC  | C2-N3 | 6.94 | 1.50        | 1.36     |
| 3   | h1    | 614  | OMU  | C2-N3 | 6.93 | 1.50        | 1.38     |
| 81  | A3    | 2738 | OMU  | C2-N3 | 6.93 | 1.50        | 1.38     |
| 81  | A3    | 1480 | OMC  | C2-N3 | 6.92 | 1.50        | 1.36     |
| 81  | A3    | 2882 | OMC  | C2-N3 | 6.92 | 1.50        | 1.36     |
| 3   | h1    | 1283 | 4AC  | C4-N3 | 6.92 | 1.44        | 1.32     |
| 81  | A3    | 2340 | OMC  | C2-N3 | 6.91 | 1.50        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 81  | A3    | 3304 | OMU  | C2-N3 | 6.90 | 1.50        | 1.38     |
| 81  | A3    | 2873 | 5MC  | C2-N3 | 6.90 | 1.50        | 1.36     |
| 3   | h1    | 1234 | OMU  | C2-N3 | 6.89 | 1.50        | 1.38     |
| 81  | A3    | 1537 | OMU  | C2-N3 | 6.89 | 1.50        | 1.38     |
| 81  | A3    | 1068 | OMU  | C2-N3 | 6.89 | 1.50        | 1.38     |
| 81  | A3    | 1448 | OMC  | C2-N3 | 6.88 | 1.50        | 1.36     |
| 81  | A3    | 2962 | OMC  | C2-N3 | 6.87 | 1.50        | 1.36     |
| 81  | A3    | 787  | OMU  | C2-N3 | 6.87 | 1.50        | 1.38     |
| 81  | A3    | 2951 | OMC  | C2-N3 | 6.87 | 1.50        | 1.36     |
| 81  | A3    | 1862 | OMC  | C2-N3 | 6.87 | 1.50        | 1.36     |
| 81  | A3    | 2368 | OMC  | C2-N3 | 6.86 | 1.50        | 1.36     |
| 81  | A3    | 2732 | OMU  | C2-N3 | 6.86 | 1.50        | 1.38     |
| 81  | A3    | 2200 | OMC  | C2-N3 | 6.86 | 1.50        | 1.36     |
| 81  | A3    | 40   | OMC  | C2-N3 | 6.86 | 1.50        | 1.36     |
| 81  | A3    | 656  | 1MA  | C4-N3 | 6.83 | 1.49        | 1.35     |
| 81  | A3    | 674  | OMC  | C2-N3 | 6.82 | 1.50        | 1.36     |
| 81  | A3    | 2413 | OMU  | C2-N3 | 6.80 | 1.50        | 1.38     |
| 81  | A3    | 48   | OMU  | C2-N3 | 6.78 | 1.50        | 1.38     |
| 81  | A3    | 1849 | OMC  | C2-N3 | 6.71 | 1.50        | 1.36     |
| 3   | h1    | 581  | OMU  | C2-N1 | 6.65 | 1.49        | 1.38     |
| 3   | h1    | 246  | OMG  | C4-N3 | 6.64 | 1.50        | 1.34     |
| 3   | h1    | 614  | OMU  | C2-N1 | 6.63 | 1.49        | 1.38     |
| 3   | h1    | 1383 | OMU  | C2-N1 | 6.63 | 1.49        | 1.38     |
| 3   | h1    | 1272 | OMU  | C2-N1 | 6.63 | 1.49        | 1.38     |
| 81  | A3    | 399  | OMG  | C4-N3 | 6.62 | 1.50        | 1.34     |
| 81  | A3    | 1537 | OMU  | C2-N1 | 6.62 | 1.49        | 1.38     |
| 81  | A3    | 1894 | OMU  | C2-N1 | 6.59 | 1.49        | 1.38     |
| 3   | h1    | 886  | OMU  | C2-N1 | 6.59 | 1.49        | 1.38     |
| 81  | A3    | 2622 | OMG  | C4-N3 | 6.58 | 1.49        | 1.34     |
| 81  | A3    | 144  | OMU  | C2-N1 | 6.58 | 1.49        | 1.38     |
| 81  | A3    | 675  | OMU  | C2-N1 | 6.58 | 1.49        | 1.38     |
| 3   | h1    | 392  | OMG  | C4-N3 | 6.57 | 1.49        | 1.34     |
| 3   | h1    | 1274 | OMG  | C4-N3 | 6.57 | 1.49        | 1.34     |
| 81  | A3    | 44   | OMU  | C2-N1 | 6.57 | 1.49        | 1.38     |
| 81  | A3    | 2239 | OMG  | C4-N3 | 6.57 | 1.49        | 1.34     |
| 81  | A3    | 2350 | OMU  | C2-N1 | 6.56 | 1.49        | 1.38     |
| 81  | A3    | 2886 | OMU  | C2-N1 | 6.56 | 1.49        | 1.38     |
| 81  | A3    | 3289 | OMU  | C2-N1 | 6.55 | 1.49        | 1.38     |
| 81  | A3    | 918  | OMG  | C4-N3 | 6.55 | 1.49        | 1.34     |
| 3   | h1    | 373  | OMU  | C2-N1 | 6.55 | 1.49        | 1.38     |
| 81  | A3    | 296  | OMG  | C4-N3 | 6.54 | 1.49        | 1.34     |
| 3   | h1    | 1283 | 4AC  | C6-C5 | 6.54 | 1.50        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | h1    | 598  | OMG  | C4-N3   | 6.53 | 1.49        | 1.34     |
| 81  | A3    | 2424 | OMU  | C2-N1   | 6.53 | 1.48        | 1.38     |
| 81  | A3    | 48   | OMU  | C2-N1   | 6.52 | 1.48        | 1.38     |
| 81  | A3    | 787  | OMU  | C2-N1   | 6.52 | 1.48        | 1.38     |
| 81  | A3    | 2925 | OMG  | C4-N3   | 6.52 | 1.49        | 1.34     |
| 82  | B3    | 78   | OMG  | C4-N3   | 6.51 | 1.49        | 1.34     |
| 81  | A3    | 1068 | OMU  | C2-N1   | 6.51 | 1.48        | 1.38     |
| 81  | A3    | 2720 | OMU  | C2-N1   | 6.51 | 1.48        | 1.38     |
| 81  | A3    | 804  | OMU  | C2-N1   | 6.51 | 1.48        | 1.38     |
| 3   | h1    | 1447 | OMU  | C2-N1   | 6.51 | 1.48        | 1.38     |
| 3   | h1    | 123  | OMU  | C2-N1   | 6.50 | 1.48        | 1.38     |
| 81  | A3    | 2291 | OMG  | C4-N3   | 6.50 | 1.49        | 1.34     |
| 81  | A3    | 3304 | OMU  | C2-N1   | 6.49 | 1.48        | 1.38     |
| 81  | A3    | 2794 | OMG  | C4-N3   | 6.48 | 1.49        | 1.34     |
| 3   | h1    | 1012 | OMU  | C2-N1   | 6.48 | 1.48        | 1.38     |
| 81  | A3    | 2738 | OMU  | C2-N1   | 6.48 | 1.48        | 1.38     |
| 81  | A3    | 2924 | OMU  | C2-N1   | 6.47 | 1.48        | 1.38     |
| 81  | A3    | 815  | OMG  | C4-N3   | 6.47 | 1.49        | 1.34     |
| 81  | A3    | 2796 | OMG  | C4-N3   | 6.46 | 1.49        | 1.34     |
| 81  | A3    | 2413 | OMU  | C2-N1   | 6.45 | 1.48        | 1.38     |
| 3   | h1    | 1433 | OMG  | C4-N3   | 6.45 | 1.49        | 1.34     |
| 3   | h1    | 1234 | OMU  | C2-N1   | 6.44 | 1.48        | 1.38     |
| 81  | A3    | 2732 | OMU  | C2-N1   | 6.43 | 1.48        | 1.38     |
| 81  | A3    | 2412 | OMG  | C4-N3   | 6.41 | 1.49        | 1.34     |
| 81  | A3    | 1461 | OMG  | C4-N3   | 6.40 | 1.49        | 1.34     |
| 3   | h1    | 1781 | 4AC  | C6-C5   | 6.39 | 1.49        | 1.35     |
| 81  | A3    | 2804 | A2M  | C3'-C2' | 6.38 | 1.67        | 1.52     |
| 81  | A3    | 2920 | OMG  | C4-N3   | 6.37 | 1.49        | 1.34     |
| 81  | A3    | 1857 | OMG  | C4-N3   | 6.37 | 1.49        | 1.34     |
| 81  | A3    | 2126 | OMG  | C4-N3   | 6.36 | 1.49        | 1.34     |
| 81  | A3    | 2127 | OMG  | C4-N3   | 6.36 | 1.49        | 1.34     |
| 81  | A3    | 2818 | OMG  | C4-N3   | 6.30 | 1.49        | 1.34     |
| 81  | A3    | 2394 | OMG  | C4-N3   | 6.25 | 1.49        | 1.34     |
| 81  | A3    | 2398 | OMG  | C4-N3   | 6.24 | 1.49        | 1.34     |
| 3   | h1    | 1645 | OMC  | C6-C5   | 6.20 | 1.49        | 1.35     |
| 81  | A3    | 2956 | UR3  | C6-C5   | 6.19 | 1.49        | 1.35     |
| 3   | h1    | 473  | OMC  | C6-C5   | 6.19 | 1.49        | 1.35     |
| 81  | A3    | 2340 | OMC  | C6-C5   | 6.19 | 1.49        | 1.35     |
| 81  | A3    | 817  | A2M  | C3'-C2' | 6.18 | 1.66        | 1.52     |
| 81  | A3    | 1852 | OMC  | C6-C5   | 6.18 | 1.49        | 1.35     |
| 3   | h1    | 544  | A2M  | C3'-C2' | 6.18 | 1.66        | 1.52     |
| 81  | A3    | 1849 | OMC  | C6-C5   | 6.17 | 1.49        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | h1    | 1218 | OMC  | C6-C5   | 6.17 | 1.49        | 1.35     |
| 81  | A3    | 2200 | OMC  | C6-C5   | 6.16 | 1.49        | 1.35     |
| 3   | h1    | 38   | OMC  | C6-C5   | 6.16 | 1.49        | 1.35     |
| 81  | A3    | 2685 | OMC  | C6-C5   | 6.16 | 1.49        | 1.35     |
| 81  | A3    | 2654 | OMG  | C4-N3   | 6.15 | 1.48        | 1.34     |
| 3   | h1    | 418  | OMC  | C6-C5   | 6.15 | 1.49        | 1.35     |
| 81  | A3    | 2368 | OMC  | C6-C5   | 6.15 | 1.49        | 1.35     |
| 81  | A3    | 1448 | OMC  | C6-C5   | 6.13 | 1.49        | 1.35     |
| 81  | A3    | 1480 | OMC  | C6-C5   | 6.13 | 1.49        | 1.35     |
| 3   | h1    | 800  | A2M  | O4'-C1' | 6.13 | 1.56        | 1.42     |
| 3   | h1    | 140  | OMC  | C6-C5   | 6.12 | 1.49        | 1.35     |
| 81  | A3    | 2296 | OMC  | C6-C5   | 6.12 | 1.49        | 1.35     |
| 81  | A3    | 2882 | OMC  | C6-C5   | 6.10 | 1.49        | 1.35     |
| 81  | A3    | 40   | OMC  | C6-C5   | 6.10 | 1.49        | 1.35     |
| 81  | A3    | 674  | OMC  | C6-C5   | 6.10 | 1.49        | 1.35     |
| 3   | h1    | 440  | A2M  | C3'-C2' | 6.10 | 1.66        | 1.52     |
| 81  | A3    | 1862 | OMC  | C6-C5   | 6.09 | 1.49        | 1.35     |
| 81  | A3    | 2962 | OMC  | C6-C5   | 6.09 | 1.49        | 1.35     |
| 3   | h1    | 162  | A2M  | O4'-C1' | 6.07 | 1.56        | 1.42     |
| 3   | h1    | 622  | A2M  | C3'-C2' | 6.06 | 1.66        | 1.52     |
| 3   | h1    | 1781 | 4AC  | C2-N3   | 6.04 | 1.48        | 1.36     |
| 81  | A3    | 2951 | OMC  | C6-C5   | 6.03 | 1.49        | 1.35     |
| 81  | A3    | 660  | A2M  | C3'-C2' | 6.02 | 1.66        | 1.52     |
| 3   | h1    | 424  | A2M  | O4'-C1' | 6.02 | 1.56        | 1.42     |
| 81  | A3    | 2839 | OMC  | C6-C5   | 6.01 | 1.49        | 1.35     |
| 3   | h1    | 468  | A2M  | O4'-C1' | 6.01 | 1.56        | 1.42     |
| 81  | A3    | 946  | A2M  | C3'-C2' | 6.01 | 1.66        | 1.52     |
| 81  | A3    | 827  | A2M  | O4'-C1' | 6.00 | 1.56        | 1.42     |
| 3   | h1    | 1579 | A2M  | C3'-C2' | 6.00 | 1.66        | 1.52     |
| 3   | h1    | 544  | A2M  | O4'-C1' | 6.00 | 1.56        | 1.42     |
| 81  | A3    | 2259 | A2M  | O4'-C1' | 6.00 | 1.56        | 1.42     |
| 81  | A3    | 2223 | A2M  | O4'-C1' | 5.99 | 1.56        | 1.42     |
| 81  | A3    | 827  | A2M  | C3'-C2' | 5.99 | 1.66        | 1.52     |
| 81  | A3    | 2129 | A2M  | O4'-C1' | 5.98 | 1.56        | 1.42     |
| 3   | h1    | 1283 | 4AC  | C2-N3   | 5.98 | 1.48        | 1.36     |
| 81  | A3    | 369  | A2M  | C3'-C2' | 5.98 | 1.66        | 1.52     |
| 81  | A3    | 2873 | 5MC  | C6-N1   | 5.97 | 1.48        | 1.38     |
| 81  | A3    | 399  | OMG  | C2-N3   | 5.96 | 1.47        | 1.33     |
| 3   | h1    | 1329 | A2M  | O4'-C1' | 5.96 | 1.56        | 1.42     |
| 81  | A3    | 2223 | A2M  | C3'-C2' | 5.95 | 1.66        | 1.52     |
| 3   | h1    | 1329 | A2M  | C3'-C2' | 5.95 | 1.66        | 1.52     |
| 81  | A3    | 1460 | A2M  | C3'-C2' | 5.95 | 1.66        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 81  | A3    | 886  | A2M  | O4'-C1' | 5.95 | 1.56        | 1.42     |
| 81  | A3    | 2949 | A2M  | O4'-C1' | 5.94 | 1.56        | 1.42     |
| 81  | A3    | 1144 | A2M  | O4'-C1' | 5.94 | 1.56        | 1.42     |
| 81  | A3    | 2914 | A2M  | O4'-C1' | 5.94 | 1.56        | 1.42     |
| 3   | h1    | 246  | OMG  | C2-N3   | 5.94 | 1.47        | 1.33     |
| 82  | B3    | 46   | A2M  | O4'-C1' | 5.94 | 1.56        | 1.42     |
| 3   | h1    | 977  | A2M  | O4'-C1' | 5.92 | 1.56        | 1.42     |
| 3   | h1    | 28   | A2M  | O4'-C1' | 5.92 | 1.56        | 1.42     |
| 81  | A3    | 2329 | A2M  | O4'-C1' | 5.92 | 1.56        | 1.42     |
| 81  | A3    | 1460 | A2M  | O4'-C1' | 5.92 | 1.56        | 1.42     |
| 81  | A3    | 2129 | A2M  | C3'-C2' | 5.91 | 1.66        | 1.52     |
| 81  | A3    | 918  | OMG  | C2-N3   | 5.90 | 1.47        | 1.33     |
| 81  | A3    | 1378 | A2M  | O4'-C1' | 5.90 | 1.56        | 1.42     |
| 3   | h1    | 28   | A2M  | C3'-C2' | 5.89 | 1.66        | 1.52     |
| 81  | A3    | 2914 | A2M  | C3'-C2' | 5.89 | 1.66        | 1.52     |
| 3   | h1    | 977  | A2M  | C3'-C2' | 5.89 | 1.66        | 1.52     |
| 81  | A3    | 2259 | A2M  | C3'-C2' | 5.89 | 1.66        | 1.52     |
| 81  | A3    | 660  | A2M  | O4'-C1' | 5.89 | 1.55        | 1.42     |
| 3   | h1    | 1274 | OMG  | C2-N3   | 5.87 | 1.47        | 1.33     |
| 3   | h1    | 440  | A2M  | O4'-C1' | 5.87 | 1.55        | 1.42     |
| 81  | A3    | 2643 | A2M  | O4'-C1' | 5.87 | 1.55        | 1.42     |
| 81  | A3    | 886  | A2M  | C3'-C2' | 5.87 | 1.66        | 1.52     |
| 81  | A3    | 369  | A2M  | O4'-C1' | 5.87 | 1.55        | 1.42     |
| 3   | h1    | 1293 | PSU  | C6-N1   | 5.87 | 1.46        | 1.36     |
| 81  | A3    | 2324 | A2M  | O4'-C1' | 5.87 | 1.55        | 1.42     |
| 3   | h1    | 424  | A2M  | C3'-C2' | 5.87 | 1.66        | 1.52     |
| 81  | A3    | 2239 | OMG  | C2-N3   | 5.86 | 1.47        | 1.33     |
| 81  | A3    | 2284 | A2M  | C3'-C2' | 5.86 | 1.66        | 1.52     |
| 81  | A3    | 2643 | A2M  | C3'-C2' | 5.86 | 1.66        | 1.52     |
| 3   | h1    | 95   | PSU  | C6-N1   | 5.85 | 1.45        | 1.36     |
| 81  | A3    | 1144 | A2M  | C3'-C2' | 5.85 | 1.66        | 1.52     |
| 3   | h1    | 1758 | A2M  | O4'-C1' | 5.84 | 1.55        | 1.42     |
| 3   | h1    | 584  | PSU  | C6-N1   | 5.84 | 1.45        | 1.36     |
| 3   | h1    | 809  | PSU  | C6-N1   | 5.84 | 1.45        | 1.36     |
| 3   | h1    | 1758 | A2M  | C3'-C2' | 5.84 | 1.66        | 1.52     |
| 3   | h1    | 598  | OMG  | C2-N3   | 5.83 | 1.47        | 1.33     |
| 3   | h1    | 1308 | PSU  | C6-N1   | 5.83 | 1.45        | 1.36     |
| 81  | A3    | 510  | PSU  | C6-N1   | 5.83 | 1.45        | 1.36     |
| 81  | A3    | 817  | A2M  | O4'-C1' | 5.83 | 1.55        | 1.42     |
| 81  | A3    | 2949 | A2M  | C3'-C2' | 5.83 | 1.65        | 1.52     |
| 3   | h1    | 1524 | PSU  | C6-N1   | 5.83 | 1.45        | 1.36     |
| 81  | A3    | 1056 | PSU  | C6-N1   | 5.83 | 1.45        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | h1    | 1579 | A2M  | O4'-C1' | 5.83 | 1.55        | 1.42     |
| 3   | h1    | 417  | PSU  | C6-N1   | 5.83 | 1.45        | 1.36     |
| 81  | A3    | 2622 | OMG  | C2-N3   | 5.82 | 1.47        | 1.33     |
| 3   | h1    | 763  | PSU  | C6-N1   | 5.82 | 1.45        | 1.36     |
| 81  | A3    | 228  | PSU  | C6-N1   | 5.82 | 1.45        | 1.36     |
| 3   | h1    | 258  | PSU  | C6-N1   | 5.82 | 1.45        | 1.36     |
| 81  | A3    | 2257 | PSU  | C6-N1   | 5.81 | 1.45        | 1.36     |
| 3   | h1    | 1027 | PSU  | C6-N1   | 5.81 | 1.45        | 1.36     |
| 3   | h1    | 1184 | PSU  | C6-N1   | 5.81 | 1.45        | 1.36     |
| 81  | A3    | 946  | A2M  | O4'-C1' | 5.81 | 1.55        | 1.42     |
| 3   | h1    | 1190 | PSU  | C6-N1   | 5.81 | 1.45        | 1.36     |
| 3   | h1    | 762  | PSU  | C6-N1   | 5.81 | 1.45        | 1.36     |
| 3   | h1    | 1535 | PSU  | C6-N1   | 5.80 | 1.45        | 1.36     |
| 3   | h1    | 1634 | PSU  | C6-N1   | 5.80 | 1.45        | 1.36     |
| 81  | A3    | 2269 | PSU  | C6-N1   | 5.80 | 1.45        | 1.36     |
| 3   | h1    | 1002 | PSU  | C6-N1   | 5.80 | 1.45        | 1.36     |
| 3   | h1    | 468  | A2M  | C3'-C2' | 5.80 | 1.65        | 1.52     |
| 81  | A3    | 2137 | PSU  | C6-N1   | 5.80 | 1.45        | 1.36     |
| 81  | A3    | 2291 | OMG  | C2-N3   | 5.79 | 1.47        | 1.33     |
| 81  | A3    | 684  | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 82  | B3    | 96   | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 3   | h1    | 1304 | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 81  | A3    | 2324 | A2M  | C3'-C2' | 5.79 | 1.65        | 1.52     |
| 3   | h1    | 961  | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 3   | h1    | 1787 | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 82  | B3    | 78   | OMG  | C2-N3   | 5.79 | 1.47        | 1.33     |
| 81  | A3    | 976  | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 3   | h1    | 306  | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 81  | A3    | 42   | PSU  | C6-N1   | 5.79 | 1.45        | 1.36     |
| 81  | A3    | 34   | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 81  | A3    | 2958 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 81  | A3    | 2868 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 81  | A3    | 2978 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 81  | A3    | 2281 | 5MC  | C6-N1   | 5.78 | 1.47        | 1.38     |
| 3   | h1    | 1217 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 81  | A3    | 1133 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 81  | A3    | 2194 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 3   | h1    | 950  | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 3   | h1    | 392  | OMG  | C2-N3   | 5.78 | 1.47        | 1.33     |
| 81  | A3    | 2263 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 3   | h1    | 1433 | OMG  | C2-N3   | 5.78 | 1.47        | 1.33     |
| 3   | h1    | 1567 | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 81  | A3    | 970  | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 3   | h1    | 121  | PSU  | C6-N1   | 5.78 | 1.45        | 1.36     |
| 3   | h1    | 1485 | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 3   | h1    | 622  | A2M  | O4'-C1' | 5.77 | 1.55        | 1.42     |
| 81  | A3    | 902  | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 3   | h1    | 607  | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 81  | A3    | 2925 | OMG  | C2-N3   | 5.77 | 1.47        | 1.33     |
| 81  | A3    | 2261 | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 3   | h1    | 1615 | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 81  | A3    | 1002 | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 81  | A3    | 2267 | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 81  | A3    | 815  | OMG  | C2-N3   | 5.77 | 1.47        | 1.33     |
| 81  | A3    | 1016 | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 3   | h1    | 310  | PSU  | C6-N1   | 5.77 | 1.45        | 1.36     |
| 81  | A3    | 296  | OMG  | C2-N3   | 5.77 | 1.47        | 1.33     |
| 81  | A3    | 2329 | A2M  | C3'-C2' | 5.76 | 1.65        | 1.52     |
| 81  | A3    | 2419 | PSU  | C6-N1   | 5.76 | 1.45        | 1.36     |
| 3   | h1    | 470  | PSU  | C6-N1   | 5.76 | 1.45        | 1.36     |
| 81  | A3    | 2317 | PSU  | C6-N1   | 5.76 | 1.45        | 1.36     |
| 81  | A3    | 2926 | PSU  | C6-N1   | 5.76 | 1.45        | 1.36     |
| 81  | A3    | 311  | PSU  | C6-N1   | 5.75 | 1.45        | 1.36     |
| 81  | A3    | 1064 | PSU  | C6-N1   | 5.75 | 1.45        | 1.36     |
| 3   | h1    | 162  | A2M  | C3'-C2' | 5.75 | 1.65        | 1.52     |
| 82  | B3    | 46   | A2M  | C3'-C2' | 5.75 | 1.65        | 1.52     |
| 81  | A3    | 2214 | PSU  | C6-N1   | 5.75 | 1.45        | 1.36     |
| 81  | A3    | 2281 | 5MC  | C4-N4   | 5.75 | 1.49        | 1.34     |
| 81  | A3    | 2796 | OMG  | C2-N3   | 5.75 | 1.47        | 1.33     |
| 3   | h1    | 605  | PSU  | C6-N1   | 5.75 | 1.45        | 1.36     |
| 81  | A3    | 1134 | PSU  | C6-N1   | 5.75 | 1.45        | 1.36     |
| 3   | h1    | 1106 | PSU  | C6-N1   | 5.75 | 1.45        | 1.36     |
| 81  | A3    | 2857 | PSU  | C6-N1   | 5.75 | 1.45        | 1.36     |
| 3   | h1    | 753  | PSU  | C6-N1   | 5.74 | 1.45        | 1.36     |
| 81  | A3    | 717  | PSU  | C6-N1   | 5.74 | 1.45        | 1.36     |
| 81  | A3    | 1461 | OMG  | C2-N3   | 5.74 | 1.47        | 1.33     |
| 3   | h1    | 339  | PSU  | C6-N1   | 5.74 | 1.45        | 1.36     |
| 81  | A3    | 2794 | OMG  | C2-N3   | 5.74 | 1.47        | 1.33     |
| 81  | A3    | 150  | PSU  | C6-N1   | 5.74 | 1.45        | 1.36     |
| 81  | A3    | 3113 | PSU  | C6-N1   | 5.74 | 1.45        | 1.36     |
| 3   | h1    | 451  | PSU  | C6-N1   | 5.73 | 1.45        | 1.36     |
| 81  | A3    | 464  | PSU  | C6-N1   | 5.73 | 1.45        | 1.36     |
| 81  | A3    | 2920 | OMG  | C2-N3   | 5.73 | 1.47        | 1.33     |
| 81  | A3    | 786  | PSU  | C6-N1   | 5.73 | 1.45        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 81  | A3    | 1685 | PSU  | C6-N1   | 5.73 | 1.45        | 1.36     |
| 81  | A3    | 2947 | PSU  | C6-N1   | 5.72 | 1.45        | 1.36     |
| 81  | A3    | 1378 | A2M  | C3'-C2' | 5.72 | 1.65        | 1.52     |
| 3   | h1    | 606  | PSU  | C6-N1   | 5.72 | 1.45        | 1.36     |
| 3   | h1    | 1178 | PSU  | C6-N1   | 5.72 | 1.45        | 1.36     |
| 81  | A3    | 2321 | PSU  | C6-N1   | 5.72 | 1.45        | 1.36     |
| 82  | B3    | 77   | PSU  | C6-N1   | 5.72 | 1.45        | 1.36     |
| 81  | A3    | 1135 | PSU  | C6-N1   | 5.72 | 1.45        | 1.36     |
| 81  | A3    | 1482 | PSU  | C6-N1   | 5.71 | 1.45        | 1.36     |
| 3   | h1    | 1120 | PSU  | C6-N1   | 5.71 | 1.45        | 1.36     |
| 81  | A3    | 2747 | PSU  | C6-N1   | 5.71 | 1.45        | 1.36     |
| 81  | A3    | 2139 | PSU  | C6-N1   | 5.71 | 1.45        | 1.36     |
| 81  | A3    | 895  | PSU  | C6-N1   | 5.71 | 1.45        | 1.36     |
| 81  | A3    | 2804 | A2M  | O4'-C1' | 5.70 | 1.55        | 1.42     |
| 81  | A3    | 1857 | OMG  | C2-N3   | 5.70 | 1.46        | 1.33     |
| 81  | A3    | 2897 | PSU  | C6-N1   | 5.70 | 1.45        | 1.36     |
| 3   | h1    | 103  | PSU  | C6-N1   | 5.70 | 1.45        | 1.36     |
| 81  | A3    | 2829 | PSU  | C6-N1   | 5.70 | 1.45        | 1.36     |
| 81  | A3    | 2435 | PSU  | C6-N1   | 5.70 | 1.45        | 1.36     |
| 3   | h1    | 635  | PSU  | C6-N1   | 5.70 | 1.45        | 1.36     |
| 81  | A3    | 2883 | PSU  | C6-N1   | 5.70 | 1.45        | 1.36     |
| 3   | h1    | 362  | PSU  | C6-N1   | 5.69 | 1.45        | 1.36     |
| 81  | A3    | 966  | PSU  | C6-N1   | 5.69 | 1.45        | 1.36     |
| 82  | B3    | 21   | PSU  | C6-N1   | 5.69 | 1.45        | 1.36     |
| 81  | A3    | 2412 | OMG  | C2-N3   | 5.69 | 1.46        | 1.33     |
| 3   | h1    | 800  | A2M  | C3'-C2' | 5.68 | 1.65        | 1.52     |
| 3   | h1    | 1210 | PSU  | C6-N1   | 5.67 | 1.45        | 1.36     |
| 81  | A3    | 2873 | 5MC  | C4-N4   | 5.67 | 1.48        | 1.34     |
| 81  | A3    | 1474 | PSU  | C6-N1   | 5.65 | 1.45        | 1.36     |
| 81  | A3    | 277  | PSU  | C6-N1   | 5.65 | 1.45        | 1.36     |
| 3   | h1    | 140  | OMC  | C4-N3   | 5.65 | 1.45        | 1.34     |
| 81  | A3    | 2284 | A2M  | O4'-C1' | 5.64 | 1.55        | 1.42     |
| 3   | h1    | 38   | OMC  | C4-N3   | 5.62 | 1.45        | 1.34     |
| 3   | h1    | 1194 | B8N  | C2-N1   | 5.62 | 1.55        | 1.39     |
| 81  | A3    | 2126 | OMG  | C2-N3   | 5.61 | 1.46        | 1.33     |
| 81  | A3    | 829  | PSU  | C6-N1   | 5.61 | 1.45        | 1.36     |
| 81  | A3    | 2839 | OMC  | C4-N3   | 5.59 | 1.45        | 1.34     |
| 3   | h1    | 1218 | OMC  | C4-N3   | 5.58 | 1.45        | 1.34     |
| 81  | A3    | 674  | OMC  | C4-N3   | 5.57 | 1.45        | 1.34     |
| 81  | A3    | 2818 | OMG  | C2-N3   | 5.56 | 1.46        | 1.33     |
| 3   | h1    | 473  | OMC  | C4-N3   | 5.56 | 1.45        | 1.34     |
| 81  | A3    | 2127 | OMG  | C2-N3   | 5.56 | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | h1    | 373  | OMU  | C6-C5 | 5.55 | 1.48        | 1.35     |
| 3   | h1    | 1645 | OMC  | C4-N3 | 5.55 | 1.45        | 1.34     |
| 3   | h1    | 886  | OMU  | C6-C5 | 5.54 | 1.47        | 1.35     |
| 81  | A3    | 2738 | OMU  | C6-C5 | 5.54 | 1.47        | 1.35     |
| 81  | A3    | 675  | OMU  | C6-C5 | 5.54 | 1.47        | 1.35     |
| 81  | A3    | 1894 | OMU  | C6-C5 | 5.54 | 1.47        | 1.35     |
| 81  | A3    | 1480 | OMC  | C4-N3 | 5.53 | 1.45        | 1.34     |
| 3   | h1    | 418  | OMC  | C4-N3 | 5.53 | 1.45        | 1.34     |
| 3   | h1    | 1234 | OMU  | C6-C5 | 5.53 | 1.47        | 1.35     |
| 81  | A3    | 2394 | OMG  | C2-N3 | 5.53 | 1.46        | 1.33     |
| 81  | A3    | 1068 | OMU  | C6-C5 | 5.52 | 1.47        | 1.35     |
| 81  | A3    | 2398 | OMG  | C2-N3 | 5.52 | 1.46        | 1.33     |
| 81  | A3    | 3304 | OMU  | C6-C5 | 5.52 | 1.47        | 1.35     |
| 81  | A3    | 2413 | OMU  | C6-C5 | 5.51 | 1.47        | 1.35     |
| 81  | A3    | 804  | OMU  | C6-C5 | 5.51 | 1.47        | 1.35     |
| 81  | A3    | 2368 | OMC  | C4-N3 | 5.51 | 1.45        | 1.34     |
| 81  | A3    | 2685 | OMC  | C4-N3 | 5.51 | 1.45        | 1.34     |
| 81  | A3    | 787  | OMU  | C6-C5 | 5.51 | 1.47        | 1.35     |
| 81  | A3    | 2350 | OMU  | C6-C5 | 5.51 | 1.47        | 1.35     |
| 3   | h1    | 123  | OMU  | C6-C5 | 5.50 | 1.47        | 1.35     |
| 81  | A3    | 2424 | OMU  | C6-C5 | 5.50 | 1.47        | 1.35     |
| 3   | h1    | 1383 | OMU  | C6-C5 | 5.50 | 1.47        | 1.35     |
| 81  | A3    | 2924 | OMU  | C6-C5 | 5.50 | 1.47        | 1.35     |
| 81  | A3    | 48   | OMU  | C6-C5 | 5.50 | 1.47        | 1.35     |
| 81  | A3    | 2732 | OMU  | C6-C5 | 5.49 | 1.47        | 1.35     |
| 3   | h1    | 1272 | OMU  | C6-C5 | 5.49 | 1.47        | 1.35     |
| 81  | A3    | 44   | OMU  | C6-C5 | 5.48 | 1.47        | 1.35     |
| 81  | A3    | 1862 | OMC  | C4-N3 | 5.48 | 1.45        | 1.34     |
| 81  | A3    | 1537 | OMU  | C6-C5 | 5.48 | 1.47        | 1.35     |
| 81  | A3    | 2296 | OMC  | C4-N3 | 5.48 | 1.45        | 1.34     |
| 3   | h1    | 614  | OMU  | C6-C5 | 5.48 | 1.47        | 1.35     |
| 81  | A3    | 2882 | OMC  | C4-N3 | 5.48 | 1.45        | 1.34     |
| 3   | h1    | 581  | OMU  | C6-C5 | 5.47 | 1.47        | 1.35     |
| 3   | h1    | 1012 | OMU  | C6-C5 | 5.47 | 1.47        | 1.35     |
| 81  | A3    | 2962 | OMC  | C4-N3 | 5.47 | 1.45        | 1.34     |
| 81  | A3    | 2200 | OMC  | C4-N3 | 5.47 | 1.45        | 1.34     |
| 81  | A3    | 1852 | OMC  | C4-N3 | 5.47 | 1.45        | 1.34     |
| 81  | A3    | 2239 | OMG  | C2-N2 | 5.46 | 1.47        | 1.34     |
| 81  | A3    | 1448 | OMC  | C4-N3 | 5.45 | 1.45        | 1.34     |
| 81  | A3    | 40   | OMC  | C4-N3 | 5.45 | 1.45        | 1.34     |
| 81  | A3    | 3289 | OMU  | C6-C5 | 5.45 | 1.47        | 1.35     |
| 81  | A3    | 2340 | OMC  | C4-N3 | 5.44 | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 81  | A3    | 2720 | OMU  | C6-C5   | 5.44 | 1.47        | 1.35     |
| 81  | A3    | 399  | OMG  | C2-N2   | 5.44 | 1.47        | 1.34     |
| 3   | h1    | 392  | OMG  | C2-N2   | 5.43 | 1.47        | 1.34     |
| 3   | h1    | 1274 | OMG  | C2-N2   | 5.43 | 1.47        | 1.34     |
| 3   | h1    | 1447 | OMU  | C6-C5   | 5.43 | 1.47        | 1.35     |
| 3   | h1    | 1194 | B8N  | C6-C5   | 5.43 | 1.42        | 1.34     |
| 3   | h1    | 246  | OMG  | C2-N2   | 5.40 | 1.47        | 1.34     |
| 81  | A3    | 296  | OMG  | C2-N2   | 5.40 | 1.47        | 1.34     |
| 81  | A3    | 2925 | OMG  | C2-N2   | 5.40 | 1.47        | 1.34     |
| 81  | A3    | 2886 | OMU  | C6-C5   | 5.40 | 1.47        | 1.35     |
| 81  | A3    | 144  | OMU  | C6-C5   | 5.40 | 1.47        | 1.35     |
| 81  | A3    | 2951 | OMC  | C4-N3   | 5.40 | 1.45        | 1.34     |
| 81  | A3    | 2794 | OMG  | C2-N2   | 5.39 | 1.47        | 1.34     |
| 81  | A3    | 1849 | OMC  | C4-N3   | 5.39 | 1.45        | 1.34     |
| 81  | A3    | 2654 | OMG  | C2-N2   | 5.39 | 1.47        | 1.34     |
| 81  | A3    | 2654 | OMG  | C2-N3   | 5.38 | 1.46        | 1.33     |
| 81  | A3    | 2622 | OMG  | C2-N2   | 5.38 | 1.47        | 1.34     |
| 3   | h1    | 598  | OMG  | C2-N2   | 5.38 | 1.47        | 1.34     |
| 3   | h1    | 1433 | OMG  | C2-N2   | 5.38 | 1.47        | 1.34     |
| 81  | A3    | 2394 | OMG  | C2-N2   | 5.38 | 1.47        | 1.34     |
| 81  | A3    | 918  | OMG  | C2-N2   | 5.37 | 1.47        | 1.34     |
| 82  | B3    | 78   | OMG  | C2-N2   | 5.37 | 1.46        | 1.34     |
| 81  | A3    | 2818 | OMG  | C2-N2   | 5.36 | 1.46        | 1.34     |
| 81  | A3    | 815  | OMG  | C2-N2   | 5.36 | 1.46        | 1.34     |
| 81  | A3    | 2796 | OMG  | C2-N2   | 5.36 | 1.46        | 1.34     |
| 81  | A3    | 2412 | OMG  | C2-N2   | 5.35 | 1.46        | 1.34     |
| 81  | A3    | 2126 | OMG  | C2-N2   | 5.33 | 1.46        | 1.34     |
| 81  | A3    | 1461 | OMG  | C2-N2   | 5.33 | 1.46        | 1.34     |
| 81  | A3    | 2291 | OMG  | C2-N2   | 5.33 | 1.46        | 1.34     |
| 81  | A3    | 2920 | OMG  | C2-N2   | 5.32 | 1.46        | 1.34     |
| 81  | A3    | 1857 | OMG  | C2-N2   | 5.31 | 1.46        | 1.34     |
| 81  | A3    | 2398 | OMG  | C2-N2   | 5.31 | 1.46        | 1.34     |
| 81  | A3    | 2127 | OMG  | C2-N2   | 5.28 | 1.46        | 1.34     |
| 3   | h1    | 1218 | OMC  | C4-N4   | 5.25 | 1.46        | 1.33     |
| 81  | A3    | 2653 | UY1  | C6-N1   | 5.24 | 1.44        | 1.36     |
| 3   | h1    | 140  | OMC  | C4-N4   | 5.22 | 1.46        | 1.33     |
| 3   | h1    | 38   | OMC  | C4-N4   | 5.22 | 1.46        | 1.33     |
| 3   | h1    | 418  | OMC  | C4-N4   | 5.22 | 1.46        | 1.33     |
| 81  | A3    | 1448 | OMC  | C4-N4   | 5.21 | 1.46        | 1.33     |
| 3   | h1    | 800  | A2M  | O4'-C4' | 5.20 | 1.56        | 1.45     |
| 81  | A3    | 2296 | OMC  | C4-N4   | 5.20 | 1.46        | 1.33     |
| 81  | A3    | 2962 | OMC  | C4-N4   | 5.20 | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | h1    | 603  | UY1  | C6-N1   | 5.19 | 1.44        | 1.36     |
| 81  | A3    | 2685 | OMC  | C4-N4   | 5.19 | 1.46        | 1.33     |
| 81  | A3    | 2956 | UR3  | C2-N3   | 5.19 | 1.49        | 1.39     |
| 81  | A3    | 2368 | OMC  | C4-N4   | 5.19 | 1.46        | 1.33     |
| 81  | A3    | 40   | OMC  | C4-N4   | 5.18 | 1.46        | 1.33     |
| 3   | h1    | 1645 | OMC  | C4-N4   | 5.16 | 1.46        | 1.33     |
| 82  | B3    | 46   | A2M  | O4'-C4' | 5.16 | 1.56        | 1.45     |
| 81  | A3    | 1480 | OMC  | C4-N4   | 5.16 | 1.46        | 1.33     |
| 81  | A3    | 1852 | OMC  | C4-N4   | 5.16 | 1.46        | 1.33     |
| 81  | A3    | 674  | OMC  | C4-N4   | 5.16 | 1.46        | 1.33     |
| 3   | h1    | 473  | OMC  | C4-N4   | 5.15 | 1.46        | 1.33     |
| 81  | A3    | 2951 | OMC  | C4-N4   | 5.15 | 1.46        | 1.33     |
| 3   | h1    | 468  | A2M  | O4'-C4' | 5.15 | 1.56        | 1.45     |
| 81  | A3    | 2839 | OMC  | C4-N4   | 5.15 | 1.46        | 1.33     |
| 81  | A3    | 1862 | OMC  | C4-N4   | 5.14 | 1.46        | 1.33     |
| 81  | A3    | 2340 | OMC  | C4-N4   | 5.14 | 1.46        | 1.33     |
| 81  | A3    | 2324 | A2M  | O4'-C4' | 5.13 | 1.56        | 1.45     |
| 81  | A3    | 2329 | A2M  | O4'-C4' | 5.13 | 1.56        | 1.45     |
| 81  | A3    | 1849 | OMC  | C4-N4   | 5.13 | 1.46        | 1.33     |
| 81  | A3    | 2882 | OMC  | C4-N4   | 5.12 | 1.46        | 1.33     |
| 81  | A3    | 2200 | OMC  | C4-N4   | 5.11 | 1.46        | 1.33     |
| 81  | A3    | 2949 | A2M  | O4'-C4' | 5.10 | 1.56        | 1.45     |
| 81  | A3    | 2129 | A2M  | O4'-C4' | 5.08 | 1.56        | 1.45     |
| 81  | A3    | 2284 | A2M  | O4'-C4' | 5.07 | 1.56        | 1.45     |
| 81  | A3    | 1378 | A2M  | O4'-C4' | 5.07 | 1.56        | 1.45     |
| 3   | h1    | 162  | A2M  | O4'-C4' | 5.07 | 1.56        | 1.45     |
| 3   | h1    | 977  | A2M  | O4'-C4' | 5.06 | 1.56        | 1.45     |
| 3   | h1    | 440  | A2M  | O4'-C4' | 5.05 | 1.56        | 1.45     |
| 81  | A3    | 2259 | A2M  | O4'-C4' | 5.04 | 1.56        | 1.45     |
| 3   | h1    | 424  | A2M  | O4'-C4' | 5.03 | 1.56        | 1.45     |
| 81  | A3    | 886  | A2M  | O4'-C4' | 5.02 | 1.56        | 1.45     |
| 81  | A3    | 660  | A2M  | O4'-C4' | 5.02 | 1.56        | 1.45     |
| 81  | A3    | 2643 | A2M  | O4'-C4' | 5.01 | 1.56        | 1.45     |
| 81  | A3    | 1144 | A2M  | O4'-C4' | 5.01 | 1.56        | 1.45     |
| 81  | A3    | 1460 | A2M  | O4'-C4' | 5.01 | 1.56        | 1.45     |
| 3   | h1    | 1579 | A2M  | O4'-C4' | 5.00 | 1.56        | 1.45     |
| 3   | h1    | 1758 | A2M  | O4'-C4' | 4.99 | 1.56        | 1.45     |
| 81  | A3    | 369  | A2M  | O4'-C4' | 4.99 | 1.56        | 1.45     |
| 81  | A3    | 946  | A2M  | O4'-C4' | 4.96 | 1.56        | 1.45     |
| 81  | A3    | 2223 | A2M  | O4'-C4' | 4.96 | 1.56        | 1.45     |
| 3   | h1    | 28   | A2M  | O4'-C4' | 4.95 | 1.56        | 1.45     |
| 81  | A3    | 827  | A2M  | O4'-C4' | 4.93 | 1.56        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | A3    | 2914 | A2M  | O4'-C4' | 4.92  | 1.56        | 1.45     |
| 3   | h1    | 1329 | A2M  | O4'-C4' | 4.91  | 1.56        | 1.45     |
| 81  | A3    | 656  | 1MA  | C2-N1   | 4.91  | 1.45        | 1.35     |
| 81  | A3    | 817  | A2M  | O4'-C4' | 4.80  | 1.55        | 1.45     |
| 3   | h1    | 544  | A2M  | O4'-C4' | 4.75  | 1.55        | 1.45     |
| 3   | h1    | 622  | A2M  | O4'-C4' | 4.74  | 1.55        | 1.45     |
| 81  | A3    | 2873 | 5MC  | C2-N1   | 4.71  | 1.50        | 1.40     |
| 81  | A3    | 2804 | A2M  | O4'-C4' | 4.69  | 1.55        | 1.45     |
| 3   | h1    | 1234 | OMU  | C4-N3   | 4.68  | 1.46        | 1.38     |
| 81  | A3    | 44   | OMU  | C4-N3   | 4.66  | 1.46        | 1.38     |
| 3   | h1    | 581  | OMU  | C4-N3   | 4.65  | 1.46        | 1.38     |
| 81  | A3    | 2281 | 5MC  | C2-N1   | 4.64  | 1.50        | 1.40     |
| 3   | h1    | 1383 | OMU  | C4-N3   | 4.63  | 1.46        | 1.38     |
| 3   | h1    | 373  | OMU  | C4-N3   | 4.63  | 1.46        | 1.38     |
| 3   | h1    | 886  | OMU  | C4-N3   | 4.63  | 1.46        | 1.38     |
| 81  | A3    | 2924 | OMU  | C4-N3   | 4.61  | 1.46        | 1.38     |
| 81  | A3    | 144  | OMU  | C4-N3   | 4.61  | 1.46        | 1.38     |
| 3   | h1    | 123  | OMU  | C4-N3   | 4.61  | 1.46        | 1.38     |
| 3   | h1    | 424  | A2M  | C6-N6   | 4.61  | 1.45        | 1.34     |
| 81  | A3    | 2350 | OMU  | C4-N3   | 4.60  | 1.46        | 1.38     |
| 81  | A3    | 2738 | OMU  | C4-N3   | 4.60  | 1.46        | 1.38     |
| 3   | h1    | 1272 | OMU  | C4-N3   | 4.60  | 1.46        | 1.38     |
| 3   | h1    | 162  | A2M  | C6-N6   | 4.60  | 1.45        | 1.34     |
| 3   | h1    | 1012 | OMU  | C4-N3   | 4.60  | 1.46        | 1.38     |
| 81  | A3    | 804  | OMU  | C4-N3   | 4.59  | 1.46        | 1.38     |
| 81  | A3    | 3304 | OMU  | C4-N3   | 4.59  | 1.46        | 1.38     |
| 3   | h1    | 544  | A2M  | C6-N6   | 4.59  | 1.45        | 1.34     |
| 81  | A3    | 2424 | OMU  | O4-C4   | -4.58 | 1.15        | 1.24     |
| 81  | A3    | 2886 | OMU  | C4-N3   | 4.58  | 1.46        | 1.38     |
| 81  | A3    | 1537 | OMU  | C4-N3   | 4.57  | 1.46        | 1.38     |
| 3   | h1    | 1447 | OMU  | C4-N3   | 4.56  | 1.46        | 1.38     |
| 3   | h1    | 1329 | A2M  | C6-N6   | 4.56  | 1.45        | 1.34     |
| 3   | h1    | 1579 | A2M  | C6-N6   | 4.56  | 1.45        | 1.34     |
| 3   | h1    | 440  | A2M  | C6-N6   | 4.55  | 1.45        | 1.34     |
| 81  | A3    | 787  | OMU  | O4-C4   | -4.55 | 1.15        | 1.24     |
| 81  | A3    | 1448 | OMC  | C2-N1   | 4.55  | 1.49        | 1.40     |
| 81  | A3    | 946  | A2M  | C6-N6   | 4.55  | 1.45        | 1.34     |
| 81  | A3    | 2643 | A2M  | C6-N6   | 4.55  | 1.45        | 1.34     |
| 81  | A3    | 2129 | A2M  | C6-N6   | 4.55  | 1.45        | 1.34     |
| 81  | A3    | 2732 | OMU  | O4-C4   | -4.55 | 1.15        | 1.24     |
| 81  | A3    | 1068 | OMU  | C4-N3   | 4.54  | 1.46        | 1.38     |
| 81  | A3    | 2424 | OMU  | C4-N3   | 4.54  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | h1    | 468  | A2M  | C6-N6 | 4.54  | 1.45        | 1.34     |
| 81  | A3    | 2324 | A2M  | C6-N6 | 4.54  | 1.45        | 1.34     |
| 81  | A3    | 1480 | OMC  | C2-N1 | 4.54  | 1.49        | 1.40     |
| 3   | h1    | 28   | A2M  | C6-N6 | 4.54  | 1.45        | 1.34     |
| 81  | A3    | 1894 | OMU  | C4-N3 | 4.54  | 1.46        | 1.38     |
| 81  | A3    | 2914 | A2M  | C6-N6 | 4.54  | 1.45        | 1.34     |
| 3   | h1    | 800  | A2M  | C6-N6 | 4.54  | 1.45        | 1.34     |
| 81  | A3    | 1460 | A2M  | C6-N6 | 4.53  | 1.45        | 1.34     |
| 3   | h1    | 1758 | A2M  | C6-N6 | 4.53  | 1.45        | 1.34     |
| 3   | h1    | 622  | A2M  | C6-N6 | 4.53  | 1.45        | 1.34     |
| 81  | A3    | 2223 | A2M  | C6-N6 | 4.53  | 1.45        | 1.34     |
| 81  | A3    | 2949 | A2M  | C6-N6 | 4.53  | 1.45        | 1.34     |
| 81  | A3    | 369  | A2M  | C6-N6 | 4.53  | 1.45        | 1.34     |
| 81  | A3    | 1852 | OMC  | C2-N1 | 4.53  | 1.49        | 1.40     |
| 3   | h1    | 614  | OMU  | C4-N3 | 4.52  | 1.46        | 1.38     |
| 81  | A3    | 675  | OMU  | C4-N3 | 4.52  | 1.46        | 1.38     |
| 81  | A3    | 787  | OMU  | C4-N3 | 4.52  | 1.46        | 1.38     |
| 81  | A3    | 886  | A2M  | C6-N6 | 4.52  | 1.45        | 1.34     |
| 81  | A3    | 2259 | A2M  | C6-N6 | 4.52  | 1.45        | 1.34     |
| 81  | A3    | 827  | A2M  | C6-N6 | 4.52  | 1.45        | 1.34     |
| 81  | A3    | 48   | OMU  | O4-C4 | -4.52 | 1.15        | 1.24     |
| 81  | A3    | 2200 | OMC  | C2-N1 | 4.52  | 1.49        | 1.40     |
| 81  | A3    | 1144 | A2M  | C6-N6 | 4.52  | 1.45        | 1.34     |
| 81  | A3    | 44   | OMU  | O4-C4 | -4.52 | 1.15        | 1.24     |
| 81  | A3    | 804  | OMU  | O4-C4 | -4.52 | 1.15        | 1.24     |
| 82  | B3    | 46   | A2M  | C6-N6 | 4.51  | 1.45        | 1.34     |
| 81  | A3    | 1378 | A2M  | C6-N6 | 4.51  | 1.45        | 1.34     |
| 81  | A3    | 2804 | A2M  | C6-N6 | 4.51  | 1.45        | 1.34     |
| 81  | A3    | 2350 | OMU  | O4-C4 | -4.51 | 1.15        | 1.24     |
| 81  | A3    | 2886 | OMU  | O4-C4 | -4.51 | 1.15        | 1.24     |
| 81  | A3    | 3289 | OMU  | O4-C4 | -4.51 | 1.15        | 1.24     |
| 81  | A3    | 2720 | OMU  | C4-N3 | 4.51  | 1.46        | 1.38     |
| 81  | A3    | 2738 | OMU  | O4-C4 | -4.51 | 1.15        | 1.24     |
| 81  | A3    | 1894 | OMU  | O4-C4 | -4.50 | 1.15        | 1.24     |
| 81  | A3    | 2413 | OMU  | O4-C4 | -4.50 | 1.15        | 1.24     |
| 81  | A3    | 2329 | A2M  | C6-N6 | 4.50  | 1.45        | 1.34     |
| 81  | A3    | 3289 | OMU  | C4-N3 | 4.50  | 1.46        | 1.38     |
| 3   | h1    | 473  | OMC  | C2-N1 | 4.50  | 1.49        | 1.40     |
| 81  | A3    | 144  | OMU  | O4-C4 | -4.50 | 1.15        | 1.24     |
| 81  | A3    | 1537 | OMU  | O4-C4 | -4.50 | 1.15        | 1.24     |
| 3   | h1    | 38   | OMC  | C2-N1 | 4.50  | 1.49        | 1.40     |
| 3   | h1    | 977  | A2M  | C6-N6 | 4.49  | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | h1    | 140  | OMC  | C2-N1  | 4.49  | 1.49        | 1.40     |
| 81  | A3    | 817  | A2M  | C6-N6  | 4.49  | 1.45        | 1.34     |
| 81  | A3    | 2296 | OMC  | C2-N1  | 4.49  | 1.49        | 1.40     |
| 3   | h1    | 418  | OMC  | C2-N1  | 4.48  | 1.49        | 1.40     |
| 81  | A3    | 2882 | OMC  | C2-N1  | 4.48  | 1.49        | 1.40     |
| 3   | h1    | 1218 | OMC  | C2-N1  | 4.48  | 1.49        | 1.40     |
| 81  | A3    | 1068 | OMU  | O4-C4  | -4.48 | 1.15        | 1.24     |
| 81  | A3    | 3304 | OMU  | O4-C4  | -4.47 | 1.15        | 1.24     |
| 3   | h1    | 607  | PSU  | C4-N3  | 4.47  | 1.47        | 1.38     |
| 3   | h1    | 1194 | B8N  | C1'-C5 | -4.47 | 1.40        | 1.50     |
| 81  | A3    | 2732 | OMU  | C4-N3  | 4.46  | 1.46        | 1.38     |
| 3   | h1    | 1524 | PSU  | C4-N3  | 4.46  | 1.47        | 1.38     |
| 81  | A3    | 40   | OMC  | C2-N1  | 4.46  | 1.49        | 1.40     |
| 81  | A3    | 2720 | OMU  | O4-C4  | -4.46 | 1.15        | 1.24     |
| 81  | A3    | 2839 | OMC  | C2-N1  | 4.45  | 1.49        | 1.40     |
| 81  | A3    | 2924 | OMU  | O4-C4  | -4.45 | 1.15        | 1.24     |
| 3   | h1    | 581  | OMU  | O4-C4  | -4.45 | 1.15        | 1.24     |
| 81  | A3    | 675  | OMU  | O4-C4  | -4.45 | 1.15        | 1.24     |
| 3   | h1    | 753  | PSU  | C4-N3  | 4.45  | 1.47        | 1.38     |
| 3   | h1    | 1645 | OMC  | C2-N1  | 4.45  | 1.49        | 1.40     |
| 3   | h1    | 1272 | OMU  | O4-C4  | -4.45 | 1.15        | 1.24     |
| 81  | A3    | 48   | OMU  | C4-N3  | 4.44  | 1.46        | 1.38     |
| 81  | A3    | 2413 | OMU  | C4-N3  | 4.44  | 1.46        | 1.38     |
| 3   | h1    | 614  | OMU  | O4-C4  | -4.43 | 1.15        | 1.24     |
| 3   | h1    | 886  | OMU  | O4-C4  | -4.43 | 1.15        | 1.24     |
| 3   | h1    | 1217 | PSU  | C4-N3  | 4.43  | 1.47        | 1.38     |
| 81  | A3    | 464  | PSU  | C4-N3  | 4.43  | 1.47        | 1.38     |
| 3   | h1    | 1447 | OMU  | O4-C4  | -4.43 | 1.15        | 1.24     |
| 3   | h1    | 1535 | PSU  | C4-N3  | 4.43  | 1.47        | 1.38     |
| 3   | h1    | 1567 | PSU  | C4-N3  | 4.42  | 1.47        | 1.38     |
| 81  | A3    | 660  | A2M  | C6-N6  | 4.42  | 1.45        | 1.34     |
| 3   | h1    | 1012 | OMU  | O4-C4  | -4.42 | 1.15        | 1.24     |
| 3   | h1    | 123  | OMU  | O4-C4  | -4.42 | 1.15        | 1.24     |
| 3   | h1    | 1383 | OMU  | O4-C4  | -4.42 | 1.15        | 1.24     |
| 3   | h1    | 950  | PSU  | C4-N3  | 4.42  | 1.47        | 1.38     |
| 3   | h1    | 373  | OMU  | O4-C4  | -4.42 | 1.15        | 1.24     |
| 81  | A3    | 2747 | PSU  | C4-N3  | 4.42  | 1.47        | 1.38     |
| 3   | h1    | 339  | PSU  | C4-N3  | 4.42  | 1.47        | 1.38     |
| 81  | A3    | 1002 | PSU  | C4-N3  | 4.42  | 1.47        | 1.38     |
| 3   | h1    | 763  | PSU  | C4-N3  | 4.41  | 1.47        | 1.38     |
| 82  | B3    | 96   | PSU  | C4-N3  | 4.41  | 1.47        | 1.38     |
| 3   | h1    | 1210 | PSU  | C4-N3  | 4.41  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 81  | A3    | 2269 | PSU  | C4-N3 | 4.41  | 1.47        | 1.38     |
| 82  | B3    | 77   | PSU  | C4-N3 | 4.41  | 1.47        | 1.38     |
| 3   | h1    | 451  | PSU  | C4-N3 | 4.40  | 1.47        | 1.38     |
| 81  | A3    | 2340 | OMC  | C2-N1 | 4.40  | 1.49        | 1.40     |
| 3   | h1    | 103  | PSU  | C4-N3 | 4.40  | 1.47        | 1.38     |
| 81  | A3    | 2685 | OMC  | C2-N1 | 4.40  | 1.49        | 1.40     |
| 3   | h1    | 809  | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 1485 | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 1787 | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 417  | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 1106 | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 95   | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 1304 | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 258  | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 3   | h1    | 1190 | PSU  | C4-N3 | 4.38  | 1.47        | 1.38     |
| 3   | h1    | 121  | PSU  | C4-N3 | 4.38  | 1.47        | 1.38     |
| 3   | h1    | 1293 | PSU  | C4-N3 | 4.38  | 1.47        | 1.38     |
| 3   | h1    | 762  | PSU  | C4-N3 | 4.38  | 1.47        | 1.38     |
| 81  | A3    | 2261 | PSU  | C4-N3 | 4.38  | 1.47        | 1.38     |
| 3   | h1    | 1634 | PSU  | C4-N3 | 4.38  | 1.47        | 1.38     |
| 3   | h1    | 584  | PSU  | C4-N3 | 4.37  | 1.47        | 1.38     |
| 3   | h1    | 606  | PSU  | C4-N3 | 4.37  | 1.47        | 1.38     |
| 3   | h1    | 1178 | PSU  | C4-N3 | 4.37  | 1.47        | 1.38     |
| 3   | h1    | 1120 | PSU  | C4-N3 | 4.37  | 1.46        | 1.38     |
| 81  | A3    | 1482 | PSU  | C4-N3 | 4.37  | 1.46        | 1.38     |
| 81  | A3    | 150  | PSU  | C4-N3 | 4.37  | 1.46        | 1.38     |
| 81  | A3    | 2263 | PSU  | C4-N3 | 4.37  | 1.46        | 1.38     |
| 81  | A3    | 786  | PSU  | C4-N3 | 4.37  | 1.46        | 1.38     |
| 81  | A3    | 1064 | PSU  | C4-N3 | 4.37  | 1.46        | 1.38     |
| 3   | h1    | 961  | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 81  | A3    | 311  | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 81  | A3    | 976  | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 81  | A3    | 2926 | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 81  | A3    | 2194 | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 81  | A3    | 1016 | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 81  | A3    | 2435 | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 81  | A3    | 2317 | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 3   | h1    | 1234 | OMU  | O4-C4 | -4.35 | 1.16        | 1.24     |
| 3   | h1    | 1002 | PSU  | C4-N3 | 4.35  | 1.46        | 1.38     |
| 81  | A3    | 228  | PSU  | C4-N3 | 4.35  | 1.46        | 1.38     |
| 3   | h1    | 1615 | PSU  | C4-N3 | 4.35  | 1.46        | 1.38     |
| 81  | A3    | 829  | PSU  | C4-N3 | 4.35  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 81  | A3    | 1474 | PSU  | C4-N3 | 4.35  | 1.46        | 1.38     |
| 3   | h1    | 306  | PSU  | C4-N3 | 4.35  | 1.46        | 1.38     |
| 3   | h1    | 470  | PSU  | C4-N3 | 4.34  | 1.46        | 1.38     |
| 3   | h1    | 1308 | PSU  | C4-N3 | 4.34  | 1.46        | 1.38     |
| 81  | A3    | 1685 | PSU  | C4-N3 | 4.34  | 1.46        | 1.38     |
| 3   | h1    | 1184 | PSU  | C4-N3 | 4.34  | 1.46        | 1.38     |
| 81  | A3    | 2214 | PSU  | C4-N3 | 4.34  | 1.46        | 1.38     |
| 3   | h1    | 635  | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 277  | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 2419 | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 2267 | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 1849 | OMC  | C2-N1 | 4.33  | 1.49        | 1.40     |
| 81  | A3    | 2897 | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 2951 | OMC  | C2-N1 | 4.33  | 1.49        | 1.40     |
| 3   | h1    | 1027 | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 2139 | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 2368 | OMC  | C2-N1 | 4.33  | 1.49        | 1.40     |
| 81  | A3    | 1056 | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 81  | A3    | 2978 | PSU  | C4-N3 | 4.33  | 1.46        | 1.38     |
| 3   | h1    | 310  | PSU  | C4-N3 | 4.32  | 1.46        | 1.38     |
| 3   | h1    | 605  | PSU  | C4-N3 | 4.32  | 1.46        | 1.38     |
| 81  | A3    | 902  | PSU  | C4-N3 | 4.32  | 1.46        | 1.38     |
| 81  | A3    | 2857 | PSU  | C4-N3 | 4.32  | 1.46        | 1.38     |
| 81  | A3    | 1133 | PSU  | C4-N3 | 4.32  | 1.46        | 1.38     |
| 81  | A3    | 40   | OMC  | O2-C2 | -4.32 | 1.15        | 1.23     |
| 81  | A3    | 2958 | PSU  | C4-N3 | 4.31  | 1.46        | 1.38     |
| 81  | A3    | 1862 | OMC  | C2-N1 | 4.31  | 1.49        | 1.40     |
| 81  | A3    | 2284 | A2M  | C6-N6 | 4.31  | 1.44        | 1.34     |
| 81  | A3    | 717  | PSU  | C4-N3 | 4.30  | 1.46        | 1.38     |
| 81  | A3    | 2829 | PSU  | C4-N3 | 4.30  | 1.46        | 1.38     |
| 81  | A3    | 2257 | PSU  | C4-N3 | 4.30  | 1.46        | 1.38     |
| 81  | A3    | 2883 | PSU  | C4-N3 | 4.30  | 1.46        | 1.38     |
| 81  | A3    | 2947 | PSU  | C4-N3 | 4.30  | 1.46        | 1.38     |
| 81  | A3    | 970  | PSU  | C4-N3 | 4.30  | 1.46        | 1.38     |
| 81  | A3    | 2868 | PSU  | C4-N3 | 4.29  | 1.46        | 1.38     |
| 82  | B3    | 21   | PSU  | C4-N3 | 4.29  | 1.46        | 1.38     |
| 81  | A3    | 966  | PSU  | C4-N3 | 4.29  | 1.46        | 1.38     |
| 81  | A3    | 1849 | OMC  | O2-C2 | -4.28 | 1.15        | 1.23     |
| 81  | A3    | 2962 | OMC  | C2-N1 | 4.28  | 1.49        | 1.40     |
| 81  | A3    | 1135 | PSU  | C4-N3 | 4.28  | 1.46        | 1.38     |
| 81  | A3    | 2951 | OMC  | O2-C2 | -4.27 | 1.15        | 1.23     |
| 81  | A3    | 2321 | PSU  | C4-N3 | 4.26  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 81  | A3    | 1862 | OMC  | O2-C2 | -4.25 | 1.15        | 1.23     |
| 81  | A3    | 2368 | OMC  | O2-C2 | -4.25 | 1.15        | 1.23     |
| 3   | h1    | 1645 | OMC  | O2-C2 | -4.25 | 1.15        | 1.23     |
| 81  | A3    | 674  | OMC  | O2-C2 | -4.25 | 1.15        | 1.23     |
| 81  | A3    | 510  | PSU  | C4-N3 | 4.25  | 1.46        | 1.38     |
| 81  | A3    | 1448 | OMC  | O2-C2 | -4.24 | 1.15        | 1.23     |
| 3   | h1    | 1283 | 4AC  | C5-C4 | 4.24  | 1.49        | 1.40     |
| 81  | A3    | 2200 | OMC  | O2-C2 | -4.23 | 1.15        | 1.23     |
| 81  | A3    | 684  | PSU  | C4-N3 | 4.23  | 1.46        | 1.38     |
| 81  | A3    | 2962 | OMC  | O2-C2 | -4.22 | 1.15        | 1.23     |
| 81  | A3    | 895  | PSU  | C4-N3 | 4.22  | 1.46        | 1.38     |
| 81  | A3    | 1852 | OMC  | O2-C2 | -4.22 | 1.15        | 1.23     |
| 81  | A3    | 34   | PSU  | C4-N3 | 4.22  | 1.46        | 1.38     |
| 81  | A3    | 2839 | OMC  | O2-C2 | -4.22 | 1.15        | 1.23     |
| 81  | A3    | 674  | OMC  | C2-N1 | 4.22  | 1.49        | 1.40     |
| 81  | A3    | 2340 | OMC  | O2-C2 | -4.22 | 1.15        | 1.23     |
| 3   | h1    | 362  | PSU  | C4-N3 | 4.21  | 1.46        | 1.38     |
| 81  | A3    | 2296 | OMC  | O2-C2 | -4.21 | 1.15        | 1.23     |
| 3   | h1    | 38   | OMC  | O2-C2 | -4.20 | 1.15        | 1.23     |
| 81  | A3    | 1480 | OMC  | O2-C2 | -4.20 | 1.15        | 1.23     |
| 81  | A3    | 42   | PSU  | C4-N3 | 4.20  | 1.46        | 1.38     |
| 81  | A3    | 2882 | OMC  | O2-C2 | -4.20 | 1.15        | 1.23     |
| 81  | A3    | 3113 | PSU  | C4-N3 | 4.20  | 1.46        | 1.38     |
| 3   | h1    | 473  | OMC  | O2-C2 | -4.18 | 1.16        | 1.23     |
| 3   | h1    | 418  | OMC  | O2-C2 | -4.18 | 1.16        | 1.23     |
| 3   | h1    | 1781 | 4AC  | C5-C4 | 4.17  | 1.49        | 1.40     |
| 81  | A3    | 1134 | PSU  | C4-N3 | 4.17  | 1.46        | 1.38     |
| 3   | h1    | 140  | OMC  | O2-C2 | -4.17 | 1.16        | 1.23     |
| 3   | h1    | 1218 | OMC  | O2-C2 | -4.16 | 1.16        | 1.23     |
| 81  | A3    | 2685 | OMC  | O2-C2 | -4.16 | 1.16        | 1.23     |
| 81  | A3    | 2137 | PSU  | C4-N3 | 4.15  | 1.46        | 1.38     |
| 3   | h1    | 1781 | 4AC  | C7-N4 | 4.11  | 1.44        | 1.37     |
| 3   | h1    | 1283 | 4AC  | C7-N4 | 4.05  | 1.44        | 1.37     |
| 3   | h1    | 1781 | 4AC  | C2-N1 | 4.03  | 1.48        | 1.40     |
| 81  | A3    | 2200 | OMC  | C6-N1 | 4.00  | 1.47        | 1.38     |
| 81  | A3    | 1448 | OMC  | C6-N1 | 3.94  | 1.47        | 1.38     |
| 81  | A3    | 1480 | OMC  | C6-N1 | 3.91  | 1.47        | 1.38     |
| 81  | A3    | 1849 | OMC  | C6-N1 | 3.90  | 1.47        | 1.38     |
| 3   | h1    | 1645 | OMC  | C6-N1 | 3.90  | 1.47        | 1.38     |
| 81  | A3    | 2340 | OMC  | C6-N1 | 3.89  | 1.47        | 1.38     |
| 3   | h1    | 473  | OMC  | C6-N1 | 3.89  | 1.47        | 1.38     |
| 3   | h1    | 603  | UY1  | C4-N3 | 3.87  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 81  | A3    | 1852 | OMC  | C6-N1 | 3.87  | 1.47        | 1.38     |
| 3   | h1    | 38   | OMC  | C6-N1 | 3.86  | 1.47        | 1.38     |
| 3   | h1    | 1283 | 4AC  | C2-N1 | 3.86  | 1.48        | 1.40     |
| 81  | A3    | 2296 | OMC  | C6-N1 | 3.85  | 1.47        | 1.38     |
| 81  | A3    | 2685 | OMC  | C6-N1 | 3.84  | 1.47        | 1.38     |
| 3   | h1    | 418  | OMC  | C6-N1 | 3.83  | 1.47        | 1.38     |
| 81  | A3    | 2653 | UY1  | C4-N3 | 3.82  | 1.45        | 1.38     |
| 81  | A3    | 2368 | OMC  | C6-N1 | 3.82  | 1.47        | 1.38     |
| 3   | h1    | 1218 | OMC  | C6-N1 | 3.81  | 1.47        | 1.38     |
| 81  | A3    | 1862 | OMC  | C6-N1 | 3.81  | 1.47        | 1.38     |
| 3   | h1    | 140  | OMC  | C6-N1 | 3.79  | 1.47        | 1.38     |
| 81  | A3    | 674  | OMC  | C6-N1 | 3.79  | 1.47        | 1.38     |
| 81  | A3    | 2882 | OMC  | C6-N1 | 3.78  | 1.47        | 1.38     |
| 81  | A3    | 40   | OMC  | C6-N1 | 3.77  | 1.47        | 1.38     |
| 81  | A3    | 48   | OMU  | C6-N1 | 3.77  | 1.47        | 1.38     |
| 81  | A3    | 2951 | OMC  | C6-N1 | 3.77  | 1.47        | 1.38     |
| 81  | A3    | 2839 | OMC  | C6-N1 | 3.76  | 1.47        | 1.38     |
| 81  | A3    | 2886 | OMU  | C6-N1 | 3.75  | 1.47        | 1.38     |
| 3   | h1    | 1272 | OMU  | C6-N1 | 3.75  | 1.47        | 1.38     |
| 3   | h1    | 614  | OMU  | C6-N1 | 3.74  | 1.47        | 1.38     |
| 81  | A3    | 2732 | OMU  | C6-N1 | 3.74  | 1.47        | 1.38     |
| 81  | A3    | 2962 | OMC  | C6-N1 | 3.73  | 1.47        | 1.38     |
| 81  | A3    | 144  | OMU  | C6-N1 | 3.73  | 1.47        | 1.38     |
| 81  | A3    | 44   | OMU  | C6-N1 | 3.73  | 1.47        | 1.38     |
| 3   | h1    | 581  | OMU  | C6-N1 | 3.72  | 1.47        | 1.38     |
| 81  | A3    | 2738 | OMU  | C6-N1 | 3.72  | 1.47        | 1.38     |
| 3   | h1    | 886  | OMU  | C6-N1 | 3.71  | 1.47        | 1.38     |
| 3   | h1    | 373  | OMU  | C6-N1 | 3.71  | 1.47        | 1.38     |
| 3   | h1    | 1383 | OMU  | C6-N1 | 3.71  | 1.47        | 1.38     |
| 81  | A3    | 675  | OMU  | C6-N1 | 3.70  | 1.46        | 1.38     |
| 81  | A3    | 1894 | OMU  | C6-N1 | 3.70  | 1.46        | 1.38     |
| 3   | h1    | 1234 | OMU  | C6-N1 | 3.70  | 1.46        | 1.38     |
| 81  | A3    | 804  | OMU  | C6-N1 | 3.70  | 1.46        | 1.38     |
| 81  | A3    | 1537 | OMU  | C6-N1 | 3.69  | 1.46        | 1.38     |
| 81  | A3    | 3304 | OMU  | C6-N1 | 3.69  | 1.46        | 1.38     |
| 81  | A3    | 2924 | OMU  | C6-N1 | 3.68  | 1.46        | 1.38     |
| 81  | A3    | 2424 | OMU  | C6-N1 | 3.68  | 1.46        | 1.38     |
| 81  | A3    | 787  | OMU  | C6-N1 | 3.68  | 1.46        | 1.38     |
| 81  | A3    | 2732 | OMU  | O2-C2 | -3.68 | 1.16        | 1.23     |
| 3   | h1    | 1781 | 4AC  | C4-N4 | 3.67  | 1.45        | 1.39     |
| 3   | h1    | 1447 | OMU  | C6-N1 | 3.67  | 1.46        | 1.38     |
| 81  | A3    | 1068 | OMU  | C6-N1 | 3.67  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | h1    | 1012 | OMU  | C6-N1 | 3.67  | 1.46        | 1.38     |
| 81  | A3    | 2350 | OMU  | C6-N1 | 3.66  | 1.46        | 1.38     |
| 81  | A3    | 675  | OMU  | O2-C2 | -3.66 | 1.16        | 1.23     |
| 81  | A3    | 2413 | OMU  | C6-N1 | 3.65  | 1.46        | 1.38     |
| 81  | A3    | 2720 | OMU  | C6-N1 | 3.65  | 1.46        | 1.38     |
| 3   | h1    | 123  | OMU  | C6-N1 | 3.65  | 1.46        | 1.38     |
| 81  | A3    | 2350 | OMU  | O2-C2 | -3.64 | 1.16        | 1.23     |
| 81  | A3    | 804  | OMU  | O2-C2 | -3.64 | 1.16        | 1.23     |
| 81  | A3    | 3289 | OMU  | C6-N1 | 3.64  | 1.46        | 1.38     |
| 81  | A3    | 2720 | OMU  | O2-C2 | -3.63 | 1.16        | 1.23     |
| 81  | A3    | 2886 | OMU  | O2-C2 | -3.62 | 1.16        | 1.23     |
| 81  | A3    | 48   | OMU  | O2-C2 | -3.62 | 1.16        | 1.23     |
| 81  | A3    | 44   | OMU  | O2-C2 | -3.61 | 1.16        | 1.23     |
| 81  | A3    | 1068 | OMU  | O2-C2 | -3.61 | 1.16        | 1.23     |
| 81  | A3    | 2924 | OMU  | O2-C2 | -3.60 | 1.16        | 1.23     |
| 81  | A3    | 787  | OMU  | O2-C2 | -3.60 | 1.16        | 1.23     |
| 81  | A3    | 2424 | OMU  | O2-C2 | -3.60 | 1.16        | 1.23     |
| 81  | A3    | 144  | OMU  | O2-C2 | -3.60 | 1.16        | 1.23     |
| 81  | A3    | 1894 | OMU  | O2-C2 | -3.59 | 1.16        | 1.23     |
| 3   | h1    | 1283 | 4AC  | C4-N4 | 3.59  | 1.44        | 1.39     |
| 3   | h1    | 581  | OMU  | O2-C2 | -3.58 | 1.16        | 1.23     |
| 3   | h1    | 1383 | OMU  | O2-C2 | -3.58 | 1.16        | 1.23     |
| 81  | A3    | 1537 | OMU  | O2-C2 | -3.57 | 1.16        | 1.23     |
| 3   | h1    | 1234 | OMU  | O2-C2 | -3.57 | 1.16        | 1.23     |
| 3   | h1    | 1012 | OMU  | O2-C2 | -3.56 | 1.16        | 1.23     |
| 81  | A3    | 3289 | OMU  | O2-C2 | -3.56 | 1.16        | 1.23     |
| 81  | A3    | 2738 | OMU  | O2-C2 | -3.55 | 1.16        | 1.23     |
| 3   | h1    | 614  | OMU  | O2-C2 | -3.55 | 1.16        | 1.23     |
| 3   | h1    | 1272 | OMU  | O2-C2 | -3.55 | 1.16        | 1.23     |
| 81  | A3    | 2413 | OMU  | O2-C2 | -3.54 | 1.16        | 1.23     |
| 81  | A3    | 3304 | OMU  | O2-C2 | -3.54 | 1.16        | 1.23     |
| 3   | h1    | 1447 | OMU  | O2-C2 | -3.53 | 1.16        | 1.23     |
| 3   | h1    | 123  | OMU  | O2-C2 | -3.50 | 1.16        | 1.23     |
| 3   | h1    | 886  | OMU  | O2-C2 | -3.50 | 1.16        | 1.23     |
| 3   | h1    | 373  | OMU  | O2-C2 | -3.50 | 1.16        | 1.23     |
| 3   | h1    | 1781 | 4AC  | O2-C2 | -3.40 | 1.17        | 1.23     |
| 3   | h1    | 1283 | 4AC  | O2-C2 | -3.40 | 1.17        | 1.23     |
| 3   | h1    | 1283 | 4AC  | C6-N1 | 3.32  | 1.46        | 1.38     |
| 81  | A3    | 786  | PSU  | O4-C4 | -3.32 | 1.17        | 1.23     |
| 81  | A3    | 829  | PSU  | O4-C4 | -3.31 | 1.17        | 1.23     |
| 81  | A3    | 684  | PSU  | O4-C4 | -3.29 | 1.17        | 1.23     |
| 81  | A3    | 2958 | PSU  | O4-C4 | -3.29 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 81  | A3    | 277  | PSU  | O4-C4 | -3.27 | 1.17        | 1.23     |
| 81  | A3    | 42   | PSU  | O4-C4 | -3.27 | 1.17        | 1.23     |
| 3   | h1    | 1106 | PSU  | O4-C4 | -3.26 | 1.17        | 1.23     |
| 81  | A3    | 1135 | PSU  | O4-C4 | -3.26 | 1.17        | 1.23     |
| 81  | A3    | 976  | PSU  | O4-C4 | -3.25 | 1.17        | 1.23     |
| 81  | A3    | 2139 | PSU  | O4-C4 | -3.25 | 1.17        | 1.23     |
| 81  | A3    | 2978 | PSU  | O4-C4 | -3.25 | 1.17        | 1.23     |
| 3   | h1    | 362  | PSU  | O4-C4 | -3.24 | 1.17        | 1.23     |
| 81  | A3    | 2947 | PSU  | O4-C4 | -3.24 | 1.17        | 1.23     |
| 82  | B3    | 96   | PSU  | O4-C4 | -3.24 | 1.17        | 1.23     |
| 3   | h1    | 306  | PSU  | O4-C4 | -3.24 | 1.17        | 1.23     |
| 81  | A3    | 2897 | PSU  | O4-C4 | -3.24 | 1.17        | 1.23     |
| 82  | B3    | 21   | PSU  | O4-C4 | -3.24 | 1.17        | 1.23     |
| 81  | A3    | 2829 | PSU  | O4-C4 | -3.24 | 1.17        | 1.23     |
| 81  | A3    | 902  | PSU  | O4-C4 | -3.23 | 1.17        | 1.23     |
| 81  | A3    | 1482 | PSU  | O4-C4 | -3.23 | 1.17        | 1.23     |
| 81  | A3    | 2435 | PSU  | O4-C4 | -3.23 | 1.17        | 1.23     |
| 81  | A3    | 2214 | PSU  | O4-C4 | -3.23 | 1.17        | 1.23     |
| 81  | A3    | 311  | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 3   | h1    | 606  | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 81  | A3    | 895  | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 81  | A3    | 510  | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 3   | h1    | 1304 | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 81  | A3    | 1134 | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 3   | h1    | 1120 | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 81  | A3    | 2194 | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 81  | A3    | 1002 | PSU  | O4-C4 | -3.22 | 1.17        | 1.23     |
| 81  | A3    | 2883 | PSU  | O4-C4 | -3.21 | 1.17        | 1.23     |
| 3   | h1    | 1781 | 4AC  | C6-N1 | 3.20  | 1.45        | 1.38     |
| 81  | A3    | 2263 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 1064 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 2137 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 3113 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 2419 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 2926 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 1474 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 966  | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 1056 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 3   | h1    | 763  | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 81  | A3    | 2269 | PSU  | O4-C4 | -3.20 | 1.17        | 1.23     |
| 82  | B3    | 77   | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 3   | h1    | 635  | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 81  | A3    | 2857 | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 81  | A3    | 2747 | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 3   | h1    | 1027 | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 81  | A3    | 656  | 1MA  | C5-C6 | 3.19  | 1.52        | 1.43     |
| 3   | h1    | 809  | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 81  | A3    | 2321 | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 81  | A3    | 2868 | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 3   | h1    | 1002 | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 81  | A3    | 970  | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 3   | h1    | 451  | PSU  | O4-C4 | -3.19 | 1.17        | 1.23     |
| 81  | A3    | 1685 | PSU  | O4-C4 | -3.18 | 1.17        | 1.23     |
| 3   | h1    | 1293 | PSU  | O4-C4 | -3.18 | 1.17        | 1.23     |
| 3   | h1    | 1178 | PSU  | O4-C4 | -3.18 | 1.17        | 1.23     |
| 3   | h1    | 103  | PSU  | O4-C4 | -3.18 | 1.17        | 1.23     |
| 81  | A3    | 1133 | PSU  | O4-C4 | -3.18 | 1.17        | 1.23     |
| 81  | A3    | 2317 | PSU  | O4-C4 | -3.18 | 1.17        | 1.23     |
| 3   | h1    | 1190 | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 81  | A3    | 34   | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 3   | h1    | 95   | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 81  | A3    | 2257 | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 3   | h1    | 1634 | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 3   | h1    | 339  | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 3   | h1    | 417  | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 3   | h1    | 753  | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 3   | h1    | 1787 | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 81  | A3    | 717  | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 3   | h1    | 1615 | PSU  | O4-C4 | -3.16 | 1.17        | 1.23     |
| 3   | h1    | 607  | PSU  | O4-C4 | -3.16 | 1.17        | 1.23     |
| 3   | h1    | 1567 | PSU  | O4-C4 | -3.16 | 1.17        | 1.23     |
| 3   | h1    | 950  | PSU  | O4-C4 | -3.16 | 1.17        | 1.23     |
| 81  | A3    | 464  | PSU  | O4-C4 | -3.16 | 1.17        | 1.23     |
| 81  | A3    | 150  | PSU  | O4-C4 | -3.16 | 1.17        | 1.23     |
| 81  | A3    | 2267 | PSU  | O4-C4 | -3.16 | 1.17        | 1.23     |
| 3   | h1    | 1210 | PSU  | O4-C4 | -3.15 | 1.17        | 1.23     |
| 3   | h1    | 1184 | PSU  | O4-C4 | -3.15 | 1.17        | 1.23     |
| 3   | h1    | 1485 | PSU  | O4-C4 | -3.15 | 1.17        | 1.23     |
| 81  | A3    | 228  | PSU  | O4-C4 | -3.15 | 1.17        | 1.23     |
| 81  | A3    | 2261 | PSU  | O4-C4 | -3.15 | 1.17        | 1.23     |
| 3   | h1    | 1524 | PSU  | O4-C4 | -3.14 | 1.17        | 1.23     |
| 3   | h1    | 1535 | PSU  | O4-C4 | -3.14 | 1.17        | 1.23     |
| 3   | h1    | 121  | PSU  | O4-C4 | -3.14 | 1.17        | 1.23     |
| 3   | h1    | 762  | PSU  | O4-C4 | -3.14 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | h1    | 1217 | PSU  | O4-C4  | -3.14 | 1.17        | 1.23     |
| 81  | A3    | 1016 | PSU  | O4-C4  | -3.14 | 1.17        | 1.23     |
| 81  | A3    | 2654 | OMG  | C2-N1  | 3.14  | 1.45        | 1.37     |
| 3   | h1    | 310  | PSU  | O4-C4  | -3.13 | 1.17        | 1.23     |
| 3   | h1    | 961  | PSU  | O4-C4  | -3.13 | 1.17        | 1.23     |
| 3   | h1    | 1308 | PSU  | O4-C4  | -3.13 | 1.17        | 1.23     |
| 3   | h1    | 470  | PSU  | O4-C4  | -3.13 | 1.17        | 1.23     |
| 81  | A3    | 2394 | OMG  | C2-N1  | 3.12  | 1.45        | 1.37     |
| 3   | h1    | 258  | PSU  | O4-C4  | -3.12 | 1.17        | 1.23     |
| 3   | h1    | 605  | PSU  | O4-C4  | -3.11 | 1.17        | 1.23     |
| 3   | h1    | 584  | PSU  | O4-C4  | -3.11 | 1.17        | 1.23     |
| 81  | A3    | 2956 | UR3  | C6-N1  | 3.09  | 1.45        | 1.38     |
| 81  | A3    | 2127 | OMG  | C2-N1  | 3.06  | 1.45        | 1.37     |
| 81  | A3    | 2818 | OMG  | C2-N1  | 3.05  | 1.45        | 1.37     |
| 3   | h1    | 392  | OMG  | C2-N1  | 3.05  | 1.45        | 1.37     |
| 81  | A3    | 2398 | OMG  | C2-N1  | 3.05  | 1.45        | 1.37     |
| 81  | A3    | 296  | OMG  | C2-N1  | 3.04  | 1.45        | 1.37     |
| 81  | A3    | 2920 | OMG  | C2-N1  | 3.04  | 1.45        | 1.37     |
| 3   | h1    | 598  | OMG  | C2-N1  | 3.04  | 1.45        | 1.37     |
| 81  | A3    | 399  | OMG  | C2-N1  | 3.04  | 1.45        | 1.37     |
| 81  | A3    | 2622 | OMG  | C2-N1  | 3.04  | 1.45        | 1.37     |
| 81  | A3    | 2398 | OMG  | C5-C6  | 3.03  | 1.55        | 1.44     |
| 81  | A3    | 2412 | OMG  | C2-N1  | 3.03  | 1.45        | 1.37     |
| 3   | h1    | 1433 | OMG  | C2-N1  | 3.03  | 1.45        | 1.37     |
| 81  | A3    | 2126 | OMG  | C2-N1  | 3.02  | 1.45        | 1.37     |
| 81  | A3    | 2654 | OMG  | C6-N1  | 3.02  | 1.44        | 1.38     |
| 81  | A3    | 2127 | OMG  | C5-C6  | 3.02  | 1.55        | 1.44     |
| 3   | h1    | 1274 | OMG  | C2-N1  | 3.02  | 1.45        | 1.37     |
| 81  | A3    | 1857 | OMG  | C2-N1  | 3.01  | 1.45        | 1.37     |
| 81  | A3    | 1461 | OMG  | C2-N1  | 3.01  | 1.45        | 1.37     |
| 3   | h1    | 246  | OMG  | C2-N1  | 3.01  | 1.45        | 1.37     |
| 3   | h1    | 584  | PSU  | C1'-C5 | 3.01  | 1.57        | 1.50     |
| 81  | A3    | 786  | PSU  | C1'-C5 | 3.01  | 1.57        | 1.50     |
| 81  | A3    | 2796 | OMG  | C2-N1  | 3.00  | 1.45        | 1.37     |
| 81  | A3    | 2394 | OMG  | C5-C6  | 3.00  | 1.55        | 1.44     |
| 81  | A3    | 2412 | OMG  | C5-C6  | 3.00  | 1.55        | 1.44     |
| 81  | A3    | 2654 | OMG  | C5-C6  | 3.00  | 1.55        | 1.44     |
| 81  | A3    | 918  | OMG  | C2-N1  | 3.00  | 1.45        | 1.37     |
| 81  | A3    | 815  | OMG  | C2-N1  | 3.00  | 1.45        | 1.37     |
| 81  | A3    | 2291 | OMG  | C2-N1  | 3.00  | 1.45        | 1.37     |
| 82  | B3    | 78   | OMG  | C2-N1  | 2.99  | 1.45        | 1.37     |
| 81  | A3    | 2925 | OMG  | C2-N1  | 2.99  | 1.45        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | h1    | 584  | PSU  | O4'-C1' | -2.98 | 1.39        | 1.43     |
| 81  | A3    | 815  | OMG  | C5-C6   | 2.97  | 1.55        | 1.44     |
| 81  | A3    | 2239 | OMG  | C2-N1   | 2.97  | 1.45        | 1.37     |
| 81  | A3    | 2818 | OMG  | C5-C6   | 2.97  | 1.55        | 1.44     |
| 81  | A3    | 1461 | OMG  | C5-C6   | 2.96  | 1.55        | 1.44     |
| 82  | B3    | 96   | PSU  | C1'-C5  | 2.95  | 1.57        | 1.50     |
| 3   | h1    | 392  | OMG  | C5-C6   | 2.95  | 1.55        | 1.44     |
| 81  | A3    | 311  | PSU  | C1'-C5  | 2.95  | 1.57        | 1.50     |
| 81  | A3    | 296  | OMG  | C5-C6   | 2.94  | 1.55        | 1.44     |
| 81  | A3    | 2394 | OMG  | C6-N1   | 2.94  | 1.44        | 1.38     |
| 3   | h1    | 1790 | MA6  | C5-C4   | -2.94 | 1.33        | 1.39     |
| 81  | A3    | 2291 | OMG  | C5-C6   | 2.94  | 1.55        | 1.44     |
| 81  | A3    | 2920 | OMG  | C5-C6   | 2.94  | 1.55        | 1.44     |
| 3   | h1    | 598  | OMG  | C5-C6   | 2.93  | 1.55        | 1.44     |
| 81  | A3    | 2239 | OMG  | C5-C6   | 2.92  | 1.55        | 1.44     |
| 81  | A3    | 399  | OMG  | C5-C6   | 2.92  | 1.55        | 1.44     |
| 81  | A3    | 2796 | OMG  | C5-C6   | 2.92  | 1.55        | 1.44     |
| 81  | A3    | 2126 | OMG  | C5-C6   | 2.92  | 1.55        | 1.44     |
| 3   | h1    | 1524 | PSU  | C1'-C5  | 2.92  | 1.56        | 1.50     |
| 3   | h1    | 1274 | OMG  | C5-C6   | 2.92  | 1.55        | 1.44     |
| 81  | A3    | 1857 | OMG  | C5-C6   | 2.91  | 1.55        | 1.44     |
| 81  | A3    | 2794 | OMG  | C2-N1   | 2.91  | 1.44        | 1.37     |
| 81  | A3    | 2398 | OMG  | C6-N1   | 2.90  | 1.44        | 1.38     |
| 81  | A3    | 2412 | OMG  | C6-N1   | 2.90  | 1.44        | 1.38     |
| 81  | A3    | 2194 | PSU  | C1'-C5  | 2.90  | 1.56        | 1.50     |
| 81  | A3    | 1480 | OMC  | C5-C4   | 2.89  | 1.49        | 1.42     |
| 3   | h1    | 246  | OMG  | C5-C6   | 2.89  | 1.55        | 1.44     |
| 81  | A3    | 2622 | OMG  | C5-C6   | 2.89  | 1.55        | 1.44     |
| 81  | A3    | 2269 | PSU  | C1'-C5  | 2.88  | 1.56        | 1.50     |
| 81  | A3    | 2263 | PSU  | C1'-C5  | 2.88  | 1.56        | 1.50     |
| 3   | h1    | 1218 | OMC  | C5-C4   | 2.88  | 1.49        | 1.42     |
| 81  | A3    | 2127 | OMG  | C6-N1   | 2.88  | 1.44        | 1.38     |
| 82  | B3    | 78   | OMG  | C5-C6   | 2.88  | 1.55        | 1.44     |
| 81  | A3    | 2818 | OMG  | O6-C6   | -2.88 | 1.18        | 1.23     |
| 81  | A3    | 2818 | OMG  | C6-N1   | 2.88  | 1.44        | 1.38     |
| 81  | A3    | 2284 | A2M  | C5-C4   | -2.88 | 1.33        | 1.39     |
| 3   | h1    | 1790 | MA6  | C6-N6   | 2.88  | 1.45        | 1.36     |
| 81  | A3    | 2296 | OMC  | C5-C4   | 2.88  | 1.49        | 1.42     |
| 3   | h1    | 1789 | MA6  | C6-N6   | 2.88  | 1.45        | 1.36     |
| 3   | h1    | 339  | PSU  | C1'-C5  | 2.87  | 1.56        | 1.50     |
| 3   | h1    | 1535 | PSU  | C1'-C5  | 2.87  | 1.56        | 1.50     |
| 81  | A3    | 2925 | OMG  | C5-C6   | 2.87  | 1.55        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | h1    | 38   | OMC  | C5-C4  | 2.87  | 1.49        | 1.42     |
| 81  | A3    | 2747 | PSU  | C1'-C5 | 2.87  | 1.56        | 1.50     |
| 3   | h1    | 418  | OMC  | C5-C4  | 2.87  | 1.49        | 1.42     |
| 3   | h1    | 1027 | PSU  | C1'-C5 | 2.87  | 1.56        | 1.50     |
| 3   | h1    | 473  | OMC  | C5-C4  | 2.87  | 1.49        | 1.42     |
| 81  | A3    | 2794 | OMG  | C5-C6  | 2.87  | 1.55        | 1.44     |
| 81  | A3    | 2200 | OMC  | C5-C4  | 2.86  | 1.49        | 1.42     |
| 81  | A3    | 2291 | OMG  | O6-C6  | -2.86 | 1.18        | 1.23     |
| 81  | A3    | 464  | PSU  | C1'-C5 | 2.86  | 1.56        | 1.50     |
| 81  | A3    | 1474 | PSU  | C1'-C5 | 2.86  | 1.56        | 1.50     |
| 81  | A3    | 918  | OMG  | C5-C6  | 2.86  | 1.55        | 1.44     |
| 81  | A3    | 1849 | OMC  | C5-C4  | 2.85  | 1.49        | 1.42     |
| 81  | A3    | 815  | OMG  | O6-C6  | -2.85 | 1.18        | 1.23     |
| 3   | h1    | 1433 | OMG  | C5-C6  | 2.85  | 1.55        | 1.44     |
| 81  | A3    | 1857 | OMG  | O6-C6  | -2.85 | 1.18        | 1.23     |
| 81  | A3    | 40   | OMC  | C5-C4  | 2.85  | 1.49        | 1.42     |
| 81  | A3    | 1852 | OMC  | C5-C4  | 2.84  | 1.49        | 1.42     |
| 3   | h1    | 392  | OMG  | C6-N1  | 2.84  | 1.44        | 1.38     |
| 3   | h1    | 1217 | PSU  | C1'-C5 | 2.84  | 1.56        | 1.50     |
| 81  | A3    | 660  | A2M  | C5-C4  | -2.84 | 1.33        | 1.39     |
| 3   | h1    | 606  | PSU  | C1'-C5 | 2.84  | 1.56        | 1.50     |
| 81  | A3    | 2261 | PSU  | C1'-C5 | 2.84  | 1.56        | 1.50     |
| 81  | A3    | 2126 | OMG  | C6-N1  | 2.84  | 1.44        | 1.38     |
| 81  | A3    | 2949 | A2M  | C5-C4  | -2.84 | 1.33        | 1.39     |
| 81  | A3    | 2321 | PSU  | C1'-C5 | 2.84  | 1.56        | 1.50     |
| 81  | A3    | 2804 | A2M  | C5-C4  | -2.84 | 1.33        | 1.39     |
| 3   | h1    | 622  | A2M  | C5-C4  | -2.83 | 1.33        | 1.39     |
| 81  | A3    | 2340 | OMC  | C5-C4  | 2.83  | 1.49        | 1.42     |
| 3   | h1    | 1789 | MA6  | C5-C4  | -2.83 | 1.33        | 1.39     |
| 81  | A3    | 2419 | PSU  | C1'-C5 | 2.83  | 1.56        | 1.50     |
| 81  | A3    | 2412 | OMG  | O6-C6  | -2.82 | 1.18        | 1.23     |
| 3   | h1    | 306  | PSU  | C1'-C5 | 2.82  | 1.56        | 1.50     |
| 81  | A3    | 2368 | OMC  | C5-C4  | 2.82  | 1.49        | 1.42     |
| 3   | h1    | 1645 | OMC  | C5-C4  | 2.82  | 1.49        | 1.42     |
| 3   | h1    | 1120 | PSU  | C1'-C5 | 2.82  | 1.56        | 1.50     |
| 3   | h1    | 950  | PSU  | C1'-C5 | 2.82  | 1.56        | 1.50     |
| 3   | h1    | 121  | PSU  | C1'-C5 | 2.82  | 1.56        | 1.50     |
| 81  | A3    | 2794 | OMG  | O6-C6  | -2.81 | 1.18        | 1.23     |
| 81  | A3    | 2398 | OMG  | O6-C6  | -2.81 | 1.18        | 1.23     |
| 81  | A3    | 2324 | A2M  | C5-C4  | -2.81 | 1.33        | 1.39     |
| 81  | A3    | 2920 | OMG  | C6-N1  | 2.81  | 1.44        | 1.38     |
| 82  | B3    | 46   | A2M  | C5-C4  | -2.81 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 81  | A3    | 815  | OMG  | C6-N1  | 2.81  | 1.44        | 1.38     |
| 3   | h1    | 605  | PSU  | C1'-C5 | 2.81  | 1.56        | 1.50     |
| 81  | A3    | 2126 | OMG  | O6-C6  | -2.81 | 1.18        | 1.23     |
| 81  | A3    | 966  | PSU  | C1'-C5 | 2.81  | 1.56        | 1.50     |
| 81  | A3    | 2958 | PSU  | C1'-C5 | 2.81  | 1.56        | 1.50     |
| 3   | h1    | 607  | PSU  | C1'-C5 | 2.80  | 1.56        | 1.50     |
| 81  | A3    | 1056 | PSU  | C1'-C5 | 2.80  | 1.56        | 1.50     |
| 81  | A3    | 296  | OMG  | C6-N1  | 2.80  | 1.44        | 1.38     |
| 3   | h1    | 310  | PSU  | C1'-C5 | 2.80  | 1.56        | 1.50     |
| 3   | h1    | 753  | PSU  | C1'-C5 | 2.80  | 1.56        | 1.50     |
| 81  | A3    | 2920 | OMG  | O6-C6  | -2.80 | 1.18        | 1.23     |
| 81  | A3    | 150  | PSU  | C1'-C5 | 2.80  | 1.56        | 1.50     |
| 81  | A3    | 2883 | PSU  | C1'-C5 | 2.79  | 1.56        | 1.50     |
| 81  | A3    | 1461 | OMG  | O6-C6  | -2.79 | 1.18        | 1.23     |
| 81  | A3    | 1144 | A2M  | C5-C4  | -2.79 | 1.33        | 1.39     |
| 81  | A3    | 1002 | PSU  | C1'-C5 | 2.79  | 1.56        | 1.50     |
| 81  | A3    | 902  | PSU  | C1'-C5 | 2.79  | 1.56        | 1.50     |
| 81  | A3    | 2214 | PSU  | C1'-C5 | 2.79  | 1.56        | 1.50     |
| 81  | A3    | 2239 | OMG  | O6-C6  | -2.79 | 1.18        | 1.23     |
| 3   | h1    | 258  | PSU  | C1'-C5 | 2.79  | 1.56        | 1.50     |
| 3   | h1    | 1178 | PSU  | C1'-C5 | 2.79  | 1.56        | 1.50     |
| 81  | A3    | 827  | A2M  | C5-C4  | -2.79 | 1.33        | 1.39     |
| 3   | h1    | 140  | OMC  | C5-C4  | 2.79  | 1.49        | 1.42     |
| 3   | h1    | 451  | PSU  | C1'-C5 | 2.78  | 1.56        | 1.50     |
| 81  | A3    | 1064 | PSU  | C1'-C5 | 2.78  | 1.56        | 1.50     |
| 3   | h1    | 1308 | PSU  | C1'-C5 | 2.78  | 1.56        | 1.50     |
| 3   | h1    | 392  | OMG  | O6-C6  | -2.78 | 1.18        | 1.23     |
| 82  | B3    | 78   | OMG  | C6-N1  | 2.78  | 1.44        | 1.38     |
| 81  | A3    | 2137 | PSU  | O2-C2  | -2.78 | 1.17        | 1.23     |
| 81  | A3    | 2685 | OMC  | C5-C4  | 2.78  | 1.49        | 1.42     |
| 81  | A3    | 2127 | OMG  | O6-C6  | -2.78 | 1.18        | 1.23     |
| 3   | h1    | 635  | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 81  | A3    | 2897 | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 81  | A3    | 1862 | OMC  | C5-C4  | 2.77  | 1.49        | 1.42     |
| 81  | A3    | 2796 | OMG  | O6-C6  | -2.77 | 1.18        | 1.23     |
| 82  | B3    | 21   | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 3   | h1    | 1634 | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 81  | A3    | 399  | OMG  | C6-N1  | 2.77  | 1.44        | 1.38     |
| 3   | h1    | 763  | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 81  | A3    | 970  | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 3   | h1    | 1567 | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 81  | A3    | 1482 | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 81  | A3    | 2868 | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 3   | h1    | 809  | PSU  | C1'-C5 | 2.77  | 1.56        | 1.50     |
| 81  | A3    | 817  | A2M  | C5-C4  | -2.77 | 1.33        | 1.39     |
| 81  | A3    | 2622 | OMG  | O6-C6  | -2.76 | 1.18        | 1.23     |
| 81  | A3    | 277  | PSU  | C1'-C5 | 2.76  | 1.56        | 1.50     |
| 3   | h1    | 1002 | PSU  | C1'-C5 | 2.76  | 1.56        | 1.50     |
| 81  | A3    | 2139 | PSU  | C1'-C5 | 2.76  | 1.56        | 1.50     |
| 81  | A3    | 2882 | OMC  | C5-C4  | 2.76  | 1.49        | 1.42     |
| 81  | A3    | 1448 | OMC  | C5-C4  | 2.76  | 1.49        | 1.42     |
| 81  | A3    | 2925 | OMG  | O6-C6  | -2.76 | 1.18        | 1.23     |
| 81  | A3    | 684  | PSU  | C1'-C5 | 2.76  | 1.56        | 1.50     |
| 3   | h1    | 1787 | PSU  | C1'-C5 | 2.76  | 1.56        | 1.50     |
| 81  | A3    | 2978 | PSU  | C1'-C5 | 2.76  | 1.56        | 1.50     |
| 3   | h1    | 1293 | PSU  | C1'-C5 | 2.76  | 1.56        | 1.50     |
| 81  | A3    | 2329 | A2M  | C5-C4  | -2.76 | 1.33        | 1.39     |
| 81  | A3    | 2643 | A2M  | C5-C4  | -2.76 | 1.33        | 1.39     |
| 81  | A3    | 918  | OMG  | O6-C6  | -2.75 | 1.18        | 1.23     |
| 81  | A3    | 2239 | OMG  | C6-N1  | 2.75  | 1.43        | 1.38     |
| 81  | A3    | 1460 | A2M  | C5-C4  | -2.75 | 1.33        | 1.39     |
| 81  | A3    | 2962 | OMC  | C5-C4  | 2.75  | 1.49        | 1.42     |
| 3   | h1    | 1274 | OMG  | C6-N1  | 2.75  | 1.43        | 1.38     |
| 3   | h1    | 1190 | PSU  | C1'-C5 | 2.75  | 1.56        | 1.50     |
| 81  | A3    | 1133 | PSU  | C1'-C5 | 2.75  | 1.56        | 1.50     |
| 81  | A3    | 886  | A2M  | C5-C4  | -2.75 | 1.33        | 1.39     |
| 81  | A3    | 2829 | PSU  | C1'-C5 | 2.75  | 1.56        | 1.50     |
| 3   | h1    | 246  | OMG  | C6-N1  | 2.75  | 1.43        | 1.38     |
| 3   | h1    | 598  | OMG  | C6-N1  | 2.75  | 1.43        | 1.38     |
| 81  | A3    | 3113 | PSU  | C1'-C5 | 2.75  | 1.56        | 1.50     |
| 3   | h1    | 1329 | A2M  | C5-C4  | -2.75 | 1.33        | 1.39     |
| 81  | A3    | 2925 | OMG  | C6-N1  | 2.75  | 1.43        | 1.38     |
| 3   | h1    | 762  | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 3   | h1    | 1433 | OMG  | O6-C6  | -2.74 | 1.18        | 1.23     |
| 3   | h1    | 1106 | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 3   | h1    | 1485 | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 82  | B3    | 78   | OMG  | O6-C6  | -2.74 | 1.18        | 1.23     |
| 3   | h1    | 1304 | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 81  | A3    | 2291 | OMG  | C6-N1  | 2.74  | 1.43        | 1.38     |
| 3   | h1    | 1184 | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 81  | A3    | 1016 | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 81  | A3    | 976  | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 81  | A3    | 2654 | OMG  | O6-C6  | -2.74 | 1.18        | 1.23     |
| 81  | A3    | 2914 | A2M  | C5-C4  | -2.74 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 81  | A3    | 674  | OMC  | C5-C4  | 2.74  | 1.49        | 1.42     |
| 81  | A3    | 1685 | PSU  | C1'-C5 | 2.74  | 1.56        | 1.50     |
| 81  | A3    | 2129 | A2M  | C5-C4  | -2.74 | 1.33        | 1.39     |
| 3   | h1    | 1274 | OMG  | O6-C6  | -2.74 | 1.18        | 1.23     |
| 3   | h1    | 246  | OMG  | O6-C6  | -2.74 | 1.18        | 1.23     |
| 81  | A3    | 2139 | PSU  | O2-C2  | -2.74 | 1.17        | 1.23     |
| 81  | A3    | 829  | PSU  | O2-C2  | -2.73 | 1.17        | 1.23     |
| 3   | h1    | 1615 | PSU  | C1'-C5 | 2.73  | 1.56        | 1.50     |
| 3   | h1    | 470  | PSU  | C1'-C5 | 2.73  | 1.56        | 1.50     |
| 81  | A3    | 1857 | OMG  | C6-N1  | 2.73  | 1.43        | 1.38     |
| 81  | A3    | 1378 | A2M  | C5-C4  | -2.73 | 1.33        | 1.39     |
| 81  | A3    | 2883 | PSU  | O2-C2  | -2.73 | 1.17        | 1.23     |
| 81  | A3    | 296  | OMG  | O6-C6  | -2.73 | 1.18        | 1.23     |
| 81  | A3    | 2394 | OMG  | O6-C6  | -2.73 | 1.18        | 1.23     |
| 3   | h1    | 103  | PSU  | C1'-C5 | 2.72  | 1.56        | 1.50     |
| 81  | A3    | 2259 | A2M  | C5-C4  | -2.72 | 1.33        | 1.39     |
| 81  | A3    | 369  | A2M  | C5-C4  | -2.72 | 1.33        | 1.39     |
| 3   | h1    | 598  | OMG  | O6-C6  | -2.72 | 1.18        | 1.23     |
| 81  | A3    | 228  | PSU  | C1'-C5 | 2.72  | 1.56        | 1.50     |
| 81  | A3    | 2926 | PSU  | C1'-C5 | 2.72  | 1.56        | 1.50     |
| 81  | A3    | 2435 | PSU  | C1'-C5 | 2.72  | 1.56        | 1.50     |
| 3   | h1    | 977  | A2M  | C5-C4  | -2.72 | 1.33        | 1.39     |
| 81  | A3    | 2796 | OMG  | C6-N1  | 2.72  | 1.43        | 1.38     |
| 81  | A3    | 1461 | OMG  | C6-N1  | 2.71  | 1.43        | 1.38     |
| 3   | h1    | 440  | A2M  | C5-C4  | -2.71 | 1.33        | 1.39     |
| 3   | h1    | 961  | PSU  | C1'-C5 | 2.71  | 1.56        | 1.50     |
| 3   | h1    | 28   | A2M  | C5-C4  | -2.71 | 1.33        | 1.39     |
| 81  | A3    | 2267 | PSU  | C1'-C5 | 2.71  | 1.56        | 1.50     |
| 81  | A3    | 2257 | PSU  | C1'-C5 | 2.71  | 1.56        | 1.50     |
| 81  | A3    | 34   | PSU  | C1'-C5 | 2.71  | 1.56        | 1.50     |
| 82  | B3    | 77   | PSU  | C1'-C5 | 2.71  | 1.56        | 1.50     |
| 81  | A3    | 399  | OMG  | O6-C6  | -2.71 | 1.18        | 1.23     |
| 3   | h1    | 162  | A2M  | C5-C4  | -2.71 | 1.34        | 1.39     |
| 3   | h1    | 1579 | A2M  | C5-C4  | -2.70 | 1.34        | 1.39     |
| 81  | A3    | 2643 | A2M  | C5-N7  | -2.70 | 1.33        | 1.39     |
| 3   | h1    | 95   | PSU  | C1'-C5 | 2.70  | 1.56        | 1.50     |
| 81  | A3    | 2839 | OMC  | C5-C4  | 2.70  | 1.49        | 1.42     |
| 81  | A3    | 2978 | PSU  | O2-C2  | -2.70 | 1.17        | 1.23     |
| 81  | A3    | 886  | A2M  | C5-N7  | -2.70 | 1.33        | 1.39     |
| 81  | A3    | 277  | PSU  | O2-C2  | -2.69 | 1.17        | 1.23     |
| 3   | h1    | 424  | A2M  | C5-C4  | -2.69 | 1.34        | 1.39     |
| 3   | h1    | 417  | PSU  | C1'-C5 | 2.69  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | h1    | 1433 | OMG  | C6-N1  | 2.69  | 1.43        | 1.38     |
| 81  | A3    | 2321 | PSU  | O2-C2  | -2.69 | 1.17        | 1.23     |
| 81  | A3    | 966  | PSU  | O2-C2  | -2.69 | 1.17        | 1.23     |
| 3   | h1    | 800  | A2M  | C5-C4  | -2.69 | 1.34        | 1.39     |
| 81  | A3    | 2419 | PSU  | O2-C2  | -2.69 | 1.17        | 1.23     |
| 81  | A3    | 1134 | PSU  | C1'-C5 | 2.68  | 1.56        | 1.50     |
| 3   | h1    | 1771 | 6MZ  | C5-N7  | -2.68 | 1.34        | 1.39     |
| 3   | h1    | 468  | A2M  | C5-C4  | -2.68 | 1.34        | 1.39     |
| 81  | A3    | 2223 | A2M  | C5-C4  | -2.68 | 1.34        | 1.39     |
| 3   | h1    | 1758 | A2M  | C5-C4  | -2.68 | 1.34        | 1.39     |
| 81  | A3    | 1460 | A2M  | C5-N7  | -2.68 | 1.34        | 1.39     |
| 81  | A3    | 1134 | PSU  | O2-C2  | -2.67 | 1.17        | 1.23     |
| 81  | A3    | 2829 | PSU  | O2-C2  | -2.67 | 1.17        | 1.23     |
| 81  | A3    | 34   | PSU  | O2-C2  | -2.67 | 1.17        | 1.23     |
| 81  | A3    | 1016 | PSU  | O2-C2  | -2.67 | 1.17        | 1.23     |
| 81  | A3    | 684  | PSU  | O2-C2  | -2.67 | 1.17        | 1.23     |
| 81  | A3    | 2897 | PSU  | O2-C2  | -2.67 | 1.17        | 1.23     |
| 3   | h1    | 103  | PSU  | O2-C2  | -2.67 | 1.17        | 1.23     |
| 81  | A3    | 1135 | PSU  | O2-C2  | -2.66 | 1.17        | 1.23     |
| 81  | A3    | 2947 | PSU  | O2-C2  | -2.66 | 1.17        | 1.23     |
| 81  | A3    | 2435 | PSU  | O2-C2  | -2.66 | 1.17        | 1.23     |
| 81  | A3    | 510  | PSU  | O2-C2  | -2.66 | 1.17        | 1.23     |
| 81  | A3    | 2958 | PSU  | O2-C2  | -2.65 | 1.17        | 1.23     |
| 82  | B3    | 96   | PSU  | O2-C2  | -2.65 | 1.17        | 1.23     |
| 81  | A3    | 2794 | OMG  | C6-N1  | 2.65  | 1.43        | 1.38     |
| 81  | A3    | 369  | A2M  | C5-N7  | -2.65 | 1.34        | 1.39     |
| 3   | h1    | 1210 | PSU  | O2-C2  | -2.65 | 1.17        | 1.23     |
| 81  | A3    | 2263 | PSU  | O2-C2  | -2.65 | 1.17        | 1.23     |
| 81  | A3    | 2622 | OMG  | C6-N1  | 2.65  | 1.43        | 1.38     |
| 81  | A3    | 2194 | PSU  | O2-C2  | -2.65 | 1.17        | 1.23     |
| 81  | A3    | 2857 | PSU  | O2-C2  | -2.65 | 1.17        | 1.23     |
| 81  | A3    | 1482 | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 81  | A3    | 946  | A2M  | C5-C4  | -2.64 | 1.34        | 1.39     |
| 3   | h1    | 635  | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 81  | A3    | 311  | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 81  | A3    | 1064 | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 81  | A3    | 2947 | PSU  | C1'-C5 | 2.64  | 1.56        | 1.50     |
| 81  | A3    | 2857 | PSU  | C1'-C5 | 2.64  | 1.56        | 1.50     |
| 81  | A3    | 902  | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 81  | A3    | 976  | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 81  | A3    | 2223 | A2M  | C5-N7  | -2.64 | 1.34        | 1.39     |
| 81  | A3    | 2317 | PSU  | C1'-C5 | 2.64  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 81  | A3    | 42   | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 81  | A3    | 895  | PSU  | O2-C2  | -2.64 | 1.17        | 1.23     |
| 3   | h1    | 977  | A2M  | C5-N7  | -2.63 | 1.34        | 1.39     |
| 81  | A3    | 829  | PSU  | C1'-C5 | 2.63  | 1.56        | 1.50     |
| 3   | h1    | 1210 | PSU  | C1'-C5 | 2.63  | 1.56        | 1.50     |
| 3   | h1    | 362  | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 81  | A3    | 228  | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 3   | h1    | 544  | A2M  | C5-N7  | -2.63 | 1.34        | 1.39     |
| 81  | A3    | 1056 | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 81  | A3    | 2868 | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 82  | B3    | 21   | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 3   | h1    | 763  | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 3   | h1    | 440  | A2M  | C5-N7  | -2.63 | 1.34        | 1.39     |
| 81  | A3    | 42   | PSU  | C1'-C5 | 2.63  | 1.56        | 1.50     |
| 3   | h1    | 607  | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 81  | A3    | 2261 | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 81  | A3    | 510  | PSU  | C1'-C5 | 2.63  | 1.56        | 1.50     |
| 3   | h1    | 1758 | A2M  | C5-N7  | -2.63 | 1.34        | 1.39     |
| 3   | h1    | 362  | PSU  | C1'-C5 | 2.63  | 1.56        | 1.50     |
| 81  | A3    | 1002 | PSU  | O2-C2  | -2.62 | 1.17        | 1.23     |
| 81  | A3    | 3113 | PSU  | O2-C2  | -2.62 | 1.17        | 1.23     |
| 3   | h1    | 1634 | PSU  | O2-C2  | -2.62 | 1.17        | 1.23     |
| 81  | A3    | 717  | PSU  | C1'-C5 | 2.62  | 1.56        | 1.50     |
| 81  | A3    | 1135 | PSU  | C1'-C5 | 2.62  | 1.56        | 1.50     |
| 3   | h1    | 809  | PSU  | O2-C2  | -2.62 | 1.17        | 1.23     |
| 3   | h1    | 1787 | PSU  | O2-C2  | -2.62 | 1.17        | 1.23     |
| 81  | A3    | 1133 | PSU  | O2-C2  | -2.62 | 1.17        | 1.23     |
| 81  | A3    | 817  | A2M  | C5-N7  | -2.62 | 1.34        | 1.39     |
| 81  | A3    | 1378 | A2M  | C5-N7  | -2.62 | 1.34        | 1.39     |
| 3   | h1    | 1120 | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 3   | h1    | 762  | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 3   | h1    | 1304 | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 81  | A3    | 918  | OMG  | C6-N1  | 2.61  | 1.43        | 1.38     |
| 81  | A3    | 2324 | A2M  | C5-N7  | -2.61 | 1.34        | 1.39     |
| 3   | h1    | 1106 | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 3   | h1    | 1178 | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 81  | A3    | 895  | PSU  | C1'-C5 | 2.61  | 1.56        | 1.50     |
| 81  | A3    | 918  | OMG  | C5-N7  | -2.61 | 1.34        | 1.39     |
| 3   | h1    | 605  | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 81  | A3    | 827  | A2M  | C5-N7  | -2.61 | 1.34        | 1.39     |
| 81  | A3    | 1474 | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 81  | A3    | 2269 | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | h1    | 961  | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 81  | A3    | 786  | PSU  | O2-C2  | -2.61 | 1.17        | 1.23     |
| 3   | h1    | 753  | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 82  | B3    | 77   | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 81  | A3    | 2267 | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 81  | A3    | 2329 | A2M  | C5-N7  | -2.60 | 1.34        | 1.39     |
| 81  | A3    | 2951 | OMC  | C5-C4  | 2.60  | 1.48        | 1.42     |
| 3   | h1    | 306  | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 81  | A3    | 2317 | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 3   | h1    | 28   | A2M  | C5-N7  | -2.60 | 1.34        | 1.39     |
| 81  | A3    | 2137 | PSU  | C1'-C5 | 2.60  | 1.56        | 1.50     |
| 81  | A3    | 2747 | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 3   | h1    | 470  | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 3   | h1    | 1308 | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 81  | A3    | 2949 | A2M  | C5-N7  | -2.60 | 1.34        | 1.39     |
| 3   | h1    | 1615 | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 81  | A3    | 150  | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 81  | A3    | 656  | 1MA  | CM1-N1 | 2.60  | 1.52        | 1.46     |
| 81  | A3    | 970  | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 81  | A3    | 2926 | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 3   | h1    | 1002 | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 81  | A3    | 1144 | A2M  | C5-N7  | -2.59 | 1.34        | 1.39     |
| 81  | A3    | 2214 | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 3   | h1    | 451  | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 81  | A3    | 2257 | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 3   | h1    | 950  | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 3   | h1    | 1184 | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 3   | h1    | 800  | A2M  | C5-N7  | -2.59 | 1.34        | 1.39     |
| 3   | h1    | 1190 | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 82  | B3    | 46   | A2M  | C5-N7  | -2.58 | 1.34        | 1.39     |
| 3   | h1    | 310  | PSU  | O2-C2  | -2.58 | 1.18        | 1.23     |
| 3   | h1    | 544  | A2M  | C5-C4  | -2.58 | 1.34        | 1.39     |
| 81  | A3    | 464  | PSU  | O2-C2  | -2.58 | 1.18        | 1.23     |
| 3   | h1    | 95   | PSU  | O2-C2  | -2.57 | 1.18        | 1.23     |
| 3   | h1    | 606  | PSU  | O2-C2  | -2.57 | 1.18        | 1.23     |
| 3   | h1    | 121  | PSU  | O2-C2  | -2.57 | 1.18        | 1.23     |
| 3   | h1    | 1293 | PSU  | O2-C2  | -2.57 | 1.18        | 1.23     |
| 3   | h1    | 1535 | PSU  | O2-C2  | -2.57 | 1.18        | 1.23     |
| 3   | h1    | 258  | PSU  | O2-C2  | -2.57 | 1.18        | 1.23     |
| 3   | h1    | 417  | PSU  | O2-C2  | -2.56 | 1.18        | 1.23     |
| 3   | h1    | 584  | PSU  | O2-C2  | -2.56 | 1.18        | 1.23     |
| 81  | A3    | 717  | PSU  | O2-C2  | -2.56 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | h1    | 1579 | A2M  | C5-N7 | -2.56 | 1.34        | 1.39     |
| 3   | h1    | 1485 | PSU  | O2-C2 | -2.56 | 1.18        | 1.23     |
| 81  | A3    | 2914 | A2M  | C5-N7 | -2.56 | 1.34        | 1.39     |
| 81  | A3    | 1685 | PSU  | O2-C2 | -2.56 | 1.18        | 1.23     |
| 3   | h1    | 1217 | PSU  | O2-C2 | -2.55 | 1.18        | 1.23     |
| 81  | A3    | 2653 | UY1  | O4-C4 | -2.55 | 1.18        | 1.23     |
| 3   | h1    | 1567 | PSU  | O2-C2 | -2.55 | 1.18        | 1.23     |
| 81  | A3    | 2804 | A2M  | C5-N7 | -2.55 | 1.34        | 1.39     |
| 3   | h1    | 1524 | PSU  | O2-C2 | -2.54 | 1.18        | 1.23     |
| 3   | h1    | 339  | PSU  | O2-C2 | -2.54 | 1.18        | 1.23     |
| 3   | h1    | 1027 | PSU  | O2-C2 | -2.54 | 1.18        | 1.23     |
| 3   | h1    | 468  | A2M  | C5-N7 | -2.53 | 1.34        | 1.39     |
| 3   | h1    | 603  | UY1  | O4-C4 | -2.52 | 1.18        | 1.23     |
| 81  | A3    | 660  | A2M  | C5-N7 | -2.52 | 1.34        | 1.39     |
| 81  | A3    | 2129 | A2M  | C5-N7 | -2.52 | 1.34        | 1.39     |
| 81  | A3    | 2284 | A2M  | C5-N7 | -2.51 | 1.34        | 1.39     |
| 81  | A3    | 2259 | A2M  | C5-N7 | -2.51 | 1.34        | 1.39     |
| 3   | h1    | 622  | A2M  | C5-N7 | -2.50 | 1.34        | 1.39     |
| 81  | A3    | 946  | A2M  | C5-N7 | -2.50 | 1.34        | 1.39     |
| 3   | h1    | 424  | A2M  | C5-N7 | -2.50 | 1.34        | 1.39     |
| 3   | h1    | 1329 | A2M  | C5-N7 | -2.45 | 1.34        | 1.39     |
| 3   | h1    | 162  | A2M  | C5-N7 | -2.44 | 1.34        | 1.39     |
| 81  | A3    | 2239 | OMG  | C5-N7 | -2.44 | 1.34        | 1.39     |
| 81  | A3    | 2873 | 5MC  | O2-C2 | -2.44 | 1.19        | 1.23     |
| 3   | h1    | 1433 | OMG  | C5-N7 | -2.43 | 1.34        | 1.39     |
| 81  | A3    | 1894 | OMU  | C5-C4 | 2.42  | 1.49        | 1.43     |
| 3   | h1    | 246  | OMG  | C5-N7 | -2.41 | 1.34        | 1.39     |
| 81  | A3    | 2622 | OMG  | C5-N7 | -2.41 | 1.34        | 1.39     |
| 81  | A3    | 787  | OMU  | C5-C4 | 2.41  | 1.49        | 1.43     |
| 3   | h1    | 373  | OMU  | C5-C4 | 2.41  | 1.49        | 1.43     |
| 81  | A3    | 2424 | OMU  | C5-C4 | 2.40  | 1.49        | 1.43     |
| 3   | h1    | 1383 | OMU  | C5-C4 | 2.40  | 1.48        | 1.43     |
| 81  | A3    | 1857 | OMG  | C5-N7 | -2.40 | 1.34        | 1.39     |
| 81  | A3    | 2796 | OMG  | C5-N7 | -2.40 | 1.34        | 1.39     |
| 81  | A3    | 2920 | OMG  | C5-N7 | -2.38 | 1.34        | 1.39     |
| 81  | A3    | 2925 | OMG  | C5-N7 | -2.38 | 1.34        | 1.39     |
| 81  | A3    | 1068 | OMU  | C5-C4 | 2.38  | 1.48        | 1.43     |
| 81  | A3    | 2732 | OMU  | C5-C4 | 2.38  | 1.48        | 1.43     |
| 81  | A3    | 44   | OMU  | C5-C4 | 2.38  | 1.48        | 1.43     |
| 3   | h1    | 1234 | OMU  | C5-C4 | 2.38  | 1.48        | 1.43     |
| 81  | A3    | 2281 | 5MC  | O2-C2 | -2.37 | 1.19        | 1.23     |
| 3   | h1    | 1274 | OMG  | C5-N7 | -2.37 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | A3    | 2794 | OMG  | C5-N7   | -2.37 | 1.34        | 1.39     |
| 82  | B3    | 78   | OMG  | C5-N7   | -2.36 | 1.34        | 1.39     |
| 3   | h1    | 1012 | OMU  | C5-C4   | 2.36  | 1.48        | 1.43     |
| 81  | A3    | 48   | OMU  | C5-C4   | 2.34  | 1.48        | 1.43     |
| 81  | A3    | 2924 | OMU  | C5-C4   | 2.34  | 1.48        | 1.43     |
| 3   | h1    | 886  | OMU  | C5-C4   | 2.34  | 1.48        | 1.43     |
| 81  | A3    | 2291 | OMG  | C5-N7   | -2.34 | 1.34        | 1.39     |
| 81  | A3    | 1537 | OMU  | C5-C4   | 2.34  | 1.48        | 1.43     |
| 3   | h1    | 598  | OMG  | C5-N7   | -2.34 | 1.34        | 1.39     |
| 81  | A3    | 399  | OMG  | C5-N7   | -2.34 | 1.34        | 1.39     |
| 3   | h1    | 392  | OMG  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 3   | h1    | 1272 | OMU  | C5-C4   | 2.33  | 1.48        | 1.43     |
| 3   | h1    | 123  | OMU  | C5-C4   | 2.33  | 1.48        | 1.43     |
| 81  | A3    | 2413 | OMU  | C5-C4   | 2.33  | 1.48        | 1.43     |
| 81  | A3    | 2738 | OMU  | C5-C4   | 2.33  | 1.48        | 1.43     |
| 81  | A3    | 2654 | OMG  | C4-N9   | -2.33 | 1.32        | 1.38     |
| 81  | A3    | 675  | OMU  | C5-C4   | 2.32  | 1.48        | 1.43     |
| 81  | A3    | 2350 | OMU  | C5-C4   | 2.32  | 1.48        | 1.43     |
| 3   | h1    | 581  | OMU  | C5-C4   | 2.32  | 1.48        | 1.43     |
| 81  | A3    | 804  | OMU  | C5-C4   | 2.32  | 1.48        | 1.43     |
| 81  | A3    | 1461 | OMG  | C5-N7   | -2.32 | 1.34        | 1.39     |
| 81  | A3    | 3304 | OMU  | C5-C4   | 2.31  | 1.48        | 1.43     |
| 81  | A3    | 2818 | OMG  | C5-N7   | -2.31 | 1.34        | 1.39     |
| 81  | A3    | 2947 | PSU  | O4'-C1' | -2.31 | 1.40        | 1.43     |
| 81  | A3    | 815  | OMG  | C5-N7   | -2.31 | 1.34        | 1.39     |
| 81  | A3    | 296  | OMG  | C5-N7   | -2.30 | 1.34        | 1.39     |
| 81  | A3    | 946  | A2M  | O5'-C5' | -2.30 | 1.39        | 1.44     |
| 3   | h1    | 614  | OMU  | C5-C4   | 2.30  | 1.48        | 1.43     |
| 81  | A3    | 2126 | OMG  | C5-N7   | -2.30 | 1.34        | 1.39     |
| 81  | A3    | 2394 | OMG  | C5-N7   | -2.28 | 1.34        | 1.39     |
| 81  | A3    | 2956 | UR3  | C5-C4   | 2.28  | 1.49        | 1.43     |
| 81  | A3    | 144  | OMU  | C5-C4   | 2.28  | 1.48        | 1.43     |
| 3   | h1    | 1789 | MA6  | C5-N7   | -2.26 | 1.34        | 1.39     |
| 81  | A3    | 2720 | OMU  | C5-C4   | 2.26  | 1.48        | 1.43     |
| 3   | h1    | 1447 | OMU  | C5-C4   | 2.25  | 1.48        | 1.43     |
| 3   | h1    | 1283 | 4AC  | CM7-C7  | 2.24  | 1.55        | 1.50     |
| 81  | A3    | 3289 | OMU  | C5-C4   | 2.23  | 1.48        | 1.43     |
| 81  | A3    | 2654 | OMG  | C5-N7   | -2.23 | 1.34        | 1.39     |
| 81  | A3    | 2956 | UR3  | C4-N3   | 2.23  | 1.45        | 1.40     |
| 81  | A3    | 2653 | UY1  | O2-C2   | -2.22 | 1.18        | 1.23     |
| 81  | A3    | 2398 | OMG  | C5-N7   | -2.22 | 1.34        | 1.39     |
| 81  | A3    | 2412 | OMG  | C5-N7   | -2.22 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | h1    | 1771 | 6MZ  | C5-C4   | -2.21 | 1.34        | 1.39     |
| 3   | h1    | 1781 | 4AC  | CM7-C7  | 2.21  | 1.55        | 1.50     |
| 3   | h1    | 603  | UY1  | O2-C2   | -2.20 | 1.18        | 1.23     |
| 81  | A3    | 2886 | OMU  | C5-C4   | 2.19  | 1.48        | 1.43     |
| 3   | h1    | 1790 | MA6  | C5-N7   | -2.17 | 1.34        | 1.39     |
| 81  | A3    | 2127 | OMG  | C5-N7   | -2.16 | 1.34        | 1.39     |
| 3   | h1    | 1194 | B8N  | O4-C4   | -2.16 | 1.18        | 1.23     |
| 81  | A3    | 2956 | UR3  | O4-C4   | -2.15 | 1.18        | 1.23     |
| 3   | h1    | 977  | A2M  | C8-N9   | -2.15 | 1.33        | 1.37     |
| 3   | h1    | 1771 | 6MZ  | C6-N1   | -2.13 | 1.31        | 1.35     |
| 3   | h1    | 1027 | PSU  | O4'-C1' | -2.11 | 1.40        | 1.43     |
| 81  | A3    | 660  | A2M  | C8-N9   | -2.11 | 1.33        | 1.37     |
| 3   | h1    | 1283 | 4AC  | O7-C7   | -2.11 | 1.18        | 1.23     |
| 81  | A3    | 2398 | OMG  | C4-N9   | -2.11 | 1.32        | 1.38     |
| 81  | A3    | 1460 | A2M  | C8-N9   | -2.11 | 1.33        | 1.37     |
| 81  | A3    | 827  | A2M  | C8-N9   | -2.11 | 1.33        | 1.37     |
| 81  | A3    | 1144 | A2M  | C8-N9   | -2.11 | 1.33        | 1.37     |
| 3   | h1    | 1781 | 4AC  | O7-C7   | -2.10 | 1.18        | 1.23     |
| 81  | A3    | 817  | A2M  | C8-N9   | -2.10 | 1.33        | 1.37     |
| 81  | A3    | 2394 | OMG  | C4-N9   | -2.09 | 1.32        | 1.38     |
| 3   | h1    | 1758 | A2M  | C8-N9   | -2.08 | 1.33        | 1.37     |
| 3   | h1    | 1194 | B8N  | O2-C2   | -2.08 | 1.18        | 1.22     |
| 81  | A3    | 2818 | OMG  | C4-N9   | -2.07 | 1.32        | 1.38     |
| 81  | A3    | 2949 | A2M  | C8-N9   | -2.06 | 1.33        | 1.37     |
| 81  | A3    | 2643 | A2M  | C8-N9   | -2.06 | 1.33        | 1.37     |
| 81  | A3    | 886  | A2M  | C8-N9   | -2.06 | 1.33        | 1.37     |
| 82  | B3    | 46   | A2M  | C8-N9   | -2.06 | 1.33        | 1.37     |
| 3   | h1    | 1329 | A2M  | C8-N9   | -2.05 | 1.33        | 1.37     |
| 81  | A3    | 2127 | OMG  | C4-N9   | -2.05 | 1.32        | 1.38     |
| 3   | h1    | 622  | A2M  | C8-N9   | -2.05 | 1.33        | 1.37     |
| 81  | A3    | 2956 | UR3  | O2-C2   | -2.05 | 1.18        | 1.22     |
| 3   | h1    | 1771 | 6MZ  | C2-N1   | 2.04  | 1.37        | 1.33     |
| 81  | A3    | 2223 | A2M  | C8-N9   | -2.04 | 1.33        | 1.37     |
| 81  | A3    | 2284 | A2M  | C8-N9   | -2.04 | 1.33        | 1.37     |
| 81  | A3    | 2259 | A2M  | C8-N9   | -2.04 | 1.33        | 1.37     |
| 3   | h1    | 1758 | A2M  | O5'-C5' | -2.04 | 1.39        | 1.44     |
| 81  | A3    | 1378 | A2M  | C8-N9   | -2.03 | 1.33        | 1.37     |
| 81  | A3    | 970  | PSU  | O4'-C1' | -2.02 | 1.41        | 1.43     |
| 3   | h1    | 800  | A2M  | C8-N9   | -2.02 | 1.33        | 1.37     |
| 81  | A3    | 2914 | A2M  | C8-N9   | -2.02 | 1.33        | 1.37     |
| 3   | h1    | 1579 | A2M  | C8-N9   | -2.01 | 1.33        | 1.37     |
| 3   | h1    | 544  | A2M  | C8-N9   | -2.01 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 81  | A3    | 2324 | A2M  | C8-N9 | -2.01 | 1.33        | 1.37     |
| 81  | A3    | 2129 | A2M  | C8-N9 | -2.00 | 1.33        | 1.37     |
| 3   | h1    | 424  | A2M  | C8-N9 | -2.00 | 1.33        | 1.37     |
| 3   | h1    | 162  | A2M  | C8-N9 | -2.00 | 1.33        | 1.37     |

All (1383) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | h1    | 1790 | MA6  | N1-C6-N6 | -8.65 | 107.62      | 117.08   |
| 3   | h1    | 1789 | MA6  | N1-C6-N6 | -8.41 | 107.89      | 117.08   |
| 81  | A3    | 2284 | A2M  | N6-C6-N1 | -7.11 | 102.77      | 118.35   |
| 81  | A3    | 946  | A2M  | N6-C6-N1 | -6.92 | 103.20      | 118.35   |
| 81  | A3    | 2804 | A2M  | N6-C6-N1 | -6.86 | 103.32      | 118.35   |
| 3   | h1    | 424  | A2M  | N6-C6-N1 | -6.85 | 103.36      | 118.35   |
| 81  | A3    | 2259 | A2M  | N6-C6-N1 | -6.84 | 103.36      | 118.35   |
| 81  | A3    | 817  | A2M  | N6-C6-N1 | -6.84 | 103.38      | 118.35   |
| 81  | A3    | 660  | A2M  | N6-C6-N1 | -6.83 | 103.39      | 118.35   |
| 3   | h1    | 162  | A2M  | N6-C6-N1 | -6.83 | 103.39      | 118.35   |
| 3   | h1    | 1579 | A2M  | N6-C6-N1 | -6.81 | 103.43      | 118.35   |
| 81  | A3    | 827  | A2M  | N6-C6-N1 | -6.79 | 103.49      | 118.35   |
| 81  | A3    | 2914 | A2M  | N6-C6-N1 | -6.78 | 103.51      | 118.35   |
| 3   | h1    | 800  | A2M  | N6-C6-N1 | -6.77 | 103.52      | 118.35   |
| 3   | h1    | 440  | A2M  | N6-C6-N1 | -6.76 | 103.55      | 118.35   |
| 3   | h1    | 1329 | A2M  | N6-C6-N1 | -6.76 | 103.55      | 118.35   |
| 81  | A3    | 2329 | A2M  | N6-C6-N1 | -6.76 | 103.55      | 118.35   |
| 3   | h1    | 622  | A2M  | N6-C6-N1 | -6.76 | 103.55      | 118.35   |
| 3   | h1    | 544  | A2M  | N6-C6-N1 | -6.76 | 103.55      | 118.35   |
| 3   | h1    | 468  | A2M  | N6-C6-N1 | -6.74 | 103.59      | 118.35   |
| 82  | B3    | 46   | A2M  | N6-C6-N1 | -6.73 | 103.61      | 118.35   |
| 81  | A3    | 2129 | A2M  | N6-C6-N1 | -6.73 | 103.61      | 118.35   |
| 81  | A3    | 1460 | A2M  | N6-C6-N1 | -6.72 | 103.64      | 118.35   |
| 3   | h1    | 28   | A2M  | N6-C6-N1 | -6.67 | 103.75      | 118.35   |
| 81  | A3    | 886  | A2M  | N6-C6-N1 | -6.66 | 103.76      | 118.35   |
| 81  | A3    | 2324 | A2M  | N6-C6-N1 | -6.66 | 103.76      | 118.35   |
| 81  | A3    | 2949 | A2M  | N6-C6-N1 | -6.66 | 103.77      | 118.35   |
| 81  | A3    | 1378 | A2M  | N6-C6-N1 | -6.66 | 103.77      | 118.35   |
| 81  | A3    | 369  | A2M  | N6-C6-N1 | -6.66 | 103.77      | 118.35   |
| 3   | h1    | 977  | A2M  | N6-C6-N1 | -6.63 | 103.83      | 118.35   |
| 3   | h1    | 1758 | A2M  | N6-C6-N1 | -6.63 | 103.83      | 118.35   |
| 81  | A3    | 1144 | A2M  | N6-C6-N1 | -6.62 | 103.86      | 118.35   |
| 81  | A3    | 2643 | A2M  | N6-C6-N1 | -6.60 | 103.89      | 118.35   |
| 81  | A3    | 2223 | A2M  | N6-C6-N1 | -6.57 | 103.97      | 118.35   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 2804 | A2M  | C4-N9-C1' | -6.56 | 110.95      | 126.59   |
| 81  | A3    | 399  | OMG  | C1'-N9-C8 | -6.38 | 108.52      | 126.70   |
| 3   | h1    | 622  | A2M  | C4-N9-C1' | -6.36 | 111.43      | 126.59   |
| 81  | A3    | 2804 | A2M  | C1'-N9-C8 | 6.17  | 141.06      | 127.14   |
| 81  | A3    | 2284 | A2M  | C5-C6-N6  | 6.17  | 136.85      | 123.43   |
| 81  | A3    | 2804 | A2M  | C5-C6-N6  | 6.13  | 136.77      | 123.43   |
| 81  | A3    | 946  | A2M  | C5-C6-N6  | 6.12  | 136.75      | 123.43   |
| 81  | A3    | 2284 | A2M  | C4-N9-C1' | -6.11 | 112.03      | 126.59   |
| 81  | A3    | 1144 | A2M  | C4-N9-C1' | -6.10 | 112.07      | 126.59   |
| 81  | A3    | 2259 | A2M  | C5-C6-N6  | 6.07  | 136.63      | 123.43   |
| 81  | A3    | 827  | A2M  | C5-C6-N6  | 6.06  | 136.61      | 123.43   |
| 3   | h1    | 424  | A2M  | C5-C6-N6  | 6.05  | 136.61      | 123.43   |
| 81  | A3    | 1144 | A2M  | C5-C6-N6  | 6.04  | 136.58      | 123.43   |
| 3   | h1    | 162  | A2M  | C5-C6-N6  | 6.03  | 136.56      | 123.43   |
| 81  | A3    | 2914 | A2M  | C5-C6-N6  | 6.03  | 136.55      | 123.43   |
| 3   | h1    | 246  | OMG  | C1'-N9-C8 | -6.02 | 109.55      | 126.70   |
| 81  | A3    | 2129 | A2M  | C5-C6-N6  | 6.02  | 136.53      | 123.43   |
| 3   | h1    | 1579 | A2M  | C5-C6-N6  | 6.02  | 136.53      | 123.43   |
| 81  | A3    | 660  | A2M  | C5-C6-N6  | 6.01  | 136.51      | 123.43   |
| 81  | A3    | 1461 | OMG  | C1'-N9-C8 | -6.01 | 109.59      | 126.70   |
| 81  | A3    | 2914 | A2M  | C4-N9-C1' | -6.01 | 112.28      | 126.59   |
| 81  | A3    | 886  | A2M  | C5-C6-N6  | 6.01  | 136.50      | 123.43   |
| 81  | A3    | 918  | OMG  | C1'-N9-C8 | -6.00 | 109.61      | 126.70   |
| 3   | h1    | 468  | A2M  | C5-C6-N6  | 6.00  | 136.48      | 123.43   |
| 81  | A3    | 817  | A2M  | C5-C6-N6  | 5.99  | 136.47      | 123.43   |
| 82  | B3    | 46   | A2M  | C5-C6-N6  | 5.99  | 136.47      | 123.43   |
| 3   | h1    | 622  | A2M  | C5-C6-N6  | 5.99  | 136.47      | 123.43   |
| 81  | A3    | 1460 | A2M  | C5-C6-N6  | 5.99  | 136.46      | 123.43   |
| 3   | h1    | 544  | A2M  | C5-C4-N3  | -5.98 | 118.94      | 126.75   |
| 81  | A3    | 2329 | A2M  | C5-C6-N6  | 5.98  | 136.45      | 123.43   |
| 81  | A3    | 2925 | OMG  | C1'-N9-C8 | -5.98 | 109.67      | 126.70   |
| 3   | h1    | 1329 | A2M  | C5-C6-N6  | 5.98  | 136.44      | 123.43   |
| 3   | h1    | 800  | A2M  | C5-C6-N6  | 5.98  | 136.44      | 123.43   |
| 3   | h1    | 440  | A2M  | C5-C6-N6  | 5.97  | 136.43      | 123.43   |
| 3   | h1    | 28   | A2M  | C5-C6-N6  | 5.96  | 136.41      | 123.43   |
| 81  | A3    | 2412 | OMG  | C1'-N9-C8 | -5.96 | 109.72      | 126.70   |
| 81  | A3    | 815  | OMG  | C1'-N9-C8 | -5.95 | 109.75      | 126.70   |
| 81  | A3    | 660  | A2M  | C4-N9-C1' | -5.95 | 112.42      | 126.59   |
| 3   | h1    | 544  | A2M  | C5-C6-N6  | 5.94  | 136.36      | 123.43   |
| 81  | A3    | 2324 | A2M  | C5-C6-N6  | 5.94  | 136.36      | 123.43   |
| 3   | h1    | 622  | A2M  | C1'-N9-C8 | 5.93  | 140.53      | 127.14   |
| 81  | A3    | 369  | A2M  | C5-C6-N6  | 5.91  | 136.30      | 123.43   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 827  | A2M  | C4-N9-C1' | -5.90 | 112.52      | 126.59   |
| 3   | h1    | 977  | A2M  | C5-C6-N6  | 5.90  | 136.28      | 123.43   |
| 81  | A3    | 2259 | A2M  | C4-N9-C1' | -5.90 | 112.54      | 126.59   |
| 81  | A3    | 1378 | A2M  | C5-C6-N6  | 5.90  | 136.27      | 123.43   |
| 3   | h1    | 1274 | OMG  | C1'-N9-C8 | -5.89 | 109.94      | 126.70   |
| 81  | A3    | 2324 | A2M  | C4-N9-C1' | -5.87 | 112.60      | 126.59   |
| 81  | A3    | 2643 | A2M  | C5-C6-N6  | 5.86  | 136.19      | 123.43   |
| 3   | h1    | 1758 | A2M  | C5-C6-N6  | 5.86  | 136.18      | 123.43   |
| 81  | A3    | 2291 | OMG  | C1'-N9-C8 | -5.86 | 110.03      | 126.70   |
| 81  | A3    | 2622 | OMG  | C1'-N9-C8 | -5.86 | 110.03      | 126.70   |
| 81  | A3    | 2223 | A2M  | C5-C6-N6  | 5.84  | 136.14      | 123.43   |
| 81  | A3    | 2949 | A2M  | C5-C6-N6  | 5.83  | 136.12      | 123.43   |
| 3   | h1    | 598  | OMG  | C1'-N9-C8 | -5.82 | 110.13      | 126.70   |
| 3   | h1    | 1433 | OMG  | C1'-N9-C8 | -5.82 | 110.13      | 126.70   |
| 3   | h1    | 424  | A2M  | C4-N9-C1' | -5.80 | 112.76      | 126.59   |
| 3   | h1    | 468  | A2M  | C4-N9-C1' | -5.80 | 112.77      | 126.59   |
| 3   | h1    | 440  | A2M  | C4-N9-C1' | -5.80 | 112.78      | 126.59   |
| 81  | A3    | 369  | A2M  | C4-N9-C1' | -5.80 | 112.78      | 126.59   |
| 3   | h1    | 1579 | A2M  | C4-N9-C1' | -5.79 | 112.81      | 126.59   |
| 3   | h1    | 28   | A2M  | C4-N9-C1' | -5.78 | 112.81      | 126.59   |
| 81  | A3    | 2129 | A2M  | C4-N9-C1' | -5.77 | 112.84      | 126.59   |
| 81  | A3    | 2239 | OMG  | C1'-N9-C8 | -5.76 | 110.31      | 126.70   |
| 82  | B3    | 78   | OMG  | C1'-N9-C8 | -5.75 | 110.33      | 126.70   |
| 3   | h1    | 1329 | A2M  | C4-N9-C1' | -5.75 | 112.90      | 126.59   |
| 3   | h1    | 162  | A2M  | C4-N9-C1' | -5.74 | 112.93      | 126.59   |
| 81  | A3    | 2949 | A2M  | C4-N9-C1' | -5.74 | 112.93      | 126.59   |
| 81  | A3    | 817  | A2M  | C5-C4-N3  | -5.72 | 119.29      | 126.75   |
| 81  | A3    | 2796 | OMG  | C1'-N9-C8 | -5.71 | 110.43      | 126.70   |
| 81  | A3    | 1378 | A2M  | C5-C4-N3  | -5.70 | 119.32      | 126.75   |
| 3   | h1    | 392  | OMG  | C1'-N9-C8 | -5.69 | 110.49      | 126.70   |
| 81  | A3    | 1144 | A2M  | C1'-N9-C8 | 5.69  | 139.99      | 127.14   |
| 81  | A3    | 2329 | A2M  | C4-N9-C1' | -5.68 | 113.06      | 126.59   |
| 81  | A3    | 946  | A2M  | C4-N9-C1' | -5.67 | 113.07      | 126.59   |
| 82  | B3    | 46   | A2M  | C4-N9-C1' | -5.66 | 113.12      | 126.59   |
| 81  | A3    | 2914 | A2M  | C1'-N9-C8 | 5.64  | 139.88      | 127.14   |
| 81  | A3    | 2920 | OMG  | C1'-N9-C8 | -5.64 | 110.64      | 126.70   |
| 81  | A3    | 2284 | A2M  | C1'-N9-C8 | 5.63  | 139.86      | 127.14   |
| 81  | A3    | 2804 | A2M  | N3-C2-N1  | -5.60 | 119.85      | 128.60   |
| 3   | h1    | 800  | A2M  | C5-C4-N3  | -5.58 | 119.47      | 126.75   |
| 81  | A3    | 2223 | A2M  | C4-N9-C1' | -5.58 | 113.31      | 126.59   |
| 81  | A3    | 1144 | A2M  | N3-C2-N1  | -5.57 | 119.89      | 128.60   |
| 81  | A3    | 296  | OMG  | C1'-N9-C8 | -5.57 | 110.84      | 126.70   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 1857 | OMG  | C1'-N9-C8 | -5.56 | 110.86      | 126.70   |
| 3   | h1    | 1790 | MA6  | N1-C2-N3  | -5.55 | 119.91      | 128.60   |
| 81  | A3    | 2223 | A2M  | C5-C4-N3  | -5.55 | 119.51      | 126.75   |
| 81  | A3    | 827  | A2M  | C1'-N9-C8 | 5.55  | 139.66      | 127.14   |
| 82  | B3    | 46   | A2M  | N3-C2-N1  | -5.54 | 119.93      | 128.60   |
| 3   | h1    | 622  | A2M  | N3-C2-N1  | -5.54 | 119.94      | 128.60   |
| 81  | A3    | 1460 | A2M  | C4-N9-C1' | -5.53 | 113.42      | 126.59   |
| 81  | A3    | 2643 | A2M  | C5-C4-N3  | -5.52 | 119.55      | 126.75   |
| 81  | A3    | 369  | A2M  | C1'-N9-C8 | 5.52  | 139.59      | 127.14   |
| 3   | h1    | 977  | A2M  | C5-C4-N3  | -5.52 | 119.55      | 126.75   |
| 81  | A3    | 2324 | A2M  | C1'-N9-C8 | 5.51  | 139.58      | 127.14   |
| 81  | A3    | 660  | A2M  | N3-C2-N1  | -5.51 | 119.98      | 128.60   |
| 81  | A3    | 886  | A2M  | N3-C2-N1  | -5.51 | 119.99      | 128.60   |
| 3   | h1    | 440  | A2M  | C1'-N9-C8 | 5.50  | 139.55      | 127.14   |
| 3   | h1    | 1758 | A2M  | C5-C4-N3  | -5.49 | 119.58      | 126.75   |
| 81  | A3    | 2259 | A2M  | N3-C2-N1  | -5.49 | 120.01      | 128.60   |
| 81  | A3    | 2329 | A2M  | N3-C2-N1  | -5.49 | 120.01      | 128.60   |
| 81  | A3    | 1460 | A2M  | C5-C4-N3  | -5.49 | 119.59      | 126.75   |
| 3   | h1    | 440  | A2M  | C5-C4-N3  | -5.49 | 119.59      | 126.75   |
| 81  | A3    | 2794 | OMG  | C1'-N9-C8 | -5.48 | 111.11      | 126.70   |
| 81  | A3    | 2126 | OMG  | C1'-N9-C8 | -5.47 | 111.12      | 126.70   |
| 3   | h1    | 468  | A2M  | N3-C2-N1  | -5.47 | 120.04      | 128.60   |
| 3   | h1    | 1789 | MA6  | N1-C2-N3  | -5.47 | 120.05      | 128.60   |
| 81  | A3    | 369  | A2M  | C5-C4-N3  | -5.47 | 119.61      | 126.75   |
| 81  | A3    | 2914 | A2M  | C5-C4-N3  | -5.46 | 119.62      | 126.75   |
| 81  | A3    | 2643 | A2M  | C4-N9-C1' | -5.45 | 113.60      | 126.59   |
| 3   | h1    | 424  | A2M  | N3-C2-N1  | -5.45 | 120.07      | 128.60   |
| 3   | h1    | 468  | A2M  | C1'-N9-C8 | 5.45  | 139.44      | 127.14   |
| 3   | h1    | 1771 | 6MZ  | N1-C2-N3  | -5.45 | 120.08      | 128.60   |
| 81  | A3    | 827  | A2M  | N3-C2-N1  | -5.44 | 120.09      | 128.60   |
| 3   | h1    | 800  | A2M  | N3-C2-N1  | -5.44 | 120.09      | 128.60   |
| 81  | A3    | 2949 | A2M  | C5-C4-N3  | -5.44 | 119.66      | 126.75   |
| 81  | A3    | 2259 | A2M  | C1'-N9-C8 | 5.43  | 139.39      | 127.14   |
| 3   | h1    | 28   | A2M  | N3-C2-N1  | -5.42 | 120.12      | 128.60   |
| 81  | A3    | 946  | A2M  | N3-C2-N1  | -5.42 | 120.12      | 128.60   |
| 3   | h1    | 28   | A2M  | C1'-N9-C8 | 5.42  | 139.37      | 127.14   |
| 3   | h1    | 1579 | A2M  | N3-C2-N1  | -5.42 | 120.12      | 128.60   |
| 3   | h1    | 162  | A2M  | N3-C2-N1  | -5.41 | 120.13      | 128.60   |
| 81  | A3    | 2284 | A2M  | N3-C2-N1  | -5.41 | 120.14      | 128.60   |
| 3   | h1    | 1771 | 6MZ  | C5-C4-N3  | -5.41 | 119.69      | 126.75   |
| 3   | h1    | 1329 | A2M  | N3-C2-N1  | -5.41 | 120.14      | 128.60   |
| 81  | A3    | 886  | A2M  | C5-C4-N3  | -5.41 | 119.70      | 126.75   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 660  | A2M  | C1'-N9-C8 | 5.40  | 139.34      | 127.14   |
| 3   | h1    | 1329 | A2M  | C5-C4-N3  | -5.40 | 119.70      | 126.75   |
| 81  | A3    | 2914 | A2M  | N3-C2-N1  | -5.40 | 120.16      | 128.60   |
| 81  | A3    | 2129 | A2M  | N3-C2-N1  | -5.40 | 120.16      | 128.60   |
| 81  | A3    | 2949 | A2M  | N3-C2-N1  | -5.39 | 120.16      | 128.60   |
| 81  | A3    | 946  | A2M  | C5-C4-N3  | -5.39 | 119.72      | 126.75   |
| 81  | A3    | 2818 | OMG  | C1'-N9-C8 | -5.39 | 111.35      | 126.70   |
| 3   | h1    | 1579 | A2M  | C1'-N9-C8 | 5.39  | 139.30      | 127.14   |
| 81  | A3    | 2129 | A2M  | C1'-N9-C8 | 5.39  | 139.30      | 127.14   |
| 3   | h1    | 1758 | A2M  | N3-C2-N1  | -5.38 | 120.18      | 128.60   |
| 3   | h1    | 440  | A2M  | N3-C2-N1  | -5.38 | 120.19      | 128.60   |
| 3   | h1    | 424  | A2M  | C1'-N9-C8 | 5.38  | 139.28      | 127.14   |
| 3   | h1    | 544  | A2M  | N3-C2-N1  | -5.37 | 120.19      | 128.60   |
| 81  | A3    | 2223 | A2M  | N3-C2-N1  | -5.36 | 120.21      | 128.60   |
| 81  | A3    | 2129 | A2M  | C5-C4-N3  | -5.36 | 119.75      | 126.75   |
| 81  | A3    | 827  | A2M  | C5-C4-N3  | -5.36 | 119.76      | 126.75   |
| 3   | h1    | 977  | A2M  | C4-N9-C1' | -5.36 | 113.83      | 126.59   |
| 81  | A3    | 2259 | A2M  | C5-C4-N3  | -5.35 | 119.76      | 126.75   |
| 81  | A3    | 369  | A2M  | N3-C2-N1  | -5.35 | 120.23      | 128.60   |
| 3   | h1    | 1579 | A2M  | C5-C4-N3  | -5.35 | 119.77      | 126.75   |
| 3   | h1    | 977  | A2M  | N3-C2-N1  | -5.34 | 120.24      | 128.60   |
| 3   | h1    | 424  | A2M  | C5-C4-N3  | -5.34 | 119.78      | 126.75   |
| 3   | h1    | 162  | A2M  | C1'-N9-C8 | 5.34  | 139.19      | 127.14   |
| 3   | h1    | 28   | A2M  | C5-C4-N3  | -5.33 | 119.79      | 126.75   |
| 81  | A3    | 2223 | A2M  | C1'-N9-C8 | 5.33  | 139.17      | 127.14   |
| 81  | A3    | 817  | A2M  | N3-C2-N1  | -5.33 | 120.27      | 128.60   |
| 3   | h1    | 162  | A2M  | C5-C4-N3  | -5.33 | 119.80      | 126.75   |
| 82  | B3    | 46   | A2M  | C5-C4-N3  | -5.31 | 119.82      | 126.75   |
| 81  | A3    | 1460 | A2M  | N3-C2-N1  | -5.31 | 120.30      | 128.60   |
| 81  | A3    | 2324 | A2M  | C5-C4-N3  | -5.30 | 119.83      | 126.75   |
| 81  | A3    | 399  | OMG  | C1'-N9-C4 | 5.30  | 142.24      | 126.50   |
| 3   | h1    | 468  | A2M  | C5-C4-N3  | -5.29 | 119.84      | 126.75   |
| 3   | h1    | 1329 | A2M  | C1'-N9-C8 | 5.29  | 139.09      | 127.14   |
| 81  | A3    | 2284 | A2M  | C5-C4-N3  | -5.29 | 119.85      | 126.75   |
| 81  | A3    | 2329 | A2M  | C1'-N9-C8 | 5.29  | 139.07      | 127.14   |
| 81  | A3    | 886  | A2M  | C4-N9-C1' | -5.28 | 114.00      | 126.59   |
| 81  | A3    | 946  | A2M  | C1'-N9-C8 | 5.28  | 139.06      | 127.14   |
| 81  | A3    | 2643 | A2M  | N3-C2-N1  | -5.28 | 120.34      | 128.60   |
| 3   | h1    | 800  | A2M  | C4-N9-C1' | -5.27 | 114.03      | 126.59   |
| 3   | h1    | 1758 | A2M  | C4-N9-C1' | -5.27 | 114.05      | 126.59   |
| 81  | A3    | 1894 | OMU  | C4-N3-C2  | -5.26 | 119.64      | 126.58   |
| 81  | A3    | 2324 | A2M  | N3-C2-N1  | -5.26 | 120.38      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 2329 | A2M  | C5-C4-N3  | -5.24 | 119.92      | 126.75   |
| 81  | A3    | 1378 | A2M  | N3-C2-N1  | -5.24 | 120.41      | 128.60   |
| 81  | A3    | 2949 | A2M  | C1'-N9-C8 | 5.20  | 138.89      | 127.14   |
| 81  | A3    | 660  | A2M  | C5-C4-N3  | -5.19 | 119.98      | 126.75   |
| 81  | A3    | 1068 | OMU  | C4-N3-C2  | -5.19 | 119.73      | 126.58   |
| 81  | A3    | 2394 | OMG  | C1'-N9-C8 | -5.19 | 111.93      | 126.70   |
| 81  | A3    | 1460 | A2M  | C1'-N9-C8 | 5.17  | 138.82      | 127.14   |
| 81  | A3    | 2924 | OMU  | C4-N3-C2  | -5.17 | 119.75      | 126.58   |
| 81  | A3    | 2804 | A2M  | C5-C4-N3  | -5.16 | 120.02      | 126.75   |
| 3   | h1    | 622  | A2M  | C5-C4-N3  | -5.16 | 120.02      | 126.75   |
| 81  | A3    | 2350 | OMU  | C4-N3-C2  | -5.16 | 119.77      | 126.58   |
| 82  | B3    | 46   | A2M  | C1'-N9-C8 | 5.15  | 138.77      | 127.14   |
| 81  | A3    | 2424 | OMU  | C4-N3-C2  | -5.14 | 119.80      | 126.58   |
| 81  | A3    | 817  | A2M  | C4-N9-C1' | -5.13 | 114.36      | 126.59   |
| 3   | h1    | 1234 | OMU  | C4-N3-C2  | -5.13 | 119.82      | 126.58   |
| 81  | A3    | 1378 | A2M  | C4-N9-C1' | -5.12 | 114.40      | 126.59   |
| 3   | h1    | 581  | OMU  | C4-N3-C2  | -5.11 | 119.83      | 126.58   |
| 3   | h1    | 1383 | OMU  | C4-N3-C2  | -5.11 | 119.83      | 126.58   |
| 3   | h1    | 1012 | OMU  | C4-N3-C2  | -5.11 | 119.84      | 126.58   |
| 3   | h1    | 886  | OMU  | C4-N3-C2  | -5.10 | 119.85      | 126.58   |
| 3   | h1    | 373  | OMU  | C4-N3-C2  | -5.10 | 119.86      | 126.58   |
| 81  | A3    | 2643 | A2M  | C1'-N9-C8 | 5.10  | 138.64      | 127.14   |
| 81  | A3    | 2738 | OMU  | C4-N3-C2  | -5.09 | 119.86      | 126.58   |
| 81  | A3    | 2398 | OMG  | C1'-N9-C8 | -5.08 | 112.23      | 126.70   |
| 81  | A3    | 918  | OMG  | C1'-N9-C4 | 5.08  | 141.60      | 126.50   |
| 81  | A3    | 144  | OMU  | C4-N3-C2  | -5.08 | 119.88      | 126.58   |
| 81  | A3    | 804  | OMU  | C4-N3-C2  | -5.07 | 119.89      | 126.58   |
| 3   | h1    | 1790 | MA6  | C5-C4-N3  | -5.07 | 120.14      | 126.75   |
| 3   | h1    | 1194 | B8N  | C5-C4-N3  | 5.06  | 125.54      | 116.17   |
| 3   | h1    | 1272 | OMU  | C4-N3-C2  | -5.06 | 119.91      | 126.58   |
| 3   | h1    | 123  | OMU  | C4-N3-C2  | -5.05 | 119.92      | 126.58   |
| 81  | A3    | 675  | OMU  | C4-N3-C2  | -5.04 | 119.93      | 126.58   |
| 81  | A3    | 3304 | OMU  | C4-N3-C2  | -5.01 | 119.97      | 126.58   |
| 81  | A3    | 48   | OMU  | C4-N3-C2  | -5.01 | 119.97      | 126.58   |
| 81  | A3    | 2127 | OMG  | C1'-N9-C8 | -5.01 | 112.44      | 126.70   |
| 81  | A3    | 1537 | OMU  | C4-N3-C2  | -5.00 | 119.98      | 126.58   |
| 81  | A3    | 1144 | A2M  | C5-C4-N3  | -5.00 | 120.23      | 126.75   |
| 81  | A3    | 787  | OMU  | C4-N3-C2  | -5.00 | 119.99      | 126.58   |
| 3   | h1    | 977  | A2M  | C1'-N9-C8 | 4.99  | 138.41      | 127.14   |
| 3   | h1    | 246  | OMG  | C1'-N9-C4 | 4.99  | 141.32      | 126.50   |
| 81  | A3    | 44   | OMU  | C4-N3-C2  | -4.97 | 120.02      | 126.58   |
| 81  | A3    | 2720 | OMU  | C4-N3-C2  | -4.97 | 120.02      | 126.58   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 656  | 1MA  | N1-C2-N3  | -4.97 | 120.09      | 126.00   |
| 3   | h1    | 800  | A2M  | C1'-N9-C8 | 4.97  | 138.35      | 127.14   |
| 81  | A3    | 1461 | OMG  | C1'-N9-C4 | 4.96  | 141.24      | 126.50   |
| 81  | A3    | 886  | A2M  | C1'-N9-C8 | 4.96  | 138.33      | 127.14   |
| 3   | h1    | 1789 | MA6  | C5-C4-N3  | -4.93 | 120.32      | 126.75   |
| 3   | h1    | 614  | OMU  | C4-N3-C2  | -4.93 | 120.08      | 126.58   |
| 81  | A3    | 2732 | OMU  | C4-N3-C2  | -4.91 | 120.10      | 126.58   |
| 81  | A3    | 918  | OMG  | C5-C4-N3  | -4.91 | 120.50      | 128.46   |
| 81  | A3    | 2413 | OMU  | C4-N3-C2  | -4.91 | 120.11      | 126.58   |
| 3   | h1    | 1274 | OMG  | C1'-N9-C4 | 4.86  | 140.93      | 126.50   |
| 81  | A3    | 2925 | OMG  | C1'-N9-C4 | 4.85  | 140.90      | 126.50   |
| 81  | A3    | 3289 | OMU  | C4-N3-C2  | -4.85 | 120.19      | 126.58   |
| 3   | h1    | 1758 | A2M  | C1'-N9-C8 | 4.84  | 138.07      | 127.14   |
| 81  | A3    | 2956 | UR3  | C4-N3-C2  | -4.82 | 120.02      | 124.56   |
| 3   | h1    | 246  | OMG  | C5-C4-N3  | -4.82 | 120.64      | 128.46   |
| 3   | h1    | 1447 | OMU  | C4-N3-C2  | -4.82 | 120.23      | 126.58   |
| 81  | A3    | 815  | OMG  | C1'-N9-C4 | 4.81  | 140.78      | 126.50   |
| 81  | A3    | 817  | A2M  | C1'-N9-C8 | 4.80  | 137.96      | 127.14   |
| 81  | A3    | 2412 | OMG  | C1'-N9-C4 | 4.79  | 140.74      | 126.50   |
| 81  | A3    | 2622 | OMG  | C1'-N9-C4 | 4.79  | 140.74      | 126.50   |
| 81  | A3    | 1378 | A2M  | C1'-N9-C8 | 4.79  | 137.95      | 127.14   |
| 81  | A3    | 2886 | OMU  | C4-N3-C2  | -4.78 | 120.27      | 126.58   |
| 81  | A3    | 399  | OMG  | C5-C4-N3  | -4.78 | 120.71      | 128.46   |
| 3   | h1    | 598  | OMG  | C1'-N9-C4 | 4.78  | 140.69      | 126.50   |
| 3   | h1    | 1433 | OMG  | C1'-N9-C4 | 4.77  | 140.68      | 126.50   |
| 81  | A3    | 2291 | OMG  | C1'-N9-C4 | 4.77  | 140.68      | 126.50   |
| 81  | A3    | 2137 | PSU  | C4-N3-C2  | -4.76 | 119.47      | 126.34   |
| 82  | B3    | 78   | OMG  | C1'-N9-C4 | 4.76  | 140.63      | 126.50   |
| 3   | h1    | 1274 | OMG  | C5-C4-N3  | -4.74 | 120.78      | 128.46   |
| 81  | A3    | 2654 | OMG  | C1'-N9-C8 | -4.73 | 113.23      | 126.70   |
| 81  | A3    | 2239 | OMG  | C1'-N9-C4 | 4.71  | 140.49      | 126.50   |
| 3   | h1    | 1790 | MA6  | N9-C8-N7  | -4.70 | 107.48      | 113.91   |
| 81  | A3    | 970  | PSU  | C4-N3-C2  | -4.68 | 119.60      | 126.34   |
| 81  | A3    | 2926 | PSU  | C4-N3-C2  | -4.67 | 119.61      | 126.34   |
| 81  | A3    | 2958 | PSU  | C4-N3-C2  | -4.67 | 119.61      | 126.34   |
| 81  | A3    | 1135 | PSU  | C4-N3-C2  | -4.66 | 119.62      | 126.34   |
| 82  | B3    | 78   | OMG  | C5-C4-N3  | -4.66 | 120.90      | 128.46   |
| 81  | A3    | 2239 | OMG  | C5-C4-N3  | -4.65 | 120.91      | 128.46   |
| 81  | A3    | 2796 | OMG  | C1'-N9-C4 | 4.65  | 140.31      | 126.50   |
| 3   | h1    | 598  | OMG  | C5-C4-N3  | -4.65 | 120.92      | 128.46   |
| 81  | A3    | 2257 | PSU  | C4-N3-C2  | -4.64 | 119.65      | 126.34   |
| 81  | A3    | 1056 | PSU  | C4-N3-C2  | -4.64 | 119.65      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 2857 | PSU  | C4-N3-C2  | -4.64 | 119.66      | 126.34   |
| 81  | A3    | 1064 | PSU  | C4-N3-C2  | -4.64 | 119.66      | 126.34   |
| 81  | A3    | 2653 | UY1  | C4-N3-C2  | -4.62 | 119.68      | 126.34   |
| 3   | h1    | 392  | OMG  | C1'-N9-C4 | 4.62  | 140.23      | 126.50   |
| 81  | A3    | 2622 | OMG  | C5-C4-N3  | -4.62 | 120.97      | 128.46   |
| 81  | A3    | 2920 | OMG  | C1'-N9-C4 | 4.62  | 140.22      | 126.50   |
| 81  | A3    | 2214 | PSU  | C4-N3-C2  | -4.62 | 119.69      | 126.34   |
| 3   | h1    | 103  | PSU  | C4-N3-C2  | -4.62 | 119.69      | 126.34   |
| 81  | A3    | 34   | PSU  | C4-N3-C2  | -4.61 | 119.69      | 126.34   |
| 81  | A3    | 2868 | PSU  | C4-N3-C2  | -4.61 | 119.69      | 126.34   |
| 81  | A3    | 717  | PSU  | C4-N3-C2  | -4.61 | 119.69      | 126.34   |
| 81  | A3    | 1685 | PSU  | C4-N3-C2  | -4.61 | 119.69      | 126.34   |
| 82  | B3    | 77   | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 81  | A3    | 2321 | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 3   | h1    | 1210 | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 3   | h1    | 961  | PSU  | C4-N3-C2  | -4.60 | 119.72      | 126.34   |
| 3   | h1    | 1217 | PSU  | C4-N3-C2  | -4.60 | 119.72      | 126.34   |
| 3   | h1    | 95   | PSU  | C4-N3-C2  | -4.59 | 119.72      | 126.34   |
| 3   | h1    | 1567 | PSU  | C4-N3-C2  | -4.59 | 119.72      | 126.34   |
| 81  | A3    | 2829 | PSU  | C4-N3-C2  | -4.59 | 119.72      | 126.34   |
| 81  | A3    | 42   | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 3   | h1    | 1184 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 3   | h1    | 1787 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 3   | h1    | 1535 | PSU  | C4-N3-C2  | -4.58 | 119.74      | 126.34   |
| 81  | A3    | 976  | PSU  | C4-N3-C2  | -4.58 | 119.74      | 126.34   |
| 81  | A3    | 1016 | PSU  | C4-N3-C2  | -4.58 | 119.74      | 126.34   |
| 81  | A3    | 2317 | PSU  | C4-N3-C2  | -4.58 | 119.74      | 126.34   |
| 81  | A3    | 1002 | PSU  | C4-N3-C2  | -4.58 | 119.74      | 126.34   |
| 3   | h1    | 392  | OMG  | C5-C4-N3  | -4.58 | 121.04      | 128.46   |
| 3   | h1    | 1293 | PSU  | C4-N3-C2  | -4.58 | 119.75      | 126.34   |
| 81  | A3    | 2435 | PSU  | C4-N3-C2  | -4.58 | 119.75      | 126.34   |
| 3   | h1    | 584  | PSU  | C4-N3-C2  | -4.58 | 119.75      | 126.34   |
| 3   | h1    | 1789 | MA6  | N9-C8-N7  | -4.57 | 107.66      | 113.91   |
| 81  | A3    | 1461 | OMG  | C5-C4-N3  | -4.57 | 121.04      | 128.46   |
| 81  | A3    | 2291 | OMG  | C5-C4-N3  | -4.57 | 121.05      | 128.46   |
| 3   | h1    | 1304 | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 81  | A3    | 2261 | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 3   | h1    | 763  | PSU  | C4-N3-C2  | -4.57 | 119.76      | 126.34   |
| 81  | A3    | 228  | PSU  | C4-N3-C2  | -4.57 | 119.76      | 126.34   |
| 81  | A3    | 1134 | PSU  | C4-N3-C2  | -4.57 | 119.76      | 126.34   |
| 81  | A3    | 150  | PSU  | C4-N3-C2  | -4.56 | 119.76      | 126.34   |
| 3   | h1    | 1190 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 1133 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 81  | A3    | 829  | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 3   | h1    | 603  | UY1  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 3   | h1    | 1178 | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 3   | h1    | 762  | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 81  | A3    | 2263 | PSU  | C4-N3-C2  | -4.55 | 119.79      | 126.34   |
| 3   | h1    | 258  | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 3   | h1    | 1106 | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 3   | h1    | 1308 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 81  | A3    | 2883 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 3   | h1    | 1524 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 3   | h1    | 1485 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 81  | A3    | 2267 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 3   | h1    | 1789 | MA6  | C1'-N9-C8 | -4.53 | 116.91      | 127.14   |
| 3   | h1    | 753  | PSU  | C4-N3-C2  | -4.53 | 119.82      | 126.34   |
| 81  | A3    | 2925 | OMG  | C5-C4-N3  | -4.53 | 121.12      | 128.46   |
| 3   | h1    | 809  | PSU  | C4-N3-C2  | -4.52 | 119.82      | 126.34   |
| 81  | A3    | 464  | PSU  | C4-N3-C2  | -4.52 | 119.82      | 126.34   |
| 81  | A3    | 786  | PSU  | C4-N3-C2  | -4.52 | 119.83      | 126.34   |
| 82  | B3    | 21   | PSU  | C4-N3-C2  | -4.52 | 119.83      | 126.34   |
| 81  | A3    | 2897 | PSU  | C4-N3-C2  | -4.52 | 119.83      | 126.34   |
| 3   | h1    | 605  | PSU  | C4-N3-C2  | -4.52 | 119.83      | 126.34   |
| 3   | h1    | 1002 | PSU  | C4-N3-C2  | -4.52 | 119.83      | 126.34   |
| 81  | A3    | 2194 | PSU  | C4-N3-C2  | -4.51 | 119.83      | 126.34   |
| 3   | h1    | 1027 | PSU  | C4-N3-C2  | -4.51 | 119.83      | 126.34   |
| 81  | A3    | 2419 | PSU  | C4-N3-C2  | -4.51 | 119.83      | 126.34   |
| 81  | A3    | 1857 | OMG  | C1'-N9-C4 | 4.51  | 139.89      | 126.50   |
| 81  | A3    | 296  | OMG  | C1'-N9-C4 | 4.50  | 139.87      | 126.50   |
| 3   | h1    | 950  | PSU  | C4-N3-C2  | -4.50 | 119.86      | 126.34   |
| 3   | h1    | 470  | PSU  | C4-N3-C2  | -4.50 | 119.86      | 126.34   |
| 3   | h1    | 607  | PSU  | C4-N3-C2  | -4.50 | 119.86      | 126.34   |
| 81  | A3    | 296  | OMG  | C5-C4-N3  | -4.49 | 121.17      | 128.46   |
| 81  | A3    | 2947 | PSU  | C4-N3-C2  | -4.49 | 119.86      | 126.34   |
| 3   | h1    | 1634 | PSU  | C4-N3-C2  | -4.49 | 119.87      | 126.34   |
| 81  | A3    | 684  | PSU  | C4-N3-C2  | -4.49 | 119.87      | 126.34   |
| 3   | h1    | 121  | PSU  | C4-N3-C2  | -4.49 | 119.87      | 126.34   |
| 81  | A3    | 2978 | PSU  | C4-N3-C2  | -4.49 | 119.87      | 126.34   |
| 3   | h1    | 417  | PSU  | C4-N3-C2  | -4.49 | 119.87      | 126.34   |
| 3   | h1    | 310  | PSU  | C4-N3-C2  | -4.49 | 119.88      | 126.34   |
| 81  | A3    | 1474 | PSU  | C4-N3-C2  | -4.48 | 119.88      | 126.34   |
| 82  | B3    | 96   | PSU  | C4-N3-C2  | -4.48 | 119.89      | 126.34   |
| 81  | A3    | 510  | PSU  | C4-N3-C2  | -4.47 | 119.89      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 902  | PSU  | C4-N3-C2  | -4.47 | 119.90      | 126.34   |
| 81  | A3    | 815  | OMG  | C5-C4-N3  | -4.47 | 121.22      | 128.46   |
| 81  | A3    | 2269 | PSU  | C4-N3-C2  | -4.47 | 119.91      | 126.34   |
| 3   | h1    | 1120 | PSU  | C4-N3-C2  | -4.46 | 119.91      | 126.34   |
| 81  | A3    | 277  | PSU  | C4-N3-C2  | -4.46 | 119.91      | 126.34   |
| 3   | h1    | 544  | A2M  | C4-N9-C1' | -4.46 | 115.97      | 126.59   |
| 81  | A3    | 2137 | PSU  | N1-C2-N3  | 4.46  | 120.18      | 115.13   |
| 3   | h1    | 1615 | PSU  | C4-N3-C2  | -4.46 | 119.92      | 126.34   |
| 81  | A3    | 2747 | PSU  | C4-N3-C2  | -4.44 | 119.94      | 126.34   |
| 81  | A3    | 2920 | OMG  | C5-C4-N3  | -4.44 | 121.25      | 128.46   |
| 3   | h1    | 451  | PSU  | C4-N3-C2  | -4.44 | 119.94      | 126.34   |
| 3   | h1    | 339  | PSU  | C4-N3-C2  | -4.44 | 119.95      | 126.34   |
| 3   | h1    | 1433 | OMG  | C5-C4-N3  | -4.42 | 121.28      | 128.46   |
| 81  | A3    | 656  | 1MA  | C5-C4-N3  | -4.42 | 120.66      | 127.26   |
| 81  | A3    | 1857 | OMG  | C5-C4-N3  | -4.41 | 121.30      | 128.46   |
| 3   | h1    | 306  | PSU  | C4-N3-C2  | -4.41 | 119.99      | 126.34   |
| 3   | h1    | 635  | PSU  | C4-N3-C2  | -4.41 | 119.99      | 126.34   |
| 3   | h1    | 606  | PSU  | C4-N3-C2  | -4.41 | 119.99      | 126.34   |
| 81  | A3    | 2139 | PSU  | C4-N3-C2  | -4.41 | 119.99      | 126.34   |
| 81  | A3    | 2949 | A2M  | N9-C8-N7  | -4.40 | 107.89      | 113.91   |
| 81  | A3    | 2796 | OMG  | C5-C4-N3  | -4.40 | 121.32      | 128.46   |
| 81  | A3    | 2126 | OMG  | C1'-N9-C4 | 4.40  | 139.57      | 126.50   |
| 81  | A3    | 660  | A2M  | N9-C8-N7  | -4.39 | 107.90      | 113.91   |
| 81  | A3    | 1482 | PSU  | C4-N3-C2  | -4.39 | 120.01      | 126.34   |
| 3   | h1    | 362  | PSU  | C4-N3-C2  | -4.37 | 120.04      | 126.34   |
| 81  | A3    | 311  | PSU  | C4-N3-C2  | -4.36 | 120.06      | 126.34   |
| 81  | A3    | 815  | OMG  | C2-N3-C4  | 4.36  | 120.06      | 112.30   |
| 81  | A3    | 2804 | A2M  | N9-C8-N7  | -4.33 | 107.99      | 113.91   |
| 81  | A3    | 2126 | OMG  | C5-C4-N3  | -4.33 | 121.44      | 128.46   |
| 81  | A3    | 2818 | OMG  | C1'-N9-C4 | 4.32  | 139.35      | 126.50   |
| 81  | A3    | 2794 | OMG  | C1'-N9-C4 | 4.32  | 139.34      | 126.50   |
| 3   | h1    | 622  | A2M  | N9-C8-N7  | -4.32 | 108.00      | 113.91   |
| 82  | B3    | 46   | A2M  | N9-C8-N7  | -4.32 | 108.00      | 113.91   |
| 81  | A3    | 918  | OMG  | C2-N3-C4  | 4.31  | 119.99      | 112.30   |
| 81  | A3    | 2291 | OMG  | C2-N3-C4  | 4.31  | 119.98      | 112.30   |
| 81  | A3    | 2259 | A2M  | N9-C8-N7  | -4.31 | 108.01      | 113.91   |
| 81  | A3    | 2412 | OMG  | C5-C4-N3  | -4.31 | 121.47      | 128.46   |
| 3   | h1    | 392  | OMG  | C2-N3-C4  | 4.31  | 119.97      | 112.30   |
| 82  | B3    | 78   | OMG  | C2-N3-C4  | 4.31  | 119.97      | 112.30   |
| 3   | h1    | 598  | OMG  | C2-N3-C4  | 4.30  | 119.97      | 112.30   |
| 81  | A3    | 399  | OMG  | C2-N3-C4  | 4.30  | 119.96      | 112.30   |
| 81  | A3    | 2412 | OMG  | C2-N3-C4  | 4.29  | 119.95      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 2394 | OMG  | C2-N3-C4  | 4.29  | 119.94      | 112.30   |
| 3   | h1    | 1274 | OMG  | C2-N3-C4  | 4.29  | 119.94      | 112.30   |
| 81  | A3    | 1461 | OMG  | C2-N3-C4  | 4.28  | 119.93      | 112.30   |
| 81  | A3    | 296  | OMG  | C2-N3-C4  | 4.28  | 119.92      | 112.30   |
| 81  | A3    | 2926 | PSU  | N1-C2-N3  | 4.28  | 119.97      | 115.13   |
| 3   | h1    | 246  | OMG  | C2-N3-C4  | 4.27  | 119.92      | 112.30   |
| 81  | A3    | 2435 | PSU  | N1-C2-N3  | 4.27  | 119.97      | 115.13   |
| 81  | A3    | 2284 | A2M  | N9-C8-N7  | -4.27 | 108.07      | 113.91   |
| 81  | A3    | 2126 | OMG  | C2-N3-C4  | 4.27  | 119.91      | 112.30   |
| 81  | A3    | 2127 | OMG  | C2-N3-C4  | 4.27  | 119.91      | 112.30   |
| 81  | A3    | 3113 | PSU  | C4-N3-C2  | -4.27 | 120.18      | 126.34   |
| 81  | A3    | 2398 | OMG  | C2-N3-C4  | 4.27  | 119.91      | 112.30   |
| 81  | A3    | 2654 | OMG  | C2-N3-C4  | 4.26  | 119.89      | 112.30   |
| 81  | A3    | 2239 | OMG  | C2-N3-C4  | 4.25  | 119.88      | 112.30   |
| 81  | A3    | 2818 | OMG  | C2-N3-C4  | 4.25  | 119.87      | 112.30   |
| 81  | A3    | 2324 | A2M  | N9-C8-N7  | -4.24 | 108.11      | 113.91   |
| 81  | A3    | 2317 | PSU  | N1-C2-N3  | 4.24  | 119.94      | 115.13   |
| 81  | A3    | 2920 | OMG  | C2-N3-C4  | 4.24  | 119.85      | 112.30   |
| 3   | h1    | 1771 | 6MZ  | C4-C5-C6  | 4.24  | 120.09      | 116.81   |
| 81  | A3    | 2868 | PSU  | N1-C2-N3  | 4.24  | 119.93      | 115.13   |
| 81  | A3    | 2214 | PSU  | N1-C2-N3  | 4.24  | 119.93      | 115.13   |
| 81  | A3    | 1134 | PSU  | N1-C2-N3  | 4.23  | 119.93      | 115.13   |
| 81  | A3    | 2925 | OMG  | C2-N3-C4  | 4.23  | 119.84      | 112.30   |
| 3   | h1    | 1790 | MA6  | C1'-N9-C8 | -4.23 | 117.59      | 127.14   |
| 3   | h1    | 544  | A2M  | C1'-N9-C8 | 4.23  | 136.68      | 127.14   |
| 81  | A3    | 2958 | PSU  | N1-C2-N3  | 4.23  | 119.92      | 115.13   |
| 81  | A3    | 2796 | OMG  | C2-N3-C4  | 4.23  | 119.83      | 112.30   |
| 81  | A3    | 2829 | PSU  | N1-C2-N3  | 4.22  | 119.92      | 115.13   |
| 81  | A3    | 1857 | OMG  | C2-N3-C4  | 4.22  | 119.82      | 112.30   |
| 3   | h1    | 1329 | A2M  | N9-C8-N7  | -4.22 | 108.14      | 113.91   |
| 81  | A3    | 829  | PSU  | N1-C2-N3  | 4.21  | 119.90      | 115.13   |
| 3   | h1    | 424  | A2M  | N9-C8-N7  | -4.21 | 108.15      | 113.91   |
| 81  | A3    | 1056 | PSU  | N1-C2-N3  | 4.21  | 119.90      | 115.13   |
| 81  | A3    | 2622 | OMG  | C2-N3-C4  | 4.21  | 119.80      | 112.30   |
| 3   | h1    | 1210 | PSU  | N1-C2-N3  | 4.21  | 119.90      | 115.13   |
| 81  | A3    | 277  | PSU  | N1-C2-N3  | 4.21  | 119.89      | 115.13   |
| 81  | A3    | 1685 | PSU  | N1-C2-N3  | 4.20  | 119.89      | 115.13   |
| 81  | A3    | 2794 | OMG  | C5-C4-N3  | -4.20 | 121.64      | 128.46   |
| 81  | A3    | 2857 | PSU  | N1-C2-N3  | 4.20  | 119.89      | 115.13   |
| 81  | A3    | 2914 | A2M  | N9-C8-N7  | -4.20 | 108.17      | 113.91   |
| 81  | A3    | 2653 | UY1  | N1-C2-N3  | 4.20  | 119.89      | 115.13   |
| 81  | A3    | 970  | PSU  | N1-C2-N3  | 4.19  | 119.88      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 81  | A3    | 966  | PSU  | C4-N3-C2 | -4.19 | 120.30      | 126.34   |
| 81  | A3    | 1016 | PSU  | N1-C2-N3 | 4.19  | 119.88      | 115.13   |
| 81  | A3    | 2257 | PSU  | N1-C2-N3 | 4.19  | 119.88      | 115.13   |
| 81  | A3    | 2329 | A2M  | N9-C8-N7 | -4.19 | 108.19      | 113.91   |
| 81  | A3    | 895  | PSU  | C4-N3-C2 | -4.18 | 120.31      | 126.34   |
| 3   | h1    | 162  | A2M  | N9-C8-N7 | -4.18 | 108.19      | 113.91   |
| 81  | A3    | 717  | PSU  | N1-C2-N3 | 4.18  | 119.87      | 115.13   |
| 81  | A3    | 1002 | PSU  | N1-C2-N3 | 4.18  | 119.87      | 115.13   |
| 81  | A3    | 228  | PSU  | N1-C2-N3 | 4.18  | 119.86      | 115.13   |
| 3   | h1    | 1787 | PSU  | N1-C2-N3 | 4.17  | 119.86      | 115.13   |
| 3   | h1    | 1579 | A2M  | N9-C8-N7 | -4.17 | 108.20      | 113.91   |
| 3   | h1    | 603  | UY1  | N1-C2-N3 | 4.17  | 119.86      | 115.13   |
| 81  | A3    | 1135 | PSU  | N1-C2-N3 | 4.17  | 119.86      | 115.13   |
| 81  | A3    | 34   | PSU  | N1-C2-N3 | 4.17  | 119.85      | 115.13   |
| 81  | A3    | 1064 | PSU  | N1-C2-N3 | 4.17  | 119.85      | 115.13   |
| 81  | A3    | 827  | A2M  | N9-C8-N7 | -4.16 | 108.22      | 113.91   |
| 81  | A3    | 946  | A2M  | N9-C8-N7 | -4.16 | 108.22      | 113.91   |
| 81  | A3    | 2129 | A2M  | N9-C8-N7 | -4.16 | 108.22      | 113.91   |
| 3   | h1    | 103  | PSU  | N1-C2-N3 | 4.16  | 119.84      | 115.13   |
| 82  | B3    | 77   | PSU  | N1-C2-N3 | 4.16  | 119.84      | 115.13   |
| 3   | h1    | 961  | PSU  | N1-C2-N3 | 4.15  | 119.84      | 115.13   |
| 81  | A3    | 150  | PSU  | N1-C2-N3 | 4.15  | 119.84      | 115.13   |
| 81  | A3    | 510  | PSU  | N1-C2-N3 | 4.15  | 119.84      | 115.13   |
| 81  | A3    | 2883 | PSU  | N1-C2-N3 | 4.15  | 119.83      | 115.13   |
| 3   | h1    | 1184 | PSU  | N1-C2-N3 | 4.15  | 119.83      | 115.13   |
| 81  | A3    | 2818 | OMG  | C5-C4-N3 | -4.15 | 121.73      | 128.46   |
| 81  | A3    | 2321 | PSU  | N1-C2-N3 | 4.15  | 119.83      | 115.13   |
| 3   | h1    | 1304 | PSU  | N1-C2-N3 | 4.14  | 119.83      | 115.13   |
| 81  | A3    | 2261 | PSU  | N1-C2-N3 | 4.14  | 119.83      | 115.13   |
| 3   | h1    | 1433 | OMG  | C2-N3-C4 | 4.14  | 119.67      | 112.30   |
| 3   | h1    | 1790 | MA6  | C5-C6-N6 | 4.14  | 132.51      | 125.30   |
| 3   | h1    | 28   | A2M  | N9-C8-N7 | -4.14 | 108.25      | 113.91   |
| 3   | h1    | 1194 | B8N  | C4-N3-C2 | -4.14 | 120.23      | 125.46   |
| 3   | h1    | 1190 | PSU  | N1-C2-N3 | 4.13  | 119.81      | 115.13   |
| 81  | A3    | 976  | PSU  | N1-C2-N3 | 4.13  | 119.81      | 115.13   |
| 3   | h1    | 607  | PSU  | N1-C2-N3 | 4.12  | 119.80      | 115.13   |
| 81  | A3    | 2794 | OMG  | C2-N3-C4 | 4.12  | 119.64      | 112.30   |
| 81  | A3    | 2978 | PSU  | N1-C2-N3 | 4.12  | 119.80      | 115.13   |
| 3   | h1    | 451  | PSU  | N1-C2-N3 | 4.12  | 119.80      | 115.13   |
| 3   | h1    | 1217 | PSU  | N1-C2-N3 | 4.12  | 119.80      | 115.13   |
| 81  | A3    | 2263 | PSU  | N1-C2-N3 | 4.11  | 119.79      | 115.13   |
| 3   | h1    | 1485 | PSU  | N1-C2-N3 | 4.11  | 119.79      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 2394 | OMG  | C1'-N9-C4 | 4.11  | 138.71      | 126.50   |
| 81  | A3    | 1460 | A2M  | N9-C8-N7  | -4.11 | 108.30      | 113.91   |
| 3   | h1    | 1002 | PSU  | N1-C2-N3  | 4.11  | 119.78      | 115.13   |
| 81  | A3    | 2267 | PSU  | N1-C2-N3  | 4.11  | 119.78      | 115.13   |
| 3   | h1    | 470  | PSU  | N1-C2-N3  | 4.11  | 119.78      | 115.13   |
| 3   | h1    | 605  | PSU  | N1-C2-N3  | 4.11  | 119.78      | 115.13   |
| 3   | h1    | 1178 | PSU  | N1-C2-N3  | 4.11  | 119.78      | 115.13   |
| 3   | h1    | 1567 | PSU  | N1-C2-N3  | 4.10  | 119.78      | 115.13   |
| 3   | h1    | 258  | PSU  | N1-C2-N3  | 4.10  | 119.78      | 115.13   |
| 3   | h1    | 1293 | PSU  | N1-C2-N3  | 4.10  | 119.77      | 115.13   |
| 3   | h1    | 1789 | MA6  | C5-C6-N6  | 4.10  | 132.44      | 125.30   |
| 3   | h1    | 1106 | PSU  | N1-C2-N3  | 4.10  | 119.77      | 115.13   |
| 81  | A3    | 2139 | PSU  | N1-C2-N3  | 4.09  | 119.77      | 115.13   |
| 81  | A3    | 42   | PSU  | N1-C2-N3  | 4.09  | 119.77      | 115.13   |
| 3   | h1    | 362  | PSU  | N1-C2-N3  | 4.09  | 119.76      | 115.13   |
| 81  | A3    | 2947 | PSU  | N1-C2-N3  | 4.09  | 119.76      | 115.13   |
| 3   | h1    | 809  | PSU  | N1-C2-N3  | 4.09  | 119.76      | 115.13   |
| 81  | A3    | 1133 | PSU  | N1-C2-N3  | 4.09  | 119.76      | 115.13   |
| 3   | h1    | 763  | PSU  | N1-C2-N3  | 4.09  | 119.76      | 115.13   |
| 81  | A3    | 2398 | OMG  | C5-C4-N3  | -4.09 | 121.83      | 128.46   |
| 81  | A3    | 2394 | OMG  | C5-C4-N3  | -4.08 | 121.83      | 128.46   |
| 81  | A3    | 817  | A2M  | N9-C8-N7  | -4.08 | 108.33      | 113.91   |
| 81  | A3    | 2194 | PSU  | N1-C2-N3  | 4.08  | 119.76      | 115.13   |
| 3   | h1    | 440  | A2M  | N9-C8-N7  | -4.08 | 108.33      | 113.91   |
| 81  | A3    | 1474 | PSU  | N1-C2-N3  | 4.08  | 119.75      | 115.13   |
| 3   | h1    | 468  | A2M  | N9-C8-N7  | -4.08 | 108.33      | 113.91   |
| 81  | A3    | 2897 | PSU  | N1-C2-N3  | 4.08  | 119.75      | 115.13   |
| 3   | h1    | 1634 | PSU  | N1-C2-N3  | 4.08  | 119.75      | 115.13   |
| 3   | h1    | 1758 | A2M  | N9-C8-N7  | -4.08 | 108.34      | 113.91   |
| 3   | h1    | 950  | PSU  | N1-C2-N3  | 4.08  | 119.75      | 115.13   |
| 81  | A3    | 902  | PSU  | N1-C2-N3  | 4.08  | 119.75      | 115.13   |
| 81  | A3    | 2269 | PSU  | N1-C2-N3  | 4.08  | 119.75      | 115.13   |
| 81  | A3    | 2747 | PSU  | N1-C2-N3  | 4.07  | 119.74      | 115.13   |
| 81  | A3    | 2419 | PSU  | N1-C2-N3  | 4.07  | 119.74      | 115.13   |
| 82  | B3    | 21   | PSU  | N1-C2-N3  | 4.07  | 119.74      | 115.13   |
| 81  | A3    | 1144 | A2M  | N9-C8-N7  | -4.06 | 108.36      | 113.91   |
| 81  | A3    | 2127 | OMG  | C5-C4-N3  | -4.06 | 121.87      | 128.46   |
| 81  | A3    | 2643 | A2M  | N9-C8-N7  | -4.06 | 108.36      | 113.91   |
| 3   | h1    | 1308 | PSU  | N1-C2-N3  | 4.06  | 119.73      | 115.13   |
| 3   | h1    | 95   | PSU  | N1-C2-N3  | 4.06  | 119.72      | 115.13   |
| 3   | h1    | 1524 | PSU  | N1-C2-N3  | 4.06  | 119.72      | 115.13   |
| 3   | h1    | 753  | PSU  | N1-C2-N3  | 4.05  | 119.72      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | h1    | 635  | PSU  | N1-C2-N3  | 4.05  | 119.72      | 115.13   |
| 3   | h1    | 121  | PSU  | N1-C2-N3  | 4.05  | 119.71      | 115.13   |
| 3   | h1    | 310  | PSU  | N1-C2-N3  | 4.05  | 119.71      | 115.13   |
| 3   | h1    | 1615 | PSU  | N1-C2-N3  | 4.04  | 119.71      | 115.13   |
| 3   | h1    | 1027 | PSU  | N1-C2-N3  | 4.04  | 119.71      | 115.13   |
| 3   | h1    | 762  | PSU  | N1-C2-N3  | 4.04  | 119.71      | 115.13   |
| 81  | A3    | 684  | PSU  | N1-C2-N3  | 4.04  | 119.71      | 115.13   |
| 3   | h1    | 1771 | 6MZ  | N9-C8-N7  | -4.04 | 108.39      | 113.91   |
| 3   | h1    | 417  | PSU  | N1-C2-N3  | 4.03  | 119.70      | 115.13   |
| 3   | h1    | 606  | PSU  | N1-C2-N3  | 4.02  | 119.68      | 115.13   |
| 3   | h1    | 1535 | PSU  | N1-C2-N3  | 4.01  | 119.68      | 115.13   |
| 81  | A3    | 464  | PSU  | N1-C2-N3  | 4.01  | 119.67      | 115.13   |
| 3   | h1    | 584  | PSU  | N1-C2-N3  | 4.01  | 119.67      | 115.13   |
| 3   | h1    | 977  | A2M  | N9-C8-N7  | -4.01 | 108.43      | 113.91   |
| 81  | A3    | 3113 | PSU  | N1-C2-N3  | 4.00  | 119.66      | 115.13   |
| 81  | A3    | 369  | A2M  | N9-C8-N7  | -3.99 | 108.45      | 113.91   |
| 81  | A3    | 1378 | A2M  | N9-C8-N7  | -3.99 | 108.45      | 113.91   |
| 3   | h1    | 800  | A2M  | N9-C8-N7  | -3.99 | 108.46      | 113.91   |
| 3   | h1    | 339  | PSU  | N1-C2-N3  | 3.98  | 119.64      | 115.13   |
| 81  | A3    | 895  | PSU  | N1-C2-N3  | 3.98  | 119.64      | 115.13   |
| 3   | h1    | 1120 | PSU  | N1-C2-N3  | 3.97  | 119.63      | 115.13   |
| 3   | h1    | 306  | PSU  | N1-C2-N3  | 3.96  | 119.62      | 115.13   |
| 81  | A3    | 2398 | OMG  | C1'-N9-C4 | 3.96  | 138.25      | 126.50   |
| 81  | A3    | 1482 | PSU  | N1-C2-N3  | 3.94  | 119.59      | 115.13   |
| 82  | B3    | 96   | PSU  | N1-C2-N3  | 3.94  | 119.59      | 115.13   |
| 81  | A3    | 311  | PSU  | N1-C2-N3  | 3.94  | 119.59      | 115.13   |
| 81  | A3    | 966  | PSU  | N1-C2-N3  | 3.91  | 119.56      | 115.13   |
| 81  | A3    | 886  | A2M  | N9-C8-N7  | -3.91 | 108.57      | 113.91   |
| 81  | A3    | 786  | PSU  | N1-C2-N3  | 3.88  | 119.53      | 115.13   |
| 81  | A3    | 2127 | OMG  | C1'-N9-C4 | 3.86  | 137.98      | 126.50   |
| 81  | A3    | 675  | OMU  | N3-C2-N1  | 3.85  | 120.00      | 114.89   |
| 81  | A3    | 1068 | OMU  | N3-C2-N1  | 3.84  | 119.99      | 114.89   |
| 81  | A3    | 804  | OMU  | N3-C2-N1  | 3.81  | 119.95      | 114.89   |
| 81  | A3    | 1894 | OMU  | N3-C2-N1  | 3.80  | 119.93      | 114.89   |
| 81  | A3    | 2924 | OMU  | N3-C2-N1  | 3.80  | 119.93      | 114.89   |
| 81  | A3    | 2738 | OMU  | N3-C2-N1  | 3.79  | 119.93      | 114.89   |
| 81  | A3    | 2350 | OMU  | N3-C2-N1  | 3.79  | 119.92      | 114.89   |
| 81  | A3    | 2223 | A2M  | N9-C8-N7  | -3.79 | 108.73      | 113.91   |
| 3   | h1    | 581  | OMU  | N3-C2-N1  | 3.78  | 119.91      | 114.89   |
| 81  | A3    | 2886 | OMU  | N3-C2-N1  | 3.78  | 119.91      | 114.89   |
| 3   | h1    | 1771 | 6MZ  | C4-N9-C1' | -3.78 | 117.60      | 126.59   |
| 3   | h1    | 544  | A2M  | N9-C8-N7  | -3.77 | 108.76      | 113.91   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | h1    | 1383 | OMU  | N3-C2-N1  | 3.75  | 119.87      | 114.89   |
| 81  | A3    | 2127 | OMG  | N9-C8-N7  | -3.75 | 106.32      | 113.39   |
| 3   | h1    | 886  | OMU  | N3-C2-N1  | 3.75  | 119.86      | 114.89   |
| 81  | A3    | 2398 | OMG  | N9-C8-N7  | -3.75 | 106.34      | 113.39   |
| 81  | A3    | 3304 | OMU  | N3-C2-N1  | 3.73  | 119.84      | 114.89   |
| 81  | A3    | 2424 | OMU  | N3-C2-N1  | 3.73  | 119.84      | 114.89   |
| 81  | A3    | 2654 | OMG  | C5-C4-N3  | -3.73 | 122.42      | 128.46   |
| 3   | h1    | 544  | A2M  | C2-N3-C4  | 3.72  | 120.54      | 111.75   |
| 3   | h1    | 123  | OMU  | N3-C2-N1  | 3.72  | 119.83      | 114.89   |
| 81  | A3    | 2654 | OMG  | N9-C8-N7  | -3.71 | 106.40      | 113.39   |
| 3   | h1    | 1012 | OMU  | N3-C2-N1  | 3.71  | 119.82      | 114.89   |
| 3   | h1    | 1272 | OMU  | N3-C2-N1  | 3.71  | 119.82      | 114.89   |
| 3   | h1    | 544  | A2M  | N3-C4-N9  | 3.71  | 133.20      | 127.08   |
| 81  | A3    | 48   | OMU  | N3-C2-N1  | 3.71  | 119.81      | 114.89   |
| 81  | A3    | 144  | OMU  | N3-C2-N1  | 3.70  | 119.81      | 114.89   |
| 3   | h1    | 1234 | OMU  | N3-C2-N1  | 3.70  | 119.80      | 114.89   |
| 81  | A3    | 787  | OMU  | N3-C2-N1  | 3.69  | 119.79      | 114.89   |
| 3   | h1    | 373  | OMU  | N3-C2-N1  | 3.68  | 119.78      | 114.89   |
| 81  | A3    | 817  | A2M  | C2-N3-C4  | 3.68  | 120.44      | 111.75   |
| 81  | A3    | 1537 | OMU  | N3-C2-N1  | 3.68  | 119.77      | 114.89   |
| 81  | A3    | 656  | 1MA  | C2-N3-C4  | 3.67  | 119.63      | 112.41   |
| 81  | A3    | 2394 | OMG  | N9-C8-N7  | -3.65 | 106.52      | 113.39   |
| 81  | A3    | 2654 | OMG  | C1'-N9-C4 | 3.64  | 137.32      | 126.50   |
| 3   | h1    | 800  | A2M  | C2-N3-C4  | 3.64  | 120.34      | 111.75   |
| 3   | h1    | 1789 | MA6  | C2-N1-C6  | 3.64  | 120.34      | 111.75   |
| 81  | A3    | 2794 | OMG  | N9-C8-N7  | -3.63 | 106.56      | 113.39   |
| 81  | A3    | 44   | OMU  | N3-C2-N1  | 3.62  | 119.70      | 114.89   |
| 81  | A3    | 2732 | OMU  | N3-C2-N1  | 3.62  | 119.69      | 114.89   |
| 3   | h1    | 1447 | OMU  | N3-C2-N1  | 3.60  | 119.67      | 114.89   |
| 81  | A3    | 2720 | OMU  | N3-C2-N1  | 3.60  | 119.66      | 114.89   |
| 3   | h1    | 1790 | MA6  | C2-N1-C6  | 3.59  | 120.24      | 111.75   |
| 81  | A3    | 296  | OMG  | N9-C8-N7  | -3.59 | 106.62      | 113.39   |
| 81  | A3    | 2317 | PSU  | C6-C5-C4  | 3.59  | 120.71      | 118.20   |
| 81  | A3    | 2818 | OMG  | N9-C8-N7  | -3.59 | 106.63      | 113.39   |
| 81  | A3    | 946  | A2M  | C2-N3-C4  | 3.58  | 120.20      | 111.75   |
| 81  | A3    | 1378 | A2M  | C2-N3-C4  | 3.58  | 120.20      | 111.75   |
| 3   | h1    | 614  | OMU  | N3-C2-N1  | 3.57  | 119.64      | 114.89   |
| 81  | A3    | 3289 | OMU  | N3-C2-N1  | 3.57  | 119.63      | 114.89   |
| 81  | A3    | 2949 | A2M  | C2-N3-C4  | 3.57  | 120.18      | 111.75   |
| 3   | h1    | 440  | A2M  | C2-N3-C4  | 3.57  | 120.18      | 111.75   |
| 81  | A3    | 2413 | OMU  | N3-C2-N1  | 3.57  | 119.63      | 114.89   |
| 81  | A3    | 2259 | A2M  | C2-N3-C4  | 3.57  | 120.17      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 81  | A3    | 2126 | OMG  | N9-C8-N7 | -3.56 | 106.69      | 113.39   |
| 81  | A3    | 2412 | OMG  | N9-C8-N7 | -3.56 | 106.69      | 113.39   |
| 81  | A3    | 2914 | A2M  | C2-N3-C4 | 3.56  | 120.16      | 111.75   |
| 81  | A3    | 827  | A2M  | C2-N3-C4 | 3.56  | 120.16      | 111.75   |
| 3   | h1    | 1771 | 6MZ  | C9-N6-C6 | -3.55 | 119.81      | 122.87   |
| 81  | A3    | 1857 | OMG  | N9-C8-N7 | -3.55 | 106.70      | 113.39   |
| 3   | h1    | 424  | A2M  | C2-N3-C4 | 3.55  | 120.14      | 111.75   |
| 3   | h1    | 1758 | A2M  | C2-N3-C4 | 3.55  | 120.14      | 111.75   |
| 3   | h1    | 392  | OMG  | N9-C8-N7 | -3.55 | 106.70      | 113.39   |
| 82  | B3    | 46   | A2M  | C2-N3-C4 | 3.55  | 120.14      | 111.75   |
| 81  | A3    | 2925 | OMG  | N9-C8-N7 | -3.55 | 106.71      | 113.39   |
| 3   | h1    | 1579 | A2M  | C2-N3-C4 | 3.55  | 120.13      | 111.75   |
| 81  | A3    | 2804 | A2M  | C2-N3-C4 | 3.54  | 120.12      | 111.75   |
| 3   | h1    | 622  | A2M  | C2-N3-C4 | 3.54  | 120.11      | 111.75   |
| 3   | h1    | 977  | A2M  | C2-N3-C4 | 3.54  | 120.11      | 111.75   |
| 81  | A3    | 886  | A2M  | C2-N3-C4 | 3.54  | 120.10      | 111.75   |
| 81  | A3    | 815  | OMG  | N9-C8-N7 | -3.53 | 106.73      | 113.39   |
| 3   | h1    | 1329 | A2M  | C2-N3-C4 | 3.53  | 120.10      | 111.75   |
| 3   | h1    | 162  | A2M  | C2-N3-C4 | 3.53  | 120.09      | 111.75   |
| 81  | A3    | 660  | A2M  | C2-N3-C4 | 3.53  | 120.08      | 111.75   |
| 3   | h1    | 1790 | MA6  | C2-N3-C4 | 3.52  | 120.08      | 111.75   |
| 3   | h1    | 1771 | 6MZ  | C2-N3-C4 | 3.52  | 120.08      | 111.75   |
| 81  | A3    | 2223 | A2M  | C2-N3-C4 | 3.52  | 120.08      | 111.75   |
| 3   | h1    | 468  | A2M  | C2-N3-C4 | 3.52  | 120.07      | 111.75   |
| 81  | A3    | 2291 | OMG  | N9-C8-N7 | -3.52 | 106.76      | 113.39   |
| 3   | h1    | 28   | A2M  | C2-N3-C4 | 3.52  | 120.06      | 111.75   |
| 81  | A3    | 2129 | A2M  | C2-N3-C4 | 3.52  | 120.06      | 111.75   |
| 3   | h1    | 598  | OMG  | N9-C8-N7 | -3.52 | 106.77      | 113.39   |
| 81  | A3    | 2329 | A2M  | C2-N3-C4 | 3.51  | 120.05      | 111.75   |
| 81  | A3    | 2643 | A2M  | C2-N3-C4 | 3.51  | 120.03      | 111.75   |
| 81  | A3    | 369  | A2M  | C2-N3-C4 | 3.50  | 120.03      | 111.75   |
| 81  | A3    | 1460 | A2M  | C2-N3-C4 | 3.50  | 120.03      | 111.75   |
| 81  | A3    | 2284 | A2M  | C2-N3-C4 | 3.50  | 120.02      | 111.75   |
| 81  | A3    | 656  | 1MA  | N9-C8-N7 | -3.50 | 106.80      | 113.39   |
| 81  | A3    | 2622 | OMG  | N9-C8-N7 | -3.50 | 106.80      | 113.39   |
| 81  | A3    | 1378 | A2M  | N3-C4-N9 | 3.50  | 132.84      | 127.08   |
| 3   | h1    | 1274 | OMG  | N9-C8-N7 | -3.49 | 106.81      | 113.39   |
| 81  | A3    | 2920 | OMG  | N9-C8-N7 | -3.49 | 106.83      | 113.39   |
| 81  | A3    | 2324 | A2M  | C2-N3-C4 | 3.48  | 119.96      | 111.75   |
| 81  | A3    | 817  | A2M  | N3-C4-N9 | 3.47  | 132.81      | 127.08   |
| 81  | A3    | 2796 | OMG  | N9-C8-N7 | -3.47 | 106.85      | 113.39   |
| 3   | h1    | 1789 | MA6  | C4-C5-C6 | 3.47  | 119.76      | 115.88   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | h1    | 1790 | MA6  | C4-C5-C6    | 3.47  | 119.76      | 115.88   |
| 81  | A3    | 1461 | OMG  | N9-C8-N7    | -3.46 | 106.87      | 113.39   |
| 81  | A3    | 2239 | OMG  | N9-C8-N7    | -3.44 | 106.91      | 113.39   |
| 3   | h1    | 1771 | 6MZ  | N3-C4-N9    | 3.44  | 132.74      | 127.08   |
| 3   | h1    | 1789 | MA6  | C2-N3-C4    | 3.43  | 119.85      | 111.75   |
| 3   | h1    | 246  | OMG  | N9-C8-N7    | -3.43 | 106.93      | 113.39   |
| 82  | B3    | 78   | OMG  | N9-C8-N7    | -3.43 | 106.94      | 113.39   |
| 3   | h1    | 1790 | MA6  | C5-N7-C8    | 3.42  | 108.37      | 103.51   |
| 3   | h1    | 544  | A2M  | C4'-O4'-C1' | -3.41 | 101.94      | 109.47   |
| 3   | h1    | 1758 | A2M  | N3-C4-N9    | 3.41  | 132.71      | 127.08   |
| 81  | A3    | 1894 | OMU  | C5-C4-N3    | 3.41  | 119.94      | 114.84   |
| 81  | A3    | 2949 | A2M  | N3-C4-N9    | 3.41  | 132.69      | 127.08   |
| 81  | A3    | 1144 | A2M  | C2-N3-C4    | 3.40  | 119.79      | 111.75   |
| 3   | h1    | 1433 | OMG  | N9-C8-N7    | -3.38 | 107.03      | 113.39   |
| 81  | A3    | 2281 | 5MC  | C5-C6-N1    | -3.37 | 119.87      | 123.34   |
| 81  | A3    | 48   | OMU  | C5-C4-N3    | 3.37  | 119.88      | 114.84   |
| 81  | A3    | 2643 | A2M  | N3-C4-N9    | 3.37  | 132.64      | 127.08   |
| 3   | h1    | 1789 | MA6  | C4-N9-C1'   | 3.36  | 134.60      | 126.59   |
| 3   | h1    | 977  | A2M  | N3-C4-N9    | 3.36  | 132.62      | 127.08   |
| 3   | h1    | 800  | A2M  | N3-C4-N9    | 3.36  | 132.62      | 127.08   |
| 81  | A3    | 399  | OMG  | N9-C8-N7    | -3.35 | 107.07      | 113.39   |
| 81  | A3    | 2424 | OMU  | C5-C4-N3    | 3.35  | 119.85      | 114.84   |
| 81  | A3    | 2223 | A2M  | N3-C4-N9    | 3.34  | 132.59      | 127.08   |
| 81  | A3    | 34   | PSU  | C6-C5-C4    | 3.33  | 120.53      | 118.20   |
| 81  | A3    | 2924 | OMU  | C5-C4-N3    | 3.33  | 119.82      | 114.84   |
| 3   | h1    | 373  | OMU  | C5-C4-N3    | 3.33  | 119.82      | 114.84   |
| 81  | A3    | 918  | OMG  | N9-C8-N7    | -3.33 | 107.13      | 113.39   |
| 3   | h1    | 1234 | OMU  | C5-C4-N3    | 3.32  | 119.81      | 114.84   |
| 81  | A3    | 829  | PSU  | C6-C5-C4    | 3.32  | 120.52      | 118.20   |
| 81  | A3    | 886  | A2M  | N3-C4-N9    | 3.32  | 132.56      | 127.08   |
| 3   | h1    | 614  | OMU  | C5-C4-N3    | 3.32  | 119.80      | 114.84   |
| 81  | A3    | 1068 | OMU  | C5-C4-N3    | 3.32  | 119.80      | 114.84   |
| 81  | A3    | 144  | OMU  | C5-C4-N3    | 3.31  | 119.80      | 114.84   |
| 3   | h1    | 886  | OMU  | C5-C4-N3    | 3.31  | 119.79      | 114.84   |
| 81  | A3    | 1537 | OMU  | C5-C4-N3    | 3.31  | 119.79      | 114.84   |
| 81  | A3    | 2413 | OMU  | C5-C4-N3    | 3.31  | 119.79      | 114.84   |
| 3   | h1    | 1272 | OMU  | C5-C4-N3    | 3.31  | 119.78      | 114.84   |
| 81  | A3    | 2829 | PSU  | C6-C5-C4    | 3.30  | 120.51      | 118.20   |
| 3   | h1    | 1789 | MA6  | C5-N7-C8    | 3.30  | 108.20      | 103.51   |
| 3   | h1    | 1383 | OMU  | C5-C4-N3    | 3.30  | 119.78      | 114.84   |
| 81  | A3    | 2653 | UY1  | C6-C5-C4    | 3.30  | 120.51      | 118.20   |
| 81  | A3    | 2949 | A2M  | C5-N7-C8    | 3.30  | 108.19      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|------|-------------|----------|
| 3   | h1    | 1012 | OMU  | C5-C4-N3  | 3.30 | 119.77      | 114.84   |
| 81  | A3    | 2738 | OMU  | C5-C4-N3  | 3.29 | 119.77      | 114.84   |
| 81  | A3    | 510  | PSU  | C6-C5-C4  | 3.29 | 120.50      | 118.20   |
| 81  | A3    | 2435 | PSU  | C6-C5-C4  | 3.28 | 120.49      | 118.20   |
| 81  | A3    | 2350 | OMU  | C5-C4-N3  | 3.28 | 119.75      | 114.84   |
| 3   | h1    | 581  | OMU  | C5-C4-N3  | 3.28 | 119.75      | 114.84   |
| 81  | A3    | 1134 | PSU  | C6-C5-C4  | 3.28 | 120.49      | 118.20   |
| 81  | A3    | 2732 | OMU  | C5-C4-N3  | 3.28 | 119.74      | 114.84   |
| 81  | A3    | 787  | OMU  | C5-C4-N3  | 3.27 | 119.74      | 114.84   |
| 81  | A3    | 1460 | A2M  | N3-C4-N9  | 3.27 | 132.48      | 127.08   |
| 3   | h1    | 440  | A2M  | N3-C4-N9  | 3.27 | 132.47      | 127.08   |
| 81  | A3    | 1135 | PSU  | C6-C5-C4  | 3.27 | 120.48      | 118.20   |
| 82  | B3    | 46   | A2M  | N3-C4-N9  | 3.26 | 132.46      | 127.08   |
| 3   | h1    | 123  | OMU  | C5-C4-N3  | 3.26 | 119.72      | 114.84   |
| 81  | A3    | 804  | OMU  | C5-C4-N3  | 3.26 | 119.72      | 114.84   |
| 81  | A3    | 3289 | OMU  | C5-C4-N3  | 3.25 | 119.71      | 114.84   |
| 81  | A3    | 2868 | PSU  | C6-C5-C4  | 3.25 | 120.47      | 118.20   |
| 81  | A3    | 3304 | OMU  | C5-C4-N3  | 3.25 | 119.70      | 114.84   |
| 81  | A3    | 44   | OMU  | C5-C4-N3  | 3.25 | 119.70      | 114.84   |
| 3   | h1    | 1771 | 6MZ  | C1'-N9-C8 | 3.24 | 134.46      | 127.14   |
| 81  | A3    | 369  | A2M  | N3-C4-N9  | 3.24 | 132.43      | 127.08   |
| 81  | A3    | 2857 | PSU  | C6-C5-C4  | 3.24 | 120.46      | 118.20   |
| 81  | A3    | 717  | PSU  | C6-C5-C4  | 3.24 | 120.46      | 118.20   |
| 81  | A3    | 2284 | A2M  | N3-C4-N9  | 3.23 | 132.41      | 127.08   |
| 81  | A3    | 2137 | PSU  | C6-C5-C4  | 3.23 | 120.46      | 118.20   |
| 81  | A3    | 2914 | A2M  | N3-C4-N9  | 3.23 | 132.41      | 127.08   |
| 81  | A3    | 2324 | A2M  | C5-N7-C8  | 3.22 | 108.09      | 103.51   |
| 81  | A3    | 2720 | OMU  | C5-C4-N3  | 3.22 | 119.66      | 114.84   |
| 3   | h1    | 1329 | A2M  | N3-C4-N9  | 3.22 | 132.40      | 127.08   |
| 81  | A3    | 675  | OMU  | C5-C4-N3  | 3.21 | 119.65      | 114.84   |
| 81  | A3    | 2259 | A2M  | N3-C4-N9  | 3.21 | 132.38      | 127.08   |
| 82  | B3    | 46   | A2M  | C5-N7-C8  | 3.21 | 108.07      | 103.51   |
| 81  | A3    | 817  | A2M  | C5-N7-C8  | 3.21 | 108.07      | 103.51   |
| 81  | A3    | 895  | PSU  | C6-C5-C4  | 3.20 | 120.44      | 118.20   |
| 81  | A3    | 660  | A2M  | C5-N7-C8  | 3.20 | 108.06      | 103.51   |
| 81  | A3    | 1460 | A2M  | C5-N7-C8  | 3.20 | 108.05      | 103.51   |
| 3   | h1    | 622  | A2M  | C5-N7-C8  | 3.19 | 108.05      | 103.51   |
| 81  | A3    | 970  | PSU  | C6-C5-C4  | 3.19 | 120.43      | 118.20   |
| 81  | A3    | 2259 | A2M  | C5-N7-C8  | 3.19 | 108.05      | 103.51   |
| 3   | h1    | 1579 | A2M  | N3-C4-N9  | 3.19 | 132.34      | 127.08   |
| 81  | A3    | 2804 | A2M  | C5-N7-C8  | 3.19 | 108.04      | 103.51   |
| 3   | h1    | 424  | A2M  | N3-C4-N9  | 3.18 | 132.33      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | h1    | 362  | PSU  | C6-C5-C4    | 3.18  | 120.42      | 118.20   |
| 81  | A3    | 2129 | A2M  | N3-C4-N9    | 3.18  | 132.32      | 127.08   |
| 81  | A3    | 2914 | A2M  | C5-N7-C8    | 3.18  | 108.02      | 103.51   |
| 81  | A3    | 946  | A2M  | N3-C4-N9    | 3.18  | 132.32      | 127.08   |
| 81  | A3    | 827  | A2M  | C5-N7-C8    | 3.18  | 108.02      | 103.51   |
| 81  | A3    | 2654 | OMG  | N2-C2-N1    | 3.18  | 123.47      | 116.71   |
| 3   | h1    | 961  | PSU  | C6-C5-C4    | 3.17  | 120.42      | 118.20   |
| 81  | A3    | 660  | A2M  | N3-C4-N9    | 3.17  | 132.31      | 127.08   |
| 82  | B3    | 77   | PSU  | C6-C5-C4    | 3.17  | 120.41      | 118.20   |
| 3   | h1    | 1210 | PSU  | C6-C5-C4    | 3.17  | 120.41      | 118.20   |
| 81  | A3    | 2926 | PSU  | C6-C5-C4    | 3.17  | 120.41      | 118.20   |
| 3   | h1    | 763  | PSU  | C6-C5-C4    | 3.16  | 120.41      | 118.20   |
| 3   | h1    | 28   | A2M  | N3-C4-N9    | 3.16  | 132.29      | 127.08   |
| 81  | A3    | 946  | A2M  | C5-N7-C8    | 3.16  | 108.00      | 103.51   |
| 3   | h1    | 886  | OMU  | CM2-O2'-C2' | 3.16  | 122.82      | 114.52   |
| 3   | h1    | 470  | PSU  | C6-C5-C4    | 3.16  | 120.41      | 118.20   |
| 81  | A3    | 827  | A2M  | N3-C4-N9    | 3.15  | 132.28      | 127.08   |
| 81  | A3    | 277  | PSU  | C6-N1-C2    | -3.15 | 119.46      | 122.68   |
| 81  | A3    | 966  | PSU  | C6-N1-C2    | -3.15 | 119.46      | 122.68   |
| 3   | h1    | 1447 | OMU  | C5-C4-N3    | 3.15  | 119.56      | 114.84   |
| 3   | h1    | 424  | A2M  | C5-N7-C8    | 3.15  | 107.98      | 103.51   |
| 3   | h1    | 162  | A2M  | C5-N7-C8    | 3.14  | 107.98      | 103.51   |
| 81  | A3    | 2329 | A2M  | N3-C4-N9    | 3.14  | 132.26      | 127.08   |
| 81  | A3    | 2257 | PSU  | C6-C5-C4    | 3.14  | 120.39      | 118.20   |
| 3   | h1    | 1002 | PSU  | C6-C5-C4    | 3.13  | 120.39      | 118.20   |
| 3   | h1    | 440  | A2M  | C5-N7-C8    | 3.13  | 107.95      | 103.51   |
| 3   | h1    | 1485 | PSU  | C6-C5-C4    | 3.13  | 120.38      | 118.20   |
| 3   | h1    | 162  | A2M  | N3-C4-N9    | 3.13  | 132.23      | 127.08   |
| 81  | A3    | 2129 | A2M  | C5-N7-C8    | 3.13  | 107.95      | 103.51   |
| 81  | A3    | 2139 | PSU  | C6-C5-C4    | 3.13  | 120.38      | 118.20   |
| 3   | h1    | 468  | A2M  | N3-C4-N9    | 3.12  | 132.23      | 127.08   |
| 81  | A3    | 2214 | PSU  | C6-C5-C4    | 3.12  | 120.38      | 118.20   |
| 3   | h1    | 417  | PSU  | C6-C5-C4    | 3.12  | 120.38      | 118.20   |
| 81  | A3    | 1685 | PSU  | C6-C5-C4    | 3.12  | 120.38      | 118.20   |
| 3   | h1    | 1329 | A2M  | C5-N7-C8    | 3.12  | 107.94      | 103.51   |
| 81  | A3    | 1378 | A2M  | C5-N7-C8    | 3.12  | 107.94      | 103.51   |
| 3   | h1    | 28   | A2M  | C5-N7-C8    | 3.12  | 107.94      | 103.51   |
| 81  | A3    | 2267 | PSU  | C6-C5-C4    | 3.12  | 120.38      | 118.20   |
| 3   | h1    | 1579 | A2M  | C5-N7-C8    | 3.11  | 107.93      | 103.51   |
| 81  | A3    | 2329 | A2M  | C5-N7-C8    | 3.11  | 107.93      | 103.51   |
| 3   | h1    | 451  | PSU  | C6-C5-C4    | 3.11  | 120.37      | 118.20   |
| 81  | A3    | 2643 | A2M  | C5-N7-C8    | 3.10  | 107.92      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 81  | A3    | 2947 | PSU  | C6-C5-C4  | 3.09  | 120.36      | 118.20   |
| 81  | A3    | 228  | PSU  | C6-C5-C4  | 3.09  | 120.36      | 118.20   |
| 81  | A3    | 2873 | 5MC  | C5-C6-N1  | -3.09 | 120.16      | 123.34   |
| 3   | h1    | 800  | A2M  | C5-N7-C8  | 3.09  | 107.89      | 103.51   |
| 81  | A3    | 1002 | PSU  | C6-C5-C4  | 3.08  | 120.35      | 118.20   |
| 81  | A3    | 369  | A2M  | C5-N7-C8  | 3.08  | 107.89      | 103.51   |
| 3   | h1    | 468  | A2M  | C5-N7-C8  | 3.08  | 107.88      | 103.51   |
| 81  | A3    | 2284 | A2M  | C5-N7-C8  | 3.08  | 107.88      | 103.51   |
| 3   | h1    | 606  | PSU  | C6-N1-C2  | -3.08 | 119.54      | 122.68   |
| 81  | A3    | 2886 | OMU  | C5-C4-N3  | 3.08  | 119.44      | 114.84   |
| 81  | A3    | 895  | PSU  | C6-N1-C2  | -3.07 | 119.54      | 122.68   |
| 3   | h1    | 544  | A2M  | C5-N7-C8  | 3.07  | 107.87      | 103.51   |
| 81  | A3    | 1064 | PSU  | C6-C5-C4  | 3.07  | 120.34      | 118.20   |
| 81  | A3    | 2897 | PSU  | C6-C5-C4  | 3.07  | 120.34      | 118.20   |
| 81  | A3    | 2883 | PSU  | C6-C5-C4  | 3.07  | 120.34      | 118.20   |
| 3   | h1    | 1304 | PSU  | C6-C5-C4  | 3.06  | 120.34      | 118.20   |
| 81  | A3    | 2324 | A2M  | N3-C4-N9  | 3.06  | 132.12      | 127.08   |
| 81  | A3    | 42   | PSU  | C6-C5-C4  | 3.06  | 120.34      | 118.20   |
| 81  | A3    | 3113 | PSU  | C6-N1-C2  | -3.06 | 119.56      | 122.68   |
| 3   | h1    | 1790 | MA6  | C4-N9-C1' | 3.06  | 133.88      | 126.59   |
| 3   | h1    | 977  | A2M  | C5-N7-C8  | 3.05  | 107.85      | 103.51   |
| 3   | h1    | 1787 | PSU  | C6-C5-C4  | 3.05  | 120.33      | 118.20   |
| 3   | h1    | 1758 | A2M  | C5-N7-C8  | 3.05  | 107.84      | 103.51   |
| 81  | A3    | 2263 | PSU  | C6-C5-C4  | 3.04  | 120.32      | 118.20   |
| 81  | A3    | 2978 | PSU  | C6-N1-C2  | -3.03 | 119.58      | 122.68   |
| 3   | h1    | 622  | A2M  | N3-C4-N9  | 3.02  | 132.06      | 127.08   |
| 81  | A3    | 150  | PSU  | C6-C5-C4  | 3.02  | 120.31      | 118.20   |
| 3   | h1    | 603  | UY1  | C6-N1-C2  | -3.01 | 119.60      | 122.68   |
| 3   | h1    | 1106 | PSU  | C6-C5-C4  | 3.01  | 120.30      | 118.20   |
| 3   | h1    | 607  | PSU  | C6-N1-C2  | -3.01 | 119.60      | 122.68   |
| 3   | h1    | 451  | PSU  | C6-N1-C2  | -3.00 | 119.61      | 122.68   |
| 3   | h1    | 1567 | PSU  | C6-C5-C4  | 3.00  | 120.30      | 118.20   |
| 81  | A3    | 2321 | PSU  | C6-C5-C4  | 3.00  | 120.30      | 118.20   |
| 81  | A3    | 2747 | PSU  | C6-N1-C2  | -3.00 | 119.62      | 122.68   |
| 3   | h1    | 1184 | PSU  | C6-C5-C4  | 3.00  | 120.29      | 118.20   |
| 81  | A3    | 1144 | A2M  | N3-C4-N9  | 3.00  | 132.02      | 127.08   |
| 3   | h1    | 1308 | PSU  | C6-C5-C4  | 3.00  | 120.29      | 118.20   |
| 81  | A3    | 1482 | PSU  | C6-N1-C2  | -2.99 | 119.62      | 122.68   |
| 81  | A3    | 2435 | PSU  | C6-N1-C2  | -2.99 | 119.62      | 122.68   |
| 3   | h1    | 635  | PSU  | C6-N1-C2  | -2.99 | 119.62      | 122.68   |
| 3   | h1    | 103  | PSU  | C6-C5-C4  | 2.99  | 120.29      | 118.20   |
| 81  | A3    | 976  | PSU  | C6-C5-C4  | 2.99  | 120.29      | 118.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | h1    | 1274 | OMG  | C2-N1-C6    | -2.98 | 119.66      | 125.10   |
| 3   | h1    | 1615 | PSU  | C6-C5-C4    | 2.98  | 120.28      | 118.20   |
| 81  | A3    | 2804 | A2M  | N3-C4-N9    | 2.98  | 131.99      | 127.08   |
| 3   | h1    | 1190 | PSU  | C6-C5-C4    | 2.97  | 120.28      | 118.20   |
| 81  | A3    | 399  | OMG  | N9-C4-N3    | 2.97  | 131.91      | 125.94   |
| 3   | h1    | 362  | PSU  | C6-N1-C2    | -2.97 | 119.64      | 122.68   |
| 3   | h1    | 950  | PSU  | C6-N1-C2    | -2.97 | 119.65      | 122.68   |
| 81  | A3    | 510  | PSU  | C6-N1-C2    | -2.97 | 119.65      | 122.68   |
| 3   | h1    | 809  | PSU  | C6-C5-C4    | 2.97  | 120.27      | 118.20   |
| 3   | h1    | 1790 | MA6  | N3-C4-N9    | 2.97  | 131.97      | 127.08   |
| 81  | A3    | 1461 | OMG  | C2-N1-C6    | -2.97 | 119.69      | 125.10   |
| 81  | A3    | 902  | PSU  | C6-N1-C2    | -2.96 | 119.65      | 122.68   |
| 81  | A3    | 2214 | PSU  | C6-N1-C2    | -2.96 | 119.65      | 122.68   |
| 81  | A3    | 918  | OMG  | N9-C4-N3    | 2.96  | 131.89      | 125.94   |
| 81  | A3    | 2139 | PSU  | C6-N1-C2    | -2.96 | 119.65      | 122.68   |
| 3   | h1    | 607  | PSU  | C6-C5-C4    | 2.96  | 120.27      | 118.20   |
| 81  | A3    | 399  | OMG  | C2-N1-C6    | -2.96 | 119.70      | 125.10   |
| 3   | h1    | 1210 | PSU  | C6-N1-C2    | -2.96 | 119.66      | 122.68   |
| 81  | A3    | 918  | OMG  | C2-N1-C6    | -2.96 | 119.71      | 125.10   |
| 81  | A3    | 2419 | PSU  | C6-C5-C4    | 2.95  | 120.26      | 118.20   |
| 81  | A3    | 1144 | A2M  | C5-N7-C8    | 2.95  | 107.71      | 103.51   |
| 81  | A3    | 1474 | PSU  | C6-N1-C2    | -2.95 | 119.66      | 122.68   |
| 3   | h1    | 310  | PSU  | C6-N1-C2    | -2.95 | 119.67      | 122.68   |
| 3   | h1    | 1634 | PSU  | C6-C5-C4    | 2.95  | 120.26      | 118.20   |
| 81  | A3    | 1016 | PSU  | C6-C5-C4    | 2.95  | 120.26      | 118.20   |
| 3   | h1    | 1789 | MA6  | N3-C4-N9    | 2.95  | 131.94      | 127.08   |
| 3   | h1    | 392  | OMG  | C2-N1-C6    | -2.95 | 119.73      | 125.10   |
| 81  | A3    | 2829 | PSU  | C6-N1-C2    | -2.94 | 119.67      | 122.68   |
| 81  | A3    | 2920 | OMG  | C2-N1-C6    | -2.94 | 119.73      | 125.10   |
| 81  | A3    | 1016 | PSU  | C6-N1-C2    | -2.94 | 119.68      | 122.68   |
| 3   | h1    | 605  | PSU  | C6-N1-C2    | -2.94 | 119.68      | 122.68   |
| 81  | A3    | 277  | PSU  | C6-C5-C4    | 2.94  | 120.25      | 118.20   |
| 81  | A3    | 886  | A2M  | C5-N7-C8    | 2.94  | 107.68      | 103.51   |
| 3   | h1    | 246  | OMG  | N9-C4-N3    | 2.94  | 131.83      | 125.94   |
| 81  | A3    | 2958 | PSU  | C6-C5-C4    | 2.93  | 120.25      | 118.20   |
| 3   | h1    | 258  | PSU  | C6-N1-C2    | -2.93 | 119.68      | 122.68   |
| 81  | A3    | 150  | PSU  | C6-N1-C2    | -2.93 | 119.68      | 122.68   |
| 81  | A3    | 1134 | PSU  | C6-N1-C2    | -2.93 | 119.68      | 122.68   |
| 3   | h1    | 339  | PSU  | C6-N1-C2    | -2.93 | 119.69      | 122.68   |
| 81  | A3    | 1056 | PSU  | C6-C5-C4    | 2.93  | 120.25      | 118.20   |
| 81  | A3    | 817  | A2M  | C4'-O4'-C1' | -2.93 | 103.01      | 109.47   |
| 3   | h1    | 246  | OMG  | C2-N1-C6    | -2.93 | 119.76      | 125.10   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 81  | A3    | 2926 | PSU  | C6-N1-C2 | -2.93 | 119.69      | 122.68   |
| 3   | h1    | 598  | OMG  | C2-N1-C6 | -2.93 | 119.76      | 125.10   |
| 81  | A3    | 228  | PSU  | C6-N1-C2 | -2.93 | 119.69      | 122.68   |
| 81  | A3    | 1002 | PSU  | C6-N1-C2 | -2.92 | 119.69      | 122.68   |
| 81  | A3    | 2269 | PSU  | C6-N1-C2 | -2.92 | 119.69      | 122.68   |
| 3   | h1    | 886  | OMU  | O4-C4-C5 | -2.92 | 120.02      | 125.16   |
| 81  | A3    | 2317 | PSU  | C6-N1-C2 | -2.92 | 119.69      | 122.68   |
| 82  | B3    | 78   | OMG  | C2-N1-C6 | -2.92 | 119.77      | 125.10   |
| 3   | h1    | 1787 | PSU  | C6-N1-C2 | -2.92 | 119.70      | 122.68   |
| 81  | A3    | 804  | OMU  | O4-C4-C5 | -2.92 | 120.03      | 125.16   |
| 81  | A3    | 2194 | PSU  | C6-N1-C2 | -2.92 | 119.70      | 122.68   |
| 81  | A3    | 2291 | OMG  | C2-N1-C6 | -2.92 | 119.78      | 125.10   |
| 81  | A3    | 815  | OMG  | C2-N1-C6 | -2.92 | 119.78      | 125.10   |
| 3   | h1    | 1194 | B8N  | N3-C2-N1 | 2.92  | 120.88      | 116.76   |
| 3   | h1    | 809  | PSU  | C6-N1-C2 | -2.92 | 119.70      | 122.68   |
| 3   | h1    | 1002 | PSU  | C6-N1-C2 | -2.91 | 119.70      | 122.68   |
| 3   | h1    | 1178 | PSU  | C6-C5-C4 | 2.91  | 120.23      | 118.20   |
| 3   | h1    | 1615 | PSU  | C6-N1-C2 | -2.91 | 119.71      | 122.68   |
| 81  | A3    | 1857 | OMG  | C2-N1-C6 | -2.91 | 119.79      | 125.10   |
| 81  | A3    | 1133 | PSU  | C6-C5-C4 | 2.91  | 120.23      | 118.20   |
| 81  | A3    | 2622 | OMG  | C2-N1-C6 | -2.91 | 119.80      | 125.10   |
| 3   | h1    | 306  | PSU  | C6-N1-C2 | -2.91 | 119.71      | 122.68   |
| 3   | h1    | 1308 | PSU  | C6-N1-C2 | -2.90 | 119.71      | 122.68   |
| 3   | h1    | 762  | PSU  | C6-C5-C4 | 2.90  | 120.23      | 118.20   |
| 81  | A3    | 684  | PSU  | C6-N1-C2 | -2.90 | 119.72      | 122.68   |
| 81  | A3    | 2223 | A2M  | C5-N7-C8 | 2.90  | 107.63      | 103.51   |
| 81  | A3    | 2261 | PSU  | C6-C5-C4 | 2.90  | 120.23      | 118.20   |
| 81  | A3    | 2412 | OMG  | C2-N1-C6 | -2.90 | 119.81      | 125.10   |
| 3   | h1    | 1190 | PSU  | C6-N1-C2 | -2.89 | 119.72      | 122.68   |
| 3   | h1    | 1771 | 6MZ  | C5-N7-C8 | 2.89  | 107.62      | 103.51   |
| 81  | A3    | 2137 | PSU  | C6-N1-C2 | -2.89 | 119.72      | 122.68   |
| 3   | h1    | 1524 | PSU  | C6-N1-C2 | -2.89 | 119.72      | 122.68   |
| 3   | h1    | 1178 | PSU  | C6-N1-C2 | -2.89 | 119.73      | 122.68   |
| 81  | A3    | 2868 | PSU  | C6-N1-C2 | -2.89 | 119.73      | 122.68   |
| 3   | h1    | 1293 | PSU  | C6-C5-C4 | 2.89  | 120.22      | 118.20   |
| 81  | A3    | 296  | OMG  | C2-N1-C6 | -2.89 | 119.83      | 125.10   |
| 81  | A3    | 2925 | OMG  | C2-N1-C6 | -2.89 | 119.83      | 125.10   |
| 3   | h1    | 603  | UY1  | C6-C5-C4 | 2.89  | 120.22      | 118.20   |
| 3   | h1    | 753  | PSU  | C6-C5-C4 | 2.89  | 120.22      | 118.20   |
| 81  | A3    | 311  | PSU  | C6-N1-C2 | -2.89 | 119.73      | 122.68   |
| 3   | h1    | 1293 | PSU  | C6-N1-C2 | -2.89 | 119.73      | 122.68   |
| 81  | A3    | 1685 | PSU  | C6-N1-C2 | -2.89 | 119.73      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 81  | A3    | 1056 | PSU  | C6-N1-C2 | -2.89 | 119.73      | 122.68   |
| 81  | A3    | 684  | PSU  | C6-C5-C4 | 2.88  | 120.22      | 118.20   |
| 3   | h1    | 470  | PSU  | C6-N1-C2 | -2.88 | 119.73      | 122.68   |
| 3   | h1    | 121  | PSU  | C6-N1-C2 | -2.88 | 119.73      | 122.68   |
| 81  | A3    | 2267 | PSU  | C6-N1-C2 | -2.88 | 119.73      | 122.68   |
| 3   | h1    | 614  | OMU  | O4-C4-C5 | -2.88 | 120.09      | 125.16   |
| 3   | h1    | 1383 | OMU  | O4-C4-C5 | -2.88 | 120.09      | 125.16   |
| 81  | A3    | 3113 | PSU  | C6-C5-C4 | 2.88  | 120.21      | 118.20   |
| 81  | A3    | 2239 | OMG  | C2-N1-C6 | -2.88 | 119.85      | 125.10   |
| 3   | h1    | 635  | PSU  | C6-C5-C4 | 2.88  | 120.21      | 118.20   |
| 3   | h1    | 103  | PSU  | C6-N1-C2 | -2.88 | 119.74      | 122.68   |
| 81  | A3    | 2818 | OMG  | C2-N1-C6 | -2.88 | 119.85      | 125.10   |
| 81  | A3    | 2897 | PSU  | C6-N1-C2 | -2.88 | 119.74      | 122.68   |
| 3   | h1    | 1194 | B8N  | O4-C4-N3 | -2.87 | 115.10      | 119.98   |
| 82  | B3    | 77   | PSU  | C6-N1-C2 | -2.87 | 119.74      | 122.68   |
| 3   | h1    | 961  | PSU  | C6-N1-C2 | -2.87 | 119.74      | 122.68   |
| 3   | h1    | 1184 | PSU  | C6-N1-C2 | -2.87 | 119.74      | 122.68   |
| 3   | h1    | 1304 | PSU  | C6-N1-C2 | -2.87 | 119.74      | 122.68   |
| 81  | A3    | 2261 | PSU  | C6-N1-C2 | -2.87 | 119.74      | 122.68   |
| 3   | h1    | 417  | PSU  | C6-N1-C2 | -2.87 | 119.75      | 122.68   |
| 3   | h1    | 1272 | OMU  | O4-C4-C5 | -2.87 | 120.11      | 125.16   |
| 81  | A3    | 3289 | OMU  | O4-C4-C5 | -2.87 | 120.12      | 125.16   |
| 81  | A3    | 902  | PSU  | C6-C5-C4 | 2.87  | 120.20      | 118.20   |
| 81  | A3    | 976  | PSU  | C6-N1-C2 | -2.87 | 119.75      | 122.68   |
| 81  | A3    | 2883 | PSU  | C6-N1-C2 | -2.86 | 119.75      | 122.68   |
| 3   | h1    | 1634 | PSU  | C6-N1-C2 | -2.86 | 119.75      | 122.68   |
| 81  | A3    | 829  | PSU  | C6-N1-C2 | -2.86 | 119.75      | 122.68   |
| 3   | h1    | 753  | PSU  | C6-N1-C2 | -2.86 | 119.76      | 122.68   |
| 81  | A3    | 2398 | OMG  | C2-N1-C6 | -2.86 | 119.89      | 125.10   |
| 81  | A3    | 464  | PSU  | C6-N1-C2 | -2.86 | 119.76      | 122.68   |
| 3   | h1    | 373  | OMU  | O4-C4-C5 | -2.86 | 120.13      | 125.16   |
| 3   | h1    | 1485 | PSU  | C6-N1-C2 | -2.86 | 119.76      | 122.68   |
| 81  | A3    | 2263 | PSU  | C6-N1-C2 | -2.86 | 119.76      | 122.68   |
| 3   | h1    | 310  | PSU  | C6-C5-C4 | 2.86  | 120.19      | 118.20   |
| 81  | A3    | 2857 | PSU  | C6-N1-C2 | -2.86 | 119.76      | 122.68   |
| 81  | A3    | 717  | PSU  | C6-N1-C2 | -2.85 | 119.77      | 122.68   |
| 81  | A3    | 2257 | PSU  | C6-N1-C2 | -2.85 | 119.77      | 122.68   |
| 3   | h1    | 1217 | PSU  | C6-C5-C4 | 2.85  | 120.19      | 118.20   |
| 81  | A3    | 2947 | PSU  | C6-N1-C2 | -2.85 | 119.77      | 122.68   |
| 81  | A3    | 2958 | PSU  | C6-N1-C2 | -2.85 | 119.77      | 122.68   |
| 81  | A3    | 2394 | OMG  | C2-N1-C6 | -2.85 | 119.90      | 125.10   |
| 82  | B3    | 96   | PSU  | C6-N1-C2 | -2.85 | 119.77      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | A3    | 1133 | PSU  | C6-N1-C2    | -2.85 | 119.77      | 122.68   |
| 81  | A3    | 2653 | UY1  | C6-N1-C2    | -2.85 | 119.77      | 122.68   |
| 81  | A3    | 2126 | OMG  | C2-N1-C6    | -2.84 | 119.92      | 125.10   |
| 3   | h1    | 95   | PSU  | C6-C5-C4    | 2.84  | 120.18      | 118.20   |
| 81  | A3    | 2738 | OMU  | O4-C4-C5    | -2.84 | 120.17      | 125.16   |
| 3   | h1    | 1234 | OMU  | O4-C4-C5    | -2.84 | 120.17      | 125.16   |
| 3   | h1    | 1106 | PSU  | C6-N1-C2    | -2.84 | 119.78      | 122.68   |
| 81  | A3    | 42   | PSU  | C6-N1-C2    | -2.84 | 119.78      | 122.68   |
| 81  | A3    | 2127 | OMG  | C2-N1-C6    | -2.84 | 119.93      | 125.10   |
| 3   | h1    | 121  | PSU  | C6-C5-C4    | 2.83  | 120.18      | 118.20   |
| 3   | h1    | 339  | PSU  | C6-C5-C4    | 2.83  | 120.18      | 118.20   |
| 3   | h1    | 1012 | OMU  | O4-C4-C5    | -2.83 | 120.18      | 125.16   |
| 3   | h1    | 1217 | PSU  | C6-N1-C2    | -2.83 | 119.79      | 122.68   |
| 3   | h1    | 584  | PSU  | C6-N1-C2    | -2.83 | 119.79      | 122.68   |
| 81  | A3    | 2720 | OMU  | O4-C4-C5    | -2.82 | 120.19      | 125.16   |
| 81  | A3    | 2796 | OMG  | C2-N1-C6    | -2.82 | 119.95      | 125.10   |
| 3   | h1    | 605  | PSU  | C6-C5-C4    | 2.82  | 120.17      | 118.20   |
| 81  | A3    | 2419 | PSU  | C6-N1-C2    | -2.82 | 119.80      | 122.68   |
| 3   | h1    | 1567 | PSU  | C6-N1-C2    | -2.81 | 119.81      | 122.68   |
| 3   | h1    | 1535 | PSU  | C6-N1-C2    | -2.81 | 119.81      | 122.68   |
| 81  | A3    | 2350 | OMU  | O4-C4-C5    | -2.81 | 120.22      | 125.16   |
| 3   | h1    | 1120 | PSU  | C6-N1-C2    | -2.80 | 119.81      | 122.68   |
| 81  | A3    | 34   | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 81  | A3    | 3304 | OMU  | O4-C4-C5    | -2.80 | 120.23      | 125.16   |
| 3   | h1    | 762  | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 3   | h1    | 1027 | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 81  | A3    | 2924 | OMU  | O4-C4-C5    | -2.80 | 120.23      | 125.16   |
| 3   | h1    | 581  | OMU  | O4-C4-C5    | -2.80 | 120.23      | 125.16   |
| 81  | A3    | 464  | PSU  | C6-C5-C4    | 2.80  | 120.16      | 118.20   |
| 81  | A3    | 1064 | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 82  | B3    | 21   | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 81  | A3    | 144  | OMU  | O4-C4-C5    | -2.79 | 120.25      | 125.16   |
| 81  | A3    | 1537 | OMU  | O4-C4-C5    | -2.79 | 120.25      | 125.16   |
| 3   | h1    | 258  | PSU  | C6-C5-C4    | 2.79  | 120.15      | 118.20   |
| 3   | h1    | 1274 | OMG  | N9-C4-N3    | 2.79  | 131.53      | 125.94   |
| 81  | A3    | 970  | PSU  | C6-N1-C2    | -2.78 | 119.84      | 122.68   |
| 81  | A3    | 2622 | OMG  | N9-C4-N3    | 2.78  | 131.53      | 125.94   |
| 3   | h1    | 1447 | OMU  | O4-C4-C5    | -2.78 | 120.27      | 125.16   |
| 81  | A3    | 1474 | PSU  | C6-C5-C4    | 2.78  | 120.14      | 118.20   |
| 81  | A3    | 2239 | OMG  | N9-C4-N3    | 2.78  | 131.52      | 125.94   |
| 81  | A3    | 660  | A2M  | C2'-C3'-C4' | 2.78  | 108.03      | 101.99   |
| 81  | A3    | 44   | OMU  | O4-C4-C5    | -2.78 | 120.28      | 125.16   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | A3    | 2804 | A2M  | C3'-C2'-C1' | 2.78  | 108.11      | 102.89   |
| 3   | h1    | 763  | PSU  | C6-N1-C2    | -2.77 | 119.85      | 122.68   |
| 81  | A3    | 2321 | PSU  | C6-N1-C2    | -2.77 | 119.85      | 122.68   |
| 3   | h1    | 95   | PSU  | C6-N1-C2    | -2.77 | 119.85      | 122.68   |
| 81  | A3    | 2424 | OMU  | O4-C4-C5    | -2.77 | 120.29      | 125.16   |
| 81  | A3    | 2978 | PSU  | C6-C5-C4    | 2.76  | 120.13      | 118.20   |
| 3   | h1    | 123  | OMU  | O4-C4-C5    | -2.76 | 120.31      | 125.16   |
| 3   | h1    | 1535 | PSU  | C6-C5-C4    | 2.75  | 120.12      | 118.20   |
| 81  | A3    | 1068 | OMU  | O4-C4-C5    | -2.75 | 120.32      | 125.16   |
| 3   | h1    | 606  | PSU  | C6-C5-C4    | 2.74  | 120.11      | 118.20   |
| 81  | A3    | 1135 | PSU  | C6-N1-C2    | -2.73 | 119.89      | 122.68   |
| 81  | A3    | 815  | OMG  | C5-C6-N1    | 2.73  | 120.12      | 113.19   |
| 81  | A3    | 787  | OMU  | O4-C4-C5    | -2.73 | 120.36      | 125.16   |
| 82  | B3    | 21   | PSU  | C6-C5-C4    | 2.73  | 120.10      | 118.20   |
| 81  | A3    | 1894 | OMU  | O4-C4-C5    | -2.72 | 120.38      | 125.16   |
| 3   | h1    | 1433 | OMG  | C2-N1-C6    | -2.72 | 120.14      | 125.10   |
| 81  | A3    | 2747 | PSU  | C6-C5-C4    | 2.72  | 120.10      | 118.20   |
| 3   | h1    | 1027 | PSU  | C6-C5-C4    | 2.71  | 120.10      | 118.20   |
| 81  | A3    | 2886 | OMU  | O4-C4-C5    | -2.71 | 120.39      | 125.16   |
| 81  | A3    | 675  | OMU  | O4-C4-C5    | -2.70 | 120.41      | 125.16   |
| 3   | h1    | 1210 | PSU  | O2-C2-N1    | -2.70 | 119.82      | 122.79   |
| 3   | h1    | 598  | OMG  | N9-C4-N3    | 2.70  | 131.35      | 125.94   |
| 81  | A3    | 2654 | OMG  | C2-N1-C6    | -2.70 | 120.18      | 125.10   |
| 81  | A3    | 2291 | OMG  | C5-C6-N1    | 2.69  | 120.03      | 113.19   |
| 81  | A3    | 2194 | PSU  | C6-C5-C4    | 2.69  | 120.08      | 118.20   |
| 81  | A3    | 2269 | PSU  | C6-C5-C4    | 2.69  | 120.08      | 118.20   |
| 81  | A3    | 966  | PSU  | C6-C5-C4    | 2.69  | 120.08      | 118.20   |
| 82  | B3    | 78   | OMG  | N9-C4-N3    | 2.69  | 131.33      | 125.94   |
| 81  | A3    | 2412 | OMG  | C5-C6-N1    | 2.68  | 120.00      | 113.19   |
| 3   | h1    | 306  | PSU  | C6-C5-C4    | 2.68  | 120.07      | 118.20   |
| 3   | h1    | 392  | OMG  | C5-C6-N1    | 2.68  | 120.00      | 113.19   |
| 81  | A3    | 399  | OMG  | C5-C6-N1    | 2.68  | 120.00      | 113.19   |
| 81  | A3    | 2732 | OMU  | O4-C4-C5    | -2.68 | 120.44      | 125.16   |
| 3   | h1    | 1274 | OMG  | C5-C6-N1    | 2.68  | 119.99      | 113.19   |
| 81  | A3    | 48   | OMU  | O4-C4-C5    | -2.68 | 120.45      | 125.16   |
| 81  | A3    | 2127 | OMG  | C5-C6-N1    | 2.67  | 119.98      | 113.19   |
| 81  | A3    | 2291 | OMG  | N9-C4-N3    | 2.67  | 131.31      | 125.94   |
| 81  | A3    | 2394 | OMG  | N2-C2-N1    | 2.67  | 122.40      | 116.71   |
| 81  | A3    | 2925 | OMG  | C5-C6-N1    | 2.67  | 119.97      | 113.19   |
| 81  | A3    | 2925 | OMG  | N9-C4-N3    | 2.67  | 131.29      | 125.94   |
| 3   | h1    | 598  | OMG  | C5-C6-N1    | 2.67  | 119.96      | 113.19   |
| 81  | A3    | 296  | OMG  | C5-C6-N1    | 2.67  | 119.96      | 113.19   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 81  | A3    | 2622 | OMG  | C5-C6-N1   | 2.66  | 119.96      | 113.19   |
| 3   | h1    | 1120 | PSU  | C6-C5-C4   | 2.66  | 120.06      | 118.20   |
| 3   | h1    | 607  | PSU  | O2-C2-N1   | -2.66 | 119.86      | 122.79   |
| 82  | B3    | 78   | OMG  | C5-C6-N1   | 2.66  | 119.94      | 113.19   |
| 81  | A3    | 2818 | OMG  | C5-C6-N1   | 2.66  | 119.94      | 113.19   |
| 81  | A3    | 1461 | OMG  | C5-C6-N1   | 2.66  | 119.94      | 113.19   |
| 81  | A3    | 918  | OMG  | C5-C6-N1   | 2.65  | 119.93      | 113.19   |
| 81  | A3    | 2796 | OMG  | C5-C6-N1   | 2.65  | 119.93      | 113.19   |
| 3   | h1    | 246  | OMG  | C5-C6-N1   | 2.65  | 119.91      | 113.19   |
| 81  | A3    | 2435 | PSU  | O2-C2-N1   | -2.64 | 119.88      | 122.79   |
| 81  | A3    | 1857 | OMG  | C5-C6-N1   | 2.64  | 119.90      | 113.19   |
| 3   | h1    | 392  | OMG  | N9-C4-N3   | 2.63  | 131.23      | 125.94   |
| 81  | A3    | 2239 | OMG  | C5-C6-N1   | 2.63  | 119.87      | 113.19   |
| 81  | A3    | 2747 | PSU  | O2-C2-N1   | -2.63 | 119.89      | 122.79   |
| 81  | A3    | 1482 | PSU  | C6-C5-C4   | 2.63  | 120.04      | 118.20   |
| 81  | A3    | 2920 | OMG  | C5-C6-N1   | 2.63  | 119.86      | 113.19   |
| 3   | h1    | 451  | PSU  | O2-C2-N1   | -2.63 | 119.90      | 122.79   |
| 81  | A3    | 1474 | PSU  | O2-C2-N1   | -2.63 | 119.90      | 122.79   |
| 81  | A3    | 2398 | OMG  | C5-C6-N1   | 2.62  | 119.85      | 113.19   |
| 81  | A3    | 150  | PSU  | O2-C2-N1   | -2.62 | 119.90      | 122.79   |
| 3   | h1    | 950  | PSU  | C6-C5-C4   | 2.62  | 120.03      | 118.20   |
| 81  | A3    | 2394 | OMG  | C5-C6-N1   | 2.61  | 119.83      | 113.19   |
| 81  | A3    | 2883 | PSU  | O2-C2-N1   | -2.61 | 119.91      | 122.79   |
| 81  | A3    | 2126 | OMG  | C5-C6-N1   | 2.61  | 119.82      | 113.19   |
| 3   | h1    | 103  | PSU  | O2-C2-N1   | -2.61 | 119.92      | 122.79   |
| 81  | A3    | 656  | 1MA  | N9-C4-N3   | 2.61  | 133.01      | 126.94   |
| 81  | A3    | 2413 | OMU  | O4-C4-C5   | -2.60 | 120.59      | 125.16   |
| 82  | B3    | 77   | PSU  | O2-C2-N1   | -2.60 | 119.93      | 122.79   |
| 81  | A3    | 2868 | PSU  | O2-C2-N1   | -2.58 | 119.95      | 122.79   |
| 81  | A3    | 815  | OMG  | N9-C4-N3   | 2.58  | 131.11      | 125.94   |
| 3   | h1    | 1433 | OMG  | N9-C4-N3   | 2.58  | 131.11      | 125.94   |
| 81  | A3    | 2654 | OMG  | C5-C6-N1   | 2.57  | 119.73      | 113.19   |
| 3   | h1    | 603  | UY1  | O2-C2-N1   | -2.57 | 119.96      | 122.79   |
| 3   | h1    | 1787 | PSU  | O2-C2-N1   | -2.57 | 119.96      | 122.79   |
| 81  | A3    | 2926 | PSU  | O2-C2-N1   | -2.57 | 119.96      | 122.79   |
| 81  | A3    | 2829 | PSU  | O2-C2-N1   | -2.57 | 119.96      | 122.79   |
| 81  | A3    | 2419 | PSU  | O2-C2-N1   | -2.56 | 119.97      | 122.79   |
| 81  | A3    | 2794 | OMG  | C5-C6-N1   | 2.56  | 119.69      | 113.19   |
| 3   | h1    | 1790 | MA6  | C4-N9-C8   | 2.56  | 108.50      | 105.73   |
| 81  | A3    | 1461 | OMG  | N9-C4-N3   | 2.55  | 131.05      | 125.94   |
| 3   | h1    | 1433 | OMG  | C5-C6-N1   | 2.55  | 119.66      | 113.19   |
| 81  | A3    | 2284 | A2M  | C2'-C1'-N9 | -2.54 | 109.25      | 113.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | A3    | 2794 | OMG  | C2-N1-C6    | -2.54 | 120.46      | 125.10   |
| 81  | A3    | 786  | PSU  | C6-N1-C2    | -2.54 | 120.08      | 122.68   |
| 82  | B3    | 21   | PSU  | O2-C2-N1    | -2.54 | 120.00      | 122.79   |
| 3   | h1    | 1789 | MA6  | C4-N9-C8    | 2.54  | 108.48      | 105.73   |
| 3   | h1    | 622  | A2M  | C3'-C2'-C1' | 2.53  | 107.65      | 102.89   |
| 81  | A3    | 277  | PSU  | O2-C2-N1    | -2.52 | 120.01      | 122.79   |
| 81  | A3    | 1685 | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 3   | h1    | 417  | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 81  | A3    | 2796 | OMG  | N9-C4-N3    | 2.52  | 130.99      | 125.94   |
| 81  | A3    | 2857 | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 3   | h1    | 1524 | PSU  | C6-C5-C4    | 2.52  | 119.96      | 118.20   |
| 81  | A3    | 2214 | PSU  | O2-C2-N1    | -2.51 | 120.03      | 122.79   |
| 81  | A3    | 296  | OMG  | N9-C4-N3    | 2.50  | 130.96      | 125.94   |
| 81  | A3    | 2127 | OMG  | N2-C2-N1    | 2.50  | 122.04      | 116.71   |
| 81  | A3    | 970  | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |
| 3   | h1    | 1106 | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |
| 81  | A3    | 717  | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |
| 81  | A3    | 2263 | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |
| 81  | A3    | 2398 | OMG  | N2-C2-N1    | 2.49  | 122.02      | 116.71   |
| 3   | h1    | 605  | PSU  | O2-C2-N1    | -2.49 | 120.05      | 122.79   |
| 3   | h1    | 1120 | PSU  | O2-C2-N1    | -2.49 | 120.05      | 122.79   |
| 81  | A3    | 2261 | PSU  | O2-C2-N1    | -2.49 | 120.05      | 122.79   |
| 3   | h1    | 1567 | PSU  | O2-C2-N1    | -2.49 | 120.05      | 122.79   |
| 81  | A3    | 2398 | OMG  | C8-N7-C5    | 2.49  | 108.74      | 104.24   |
| 81  | A3    | 829  | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 81  | A3    | 2920 | OMG  | O6-C6-C5    | -2.48 | 120.02      | 126.60   |
| 81  | A3    | 815  | OMG  | O6-C6-C5    | -2.48 | 120.02      | 126.60   |
| 3   | h1    | 1190 | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 81  | A3    | 2127 | OMG  | C8-N7-C5    | 2.48  | 108.73      | 104.24   |
| 81  | A3    | 464  | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 81  | A3    | 399  | OMG  | O6-C6-C5    | -2.48 | 120.03      | 126.60   |
| 81  | A3    | 1135 | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 3   | h1    | 809  | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 3   | h1    | 753  | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 81  | A3    | 2239 | OMG  | O6-C6-C5    | -2.47 | 120.05      | 126.60   |
| 3   | h1    | 1308 | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 81  | A3    | 2804 | A2M  | C2'-C3'-C4' | 2.47  | 107.36      | 101.99   |
| 82  | B3    | 78   | OMG  | O6-C6-C5    | -2.47 | 120.05      | 126.60   |
| 3   | h1    | 961  | PSU  | O2-C2-N1    | -2.47 | 120.08      | 122.79   |
| 82  | B3    | 96   | PSU  | C6-C5-C4    | 2.46  | 119.92      | 118.20   |
| 81  | A3    | 1016 | PSU  | O2-C2-N1    | -2.46 | 120.08      | 122.79   |
| 81  | A3    | 2284 | A2M  | O4'-C1'-N9  | 2.46  | 112.91      | 108.06   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | h1    | 1178 | PSU  | O2-C2-N1    | -2.46 | 120.08      | 122.79   |
| 81  | A3    | 2281 | 5MC  | CM5-C5-C6   | -2.46 | 119.56      | 122.85   |
| 81  | A3    | 2622 | OMG  | O6-C6-C5    | -2.46 | 120.08      | 126.60   |
| 3   | h1    | 1524 | PSU  | O2-C2-N1    | -2.46 | 120.08      | 122.79   |
| 3   | h1    | 392  | OMG  | O6-C6-C5    | -2.46 | 120.09      | 126.60   |
| 3   | h1    | 418  | OMC  | CM2-O2'-C2' | 2.46  | 120.97      | 114.52   |
| 3   | h1    | 763  | PSU  | O2-C2-N1    | -2.46 | 120.09      | 122.79   |
| 3   | h1    | 246  | OMG  | O6-C6-C5    | -2.45 | 120.09      | 126.60   |
| 81  | A3    | 1857 | OMG  | N9-C4-N3    | 2.45  | 130.87      | 125.94   |
| 81  | A3    | 2958 | PSU  | O2-C2-N1    | -2.45 | 120.09      | 122.79   |
| 81  | A3    | 1134 | PSU  | O2-C2-N1    | -2.45 | 120.09      | 122.79   |
| 81  | A3    | 2317 | PSU  | O2-C2-N1    | -2.45 | 120.09      | 122.79   |
| 3   | h1    | 1274 | OMG  | O6-C6-C5    | -2.45 | 120.11      | 126.60   |
| 3   | h1    | 544  | A2M  | C6-C5-C4    | 2.45  | 120.47      | 117.18   |
| 81  | A3    | 296  | OMG  | C8-N7-C5    | 2.45  | 108.67      | 104.24   |
| 3   | h1    | 1485 | PSU  | O2-C2-N1    | -2.45 | 120.10      | 122.79   |
| 81  | A3    | 2269 | PSU  | O2-C2-N1    | -2.44 | 120.10      | 122.79   |
| 81  | A3    | 2925 | OMG  | O6-C6-C5    | -2.44 | 120.12      | 126.60   |
| 3   | h1    | 635  | PSU  | O2-C2-N1    | -2.44 | 120.10      | 122.79   |
| 81  | A3    | 2818 | OMG  | N2-C2-N1    | 2.44  | 121.91      | 116.71   |
| 3   | h1    | 584  | PSU  | C6-C5-C4    | 2.44  | 119.90      | 118.20   |
| 3   | h1    | 598  | OMG  | O6-C6-C5    | -2.44 | 120.13      | 126.60   |
| 81  | A3    | 918  | OMG  | O6-C6-C5    | -2.44 | 120.13      | 126.60   |
| 3   | h1    | 339  | PSU  | O2-C2-N1    | -2.44 | 120.11      | 122.79   |
| 81  | A3    | 2194 | PSU  | O2-C2-N1    | -2.44 | 120.11      | 122.79   |
| 81  | A3    | 1002 | PSU  | O2-C2-N1    | -2.44 | 120.11      | 122.79   |
| 3   | h1    | 1781 | 4AC  | C5-C4-N3    | -2.44 | 118.67      | 122.59   |
| 3   | h1    | 121  | PSU  | O2-C2-N1    | -2.43 | 120.11      | 122.79   |
| 81  | A3    | 296  | OMG  | O6-C6-C5    | -2.43 | 120.14      | 126.60   |
| 81  | A3    | 2920 | OMG  | N9-C4-N3    | 2.43  | 130.82      | 125.94   |
| 81  | A3    | 2394 | OMG  | O6-C6-C5    | -2.43 | 120.15      | 126.60   |
| 81  | A3    | 2818 | OMG  | O6-C6-C5    | -2.43 | 120.16      | 126.60   |
| 3   | h1    | 1615 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 3   | h1    | 1634 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 81  | A3    | 2412 | OMG  | N9-C4-N3    | 2.42  | 130.81      | 125.94   |
| 3   | h1    | 258  | PSU  | O2-C2-N1    | -2.42 | 120.12      | 122.79   |
| 3   | h1    | 606  | PSU  | O2-C2-N1    | -2.42 | 120.12      | 122.79   |
| 81  | A3    | 1857 | OMG  | O6-C6-C5    | -2.42 | 120.18      | 126.60   |
| 81  | A3    | 1482 | PSU  | O2-C2-N1    | -2.42 | 120.13      | 122.79   |
| 3   | h1    | 1217 | PSU  | O2-C2-N1    | -2.42 | 120.13      | 122.79   |
| 81  | A3    | 1378 | A2M  | C6-C5-C4    | 2.42  | 120.43      | 117.18   |
| 3   | h1    | 584  | PSU  | O2-C2-N1    | -2.42 | 120.13      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | h1    | 598  | OMG  | C8-N7-C5    | 2.42  | 108.62      | 104.24   |
| 81  | A3    | 228  | PSU  | O2-C2-N1    | -2.42 | 120.13      | 122.79   |
| 81  | A3    | 976  | PSU  | O2-C2-N1    | -2.41 | 120.13      | 122.79   |
| 81  | A3    | 2412 | OMG  | O6-C6-C5    | -2.41 | 120.20      | 126.60   |
| 81  | A3    | 2794 | OMG  | N9-C4-N3    | 2.41  | 130.78      | 125.94   |
| 81  | A3    | 1056 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 81  | A3    | 2139 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 81  | A3    | 2126 | OMG  | N2-C2-N1    | 2.41  | 121.84      | 116.71   |
| 81  | A3    | 311  | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 81  | A3    | 786  | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 81  | A3    | 2267 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 81  | A3    | 2284 | A2M  | C4'-O4'-C1' | -2.41 | 104.16      | 109.47   |
| 81  | A3    | 2321 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 81  | A3    | 311  | PSU  | C6-C5-C4    | 2.40  | 119.88      | 118.20   |
| 3   | h1    | 1274 | OMG  | C8-N7-C5    | 2.40  | 108.59      | 104.24   |
| 3   | h1    | 1293 | PSU  | O2-C2-N1    | -2.40 | 120.15      | 122.79   |
| 81  | A3    | 2394 | OMG  | C8-N7-C5    | 2.40  | 108.59      | 104.24   |
| 3   | h1    | 392  | OMG  | C8-N7-C5    | 2.40  | 108.58      | 104.24   |
| 81  | A3    | 2654 | OMG  | O6-C6-C5    | -2.40 | 120.24      | 126.60   |
| 3   | h1    | 1535 | PSU  | O2-C2-N1    | -2.40 | 120.15      | 122.79   |
| 3   | h1    | 1304 | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 81  | A3    | 1133 | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 3   | h1    | 950  | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 81  | A3    | 2796 | OMG  | O6-C6-C5    | -2.39 | 120.26      | 126.60   |
| 3   | h1    | 1027 | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 3   | h1    | 470  | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 3   | h1    | 762  | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 81  | A3    | 817  | A2M  | C3'-C2'-C1' | 2.38  | 107.37      | 102.89   |
| 81  | A3    | 2291 | OMG  | O6-C6-C5    | -2.38 | 120.29      | 126.60   |
| 81  | A3    | 1064 | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 81  | A3    | 2126 | OMG  | O6-C6-C5    | -2.38 | 120.30      | 126.60   |
| 81  | A3    | 2949 | A2M  | C2'-C1'-N9  | -2.38 | 109.53      | 113.53   |
| 3   | h1    | 1781 | 4AC  | N4-C4-N3    | 2.37  | 117.84      | 113.85   |
| 81  | A3    | 1461 | OMG  | C8-N7-C5    | 2.37  | 108.53      | 104.24   |
| 81  | A3    | 1857 | OMG  | C8-N7-C5    | 2.37  | 108.53      | 104.24   |
| 3   | h1    | 1184 | PSU  | O2-C2-N1    | -2.37 | 120.18      | 122.79   |
| 3   | h1    | 310  | PSU  | O2-C2-N1    | -2.37 | 120.19      | 122.79   |
| 81  | A3    | 2925 | OMG  | C8-N7-C5    | 2.37  | 108.52      | 104.24   |
| 81  | A3    | 2291 | OMG  | C8-N7-C5    | 2.36  | 108.52      | 104.24   |
| 3   | h1    | 1433 | OMG  | O6-C6-C5    | -2.36 | 120.33      | 126.60   |
| 81  | A3    | 2653 | UY1  | O2-C2-N1    | -2.36 | 120.19      | 122.79   |
| 81  | A3    | 895  | PSU  | O2-C2-N1    | -2.36 | 120.19      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | h1    | 246  | OMG  | C8-N7-C5    | 2.36  | 108.51      | 104.24   |
| 81  | A3    | 2223 | A2M  | C6-C5-C4    | 2.36  | 120.35      | 117.18   |
| 81  | A3    | 2622 | OMG  | C8-N7-C5    | 2.35  | 108.50      | 104.24   |
| 3   | h1    | 1790 | MA6  | C4-C5-N7    | -2.35 | 107.75      | 110.62   |
| 81  | A3    | 2127 | OMG  | O6-C6-C5    | -2.35 | 120.36      | 126.60   |
| 81  | A3    | 918  | OMG  | C8-N7-C5    | 2.35  | 108.50      | 104.24   |
| 81  | A3    | 2126 | OMG  | C8-N7-C5    | 2.35  | 108.49      | 104.24   |
| 3   | h1    | 1002 | PSU  | O2-C2-N1    | -2.35 | 120.21      | 122.79   |
| 82  | B3    | 78   | OMG  | C8-N7-C5    | 2.35  | 108.49      | 104.24   |
| 81  | A3    | 2897 | PSU  | O2-C2-N1    | -2.35 | 120.21      | 122.79   |
| 81  | A3    | 2654 | OMG  | C8-N7-C5    | 2.34  | 108.48      | 104.24   |
| 81  | A3    | 2643 | A2M  | C6-C5-C4    | 2.34  | 120.33      | 117.18   |
| 81  | A3    | 2239 | OMG  | C8-N7-C5    | 2.34  | 108.48      | 104.24   |
| 81  | A3    | 2794 | OMG  | C8-N7-C5    | 2.34  | 108.48      | 104.24   |
| 81  | A3    | 2818 | OMG  | C8-N7-C5    | 2.34  | 108.48      | 104.24   |
| 81  | A3    | 2920 | OMG  | C8-N7-C5    | 2.34  | 108.48      | 104.24   |
| 81  | A3    | 34   | PSU  | O2-C2-N1    | -2.34 | 120.21      | 122.79   |
| 81  | A3    | 2398 | OMG  | O6-C6-C5    | -2.34 | 120.40      | 126.60   |
| 3   | h1    | 1283 | 4AC  | C6-C5-C4    | 2.34  | 119.82      | 116.96   |
| 81  | A3    | 510  | PSU  | O2-C2-N1    | -2.33 | 120.22      | 122.79   |
| 82  | B3    | 96   | PSU  | O2-C2-N1    | -2.33 | 120.22      | 122.79   |
| 81  | A3    | 902  | PSU  | O2-C2-N1    | -2.33 | 120.23      | 122.79   |
| 3   | h1    | 362  | PSU  | O2-C2-N1    | -2.32 | 120.23      | 122.79   |
| 81  | A3    | 40   | OMC  | CM2-O2'-C2' | 2.32  | 120.62      | 114.52   |
| 81  | A3    | 966  | PSU  | O2-C2-N1    | -2.32 | 120.23      | 122.79   |
| 81  | A3    | 2947 | PSU  | O2-C2-N1    | -2.32 | 120.23      | 122.79   |
| 81  | A3    | 660  | A2M  | C4-N9-C8    | 2.32  | 108.24      | 105.73   |
| 81  | A3    | 2126 | OMG  | N9-C4-N3    | 2.32  | 130.59      | 125.94   |
| 81  | A3    | 2412 | OMG  | C8-N7-C5    | 2.32  | 108.43      | 104.24   |
| 81  | A3    | 2794 | OMG  | O6-C6-C5    | -2.32 | 120.46      | 126.60   |
| 81  | A3    | 3113 | PSU  | O2-C2-N1    | -2.32 | 120.24      | 122.79   |
| 3   | h1    | 977  | A2M  | C6-C5-C4    | 2.31  | 120.29      | 117.18   |
| 81  | A3    | 815  | OMG  | C8-N7-C5    | 2.31  | 108.43      | 104.24   |
| 3   | h1    | 95   | PSU  | O2-C2-N1    | -2.31 | 120.25      | 122.79   |
| 81  | A3    | 2257 | PSU  | O2-C2-N1    | -2.30 | 120.26      | 122.79   |
| 81  | A3    | 1460 | A2M  | C6-C5-C4    | 2.30  | 120.27      | 117.18   |
| 81  | A3    | 1461 | OMG  | O6-C6-C5    | -2.30 | 120.50      | 126.60   |
| 81  | A3    | 2796 | OMG  | C8-N7-C5    | 2.29  | 108.39      | 104.24   |
| 81  | A3    | 946  | A2M  | C3'-C2'-C1' | 2.29  | 107.20      | 102.89   |
| 3   | h1    | 1781 | 4AC  | C6-C5-C4    | 2.29  | 119.76      | 116.96   |
| 81  | A3    | 399  | OMG  | C8-N7-C5    | 2.27  | 108.36      | 104.24   |
| 81  | A3    | 2329 | A2M  | C4'-O4'-C1' | -2.27 | 104.45      | 109.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | h1    | 451  | PSU  | O4'-C1'-C2' | 2.27  | 108.35      | 105.14   |
| 81  | A3    | 369  | A2M  | C6-C5-C4    | 2.27  | 120.24      | 117.18   |
| 81  | A3    | 2949 | A2M  | C4-N9-C8    | 2.27  | 108.19      | 105.73   |
| 81  | A3    | 817  | A2M  | C6-C5-C4    | 2.26  | 120.23      | 117.18   |
| 81  | A3    | 684  | PSU  | O2-C2-N1    | -2.25 | 120.31      | 122.79   |
| 81  | A3    | 369  | A2M  | C2'-C3'-C4' | 2.25  | 106.88      | 101.99   |
| 81  | A3    | 2654 | OMG  | C6-C5-N7    | 2.25  | 134.43      | 130.25   |
| 81  | A3    | 2127 | OMG  | C2'-C1'-N9  | -2.25 | 109.86      | 114.22   |
| 3   | h1    | 306  | PSU  | O2-C2-N1    | -2.24 | 120.33      | 122.79   |
| 3   | h1    | 1283 | 4AC  | C5-C4-N3    | -2.24 | 119.00      | 122.59   |
| 3   | h1    | 1433 | OMG  | C8-N7-C5    | 2.23  | 108.28      | 104.24   |
| 81  | A3    | 1144 | A2M  | C4'-O4'-C1' | -2.23 | 104.54      | 109.47   |
| 81  | A3    | 886  | A2M  | C6-C5-C4    | 2.23  | 120.19      | 117.18   |
| 3   | h1    | 1758 | A2M  | C6-C5-C4    | 2.23  | 120.18      | 117.18   |
| 81  | A3    | 2978 | PSU  | O2-C2-N1    | -2.23 | 120.34      | 122.79   |
| 81  | A3    | 2914 | A2M  | C6-C5-C4    | 2.23  | 120.17      | 117.18   |
| 81  | A3    | 2654 | OMG  | C4-C5-N7    | -2.22 | 107.21      | 110.72   |
| 3   | h1    | 1789 | MA6  | C4-C5-N7    | -2.22 | 107.92      | 110.62   |
| 3   | h1    | 1758 | A2M  | C4'-O4'-C1' | -2.21 | 104.59      | 109.47   |
| 81  | A3    | 946  | A2M  | C2'-C3'-C4' | 2.21  | 106.80      | 101.99   |
| 3   | h1    | 800  | A2M  | C6-C5-C4    | 2.21  | 120.15      | 117.18   |
| 81  | A3    | 2324 | A2M  | C6-C5-C4    | 2.21  | 120.15      | 117.18   |
| 3   | h1    | 440  | A2M  | C6-C5-C4    | 2.21  | 120.15      | 117.18   |
| 81  | A3    | 2398 | OMG  | C4-C5-N7    | -2.20 | 107.23      | 110.72   |
| 81  | A3    | 2920 | OMG  | N2-C2-N1    | 2.20  | 121.41      | 116.71   |
| 81  | A3    | 2324 | A2M  | C4-C5-N7    | -2.20 | 107.94      | 110.62   |
| 82  | B3    | 46   | A2M  | C4-N9-C8    | 2.20  | 108.11      | 105.73   |
| 3   | h1    | 162  | A2M  | C4'-O4'-C1' | -2.20 | 104.62      | 109.47   |
| 81  | A3    | 2127 | OMG  | C4-C5-N7    | -2.20 | 107.24      | 110.72   |
| 3   | h1    | 1194 | B8N  | O4'-C1'-C2' | 2.20  | 108.24      | 105.14   |
| 81  | A3    | 2412 | OMG  | N2-C2-N1    | 2.19  | 121.37      | 116.71   |
| 81  | A3    | 2284 | A2M  | C4-N9-C8    | 2.18  | 108.09      | 105.73   |
| 81  | A3    | 946  | A2M  | C4-C5-N7    | -2.18 | 107.96      | 110.62   |
| 81  | A3    | 2947 | PSU  | O4'-C1'-C2' | 2.18  | 108.22      | 105.14   |
| 81  | A3    | 2804 | A2M  | C4'-O4'-C1' | -2.18 | 104.66      | 109.47   |
| 81  | A3    | 656  | 1MA  | C8-N9-C4    | 2.18  | 110.19      | 106.05   |
| 81  | A3    | 1460 | A2M  | C4-C5-N7    | -2.17 | 107.97      | 110.62   |
| 81  | A3    | 2949 | A2M  | C6-C5-C4    | 2.17  | 120.11      | 117.18   |
| 3   | h1    | 28   | A2M  | C6-C5-C4    | 2.17  | 120.10      | 117.18   |
| 81  | A3    | 827  | A2M  | C6-C5-C4    | 2.17  | 120.10      | 117.18   |
| 81  | A3    | 2259 | A2M  | C4-N9-C8    | 2.16  | 108.07      | 105.73   |
| 3   | h1    | 162  | A2M  | C4-C5-N7    | -2.16 | 107.98      | 110.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | A3    | 827  | A2M  | C4-C5-N7    | -2.16 | 107.98      | 110.62   |
| 3   | h1    | 1329 | A2M  | C6-C5-C4    | 2.16  | 120.09      | 117.18   |
| 81  | A3    | 2883 | PSU  | O4'-C1'-C2' | 2.16  | 108.19      | 105.14   |
| 3   | h1    | 622  | A2M  | C4-C5-N7    | -2.16 | 107.99      | 110.62   |
| 81  | A3    | 2914 | A2M  | C4-C5-N7    | -2.16 | 107.99      | 110.62   |
| 81  | A3    | 42   | PSU  | O2-C2-N1    | -2.16 | 120.42      | 122.79   |
| 3   | h1    | 607  | PSU  | O4'-C1'-C2' | 2.16  | 108.18      | 105.14   |
| 81  | A3    | 2129 | A2M  | C6-C5-C4    | 2.15  | 120.08      | 117.18   |
| 81  | A3    | 2804 | A2M  | C4-C5-N7    | -2.15 | 108.00      | 110.62   |
| 81  | A3    | 2259 | A2M  | C4-C5-N7    | -2.14 | 108.01      | 110.62   |
| 81  | A3    | 786  | PSU  | C6-C5-C4    | 2.14  | 119.70      | 118.20   |
| 3   | h1    | 622  | A2M  | C4-N9-C8    | 2.14  | 108.04      | 105.73   |
| 3   | h1    | 1579 | A2M  | C2'-C3'-C4' | 2.13  | 106.63      | 101.99   |
| 81  | A3    | 817  | A2M  | C4-C5-N7    | -2.13 | 108.02      | 110.62   |
| 3   | h1    | 424  | A2M  | C4-C5-N7    | -2.13 | 108.03      | 110.62   |
| 3   | h1    | 1329 | A2M  | C4-C5-N7    | -2.13 | 108.03      | 110.62   |
| 81  | A3    | 1068 | OMU  | O2-C2-N1    | -2.12 | 119.96      | 122.79   |
| 81  | A3    | 2829 | PSU  | O4'-C1'-C2' | 2.12  | 108.14      | 105.14   |
| 81  | A3    | 2129 | A2M  | C4-C5-N7    | -2.12 | 108.04      | 110.62   |
| 81  | A3    | 2949 | A2M  | C4'-O4'-C1' | -2.12 | 104.80      | 109.47   |
| 81  | A3    | 656  | 1MA  | C8-N7-C5    | 2.11  | 108.07      | 104.24   |
| 81  | A3    | 2394 | OMG  | C4-C5-N7    | -2.11 | 107.38      | 110.72   |
| 3   | h1    | 622  | A2M  | C4'-O4'-C1' | -2.11 | 104.81      | 109.47   |
| 81  | A3    | 2818 | OMG  | N9-C4-N3    | 2.11  | 130.18      | 125.94   |
| 81  | A3    | 1894 | OMU  | O2-C2-N1    | -2.10 | 119.99      | 122.79   |
| 81  | A3    | 2868 | PSU  | O4'-C1'-C2' | 2.10  | 108.11      | 105.14   |
| 81  | A3    | 886  | A2M  | C3'-C2'-C1' | 2.10  | 106.83      | 102.89   |
| 3   | h1    | 468  | A2M  | C4-C5-N7    | -2.09 | 108.07      | 110.62   |
| 81  | A3    | 2435 | PSU  | O4'-C1'-C2' | 2.09  | 108.10      | 105.14   |
| 81  | A3    | 2654 | OMG  | N1-C2-N3    | -2.09 | 119.42      | 123.32   |
| 3   | h1    | 1329 | A2M  | C4-N9-C8    | 2.08  | 107.99      | 105.73   |
| 3   | h1    | 1579 | A2M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 81  | A3    | 2738 | OMU  | O2-C2-N1    | -2.08 | 120.02      | 122.79   |
| 3   | h1    | 28   | A2M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 81  | A3    | 660  | A2M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 81  | A3    | 2949 | A2M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 81  | A3    | 2804 | A2M  | C4-N9-C8    | 2.08  | 107.98      | 105.73   |
| 81  | A3    | 2956 | UR3  | C6-N1-C2    | -2.08 | 119.93      | 121.79   |
| 3   | h1    | 339  | PSU  | O4'-C1'-C2' | 2.08  | 108.08      | 105.14   |
| 82  | B3    | 46   | A2M  | C6-C5-C4    | 2.08  | 119.98      | 117.18   |
| 82  | B3    | 46   | A2M  | C4-C5-N7    | -2.08 | 108.09      | 110.62   |
| 81  | A3    | 2324 | A2M  | C4'-O4'-C1' | -2.07 | 104.90      | 109.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | A3    | 2127 | OMG  | C6-C5-N7    | 2.07  | 134.10      | 130.25   |
| 3   | h1    | 468  | A2M  | C6-C5-C4    | 2.07  | 119.97      | 117.18   |
| 81  | A3    | 2424 | OMU  | O2-C2-N1    | -2.07 | 120.04      | 122.79   |
| 3   | h1    | 1579 | A2M  | C6-C5-C4    | 2.06  | 119.96      | 117.18   |
| 81  | A3    | 2259 | A2M  | C6-C5-C4    | 2.06  | 119.95      | 117.18   |
| 3   | h1    | 1194 | B8N  | C31-N3-C4   | 2.06  | 120.35      | 117.31   |
| 3   | h1    | 440  | A2M  | C4-C5-N7    | -2.06 | 108.11      | 110.62   |
| 3   | h1    | 800  | A2M  | C4-C5-N7    | -2.06 | 108.11      | 110.62   |
| 3   | h1    | 162  | A2M  | C6-C5-C4    | 2.06  | 119.95      | 117.18   |
| 81  | A3    | 2350 | OMU  | O2-C2-N1    | -2.05 | 120.06      | 122.79   |
| 81  | A3    | 369  | A2M  | C4-C5-N7    | -2.05 | 108.12      | 110.62   |
| 81  | A3    | 464  | PSU  | O4'-C1'-C2' | 2.05  | 108.03      | 105.14   |
| 3   | h1    | 424  | A2M  | C4-N9-C8    | 2.05  | 107.95      | 105.73   |
| 3   | h1    | 1433 | OMG  | N2-C2-N1    | 2.05  | 121.08      | 116.71   |
| 3   | h1    | 123  | OMU  | O2-C2-N1    | -2.05 | 120.06      | 122.79   |
| 3   | h1    | 614  | OMU  | C1'-N1-C2   | 2.05  | 121.28      | 117.57   |
| 81  | A3    | 804  | OMU  | O2-C2-N1    | -2.05 | 120.06      | 122.79   |
| 81  | A3    | 660  | A2M  | C3'-C2'-C1' | 2.05  | 106.73      | 102.89   |
| 3   | h1    | 424  | A2M  | C6-C5-C4    | 2.04  | 119.93      | 117.18   |
| 81  | A3    | 815  | OMG  | N2-C2-N1    | 2.04  | 121.06      | 116.71   |
| 81  | A3    | 1378 | A2M  | C4-C5-N7    | -2.04 | 108.13      | 110.62   |
| 81  | A3    | 1685 | PSU  | O4'-C1'-C2' | 2.04  | 108.02      | 105.14   |
| 81  | A3    | 1144 | A2M  | C4-N9-C8    | 2.04  | 107.94      | 105.73   |
| 81  | A3    | 886  | A2M  | C2'-C3'-C4' | 2.04  | 106.42      | 101.99   |
| 82  | B3    | 46   | A2M  | C4'-O4'-C1' | -2.04 | 104.98      | 109.47   |
| 81  | A3    | 2818 | OMG  | C4-C5-N7    | -2.03 | 107.50      | 110.72   |
| 3   | h1    | 977  | A2M  | C4-C5-N7    | -2.03 | 108.14      | 110.62   |
| 3   | h1    | 1771 | 6MZ  | C4-N9-C8    | 2.03  | 107.93      | 105.73   |
| 81  | A3    | 2259 | A2M  | C4'-O4'-C1' | -2.03 | 104.98      | 109.47   |
| 81  | A3    | 1144 | A2M  | C6-C5-C4    | 2.03  | 119.92      | 117.18   |
| 81  | A3    | 2398 | OMG  | C6-C5-N7    | 2.03  | 134.02      | 130.25   |
| 81  | A3    | 2794 | OMG  | N1-C2-N3    | -2.03 | 119.54      | 123.32   |
| 3   | h1    | 424  | A2M  | C4'-O4'-C1' | -2.03 | 105.00      | 109.47   |
| 81  | A3    | 946  | A2M  | C6-C5-C4    | 2.02  | 119.90      | 117.18   |
| 81  | A3    | 2394 | OMG  | N9-C4-N3    | 2.02  | 130.00      | 125.94   |
| 81  | A3    | 2137 | PSU  | O2-C2-N1    | -2.02 | 120.57      | 122.79   |
| 81  | A3    | 787  | OMU  | O2-C2-N1    | -2.02 | 120.10      | 122.79   |
| 81  | A3    | 2796 | OMG  | N2-C2-N1    | 2.02  | 121.00      | 116.71   |
| 3   | h1    | 544  | A2M  | C4-C5-N7    | -2.01 | 108.17      | 110.62   |
| 81  | A3    | 1461 | OMG  | C4-C5-N7    | -2.01 | 107.54      | 110.72   |
| 81  | A3    | 675  | OMU  | O2-C2-N1    | -2.01 | 120.12      | 122.79   |
| 81  | A3    | 2398 | OMG  | N9-C4-N3    | 2.01  | 129.97      | 125.94   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 81  | A3    | 2643 | A2M  | C4-C5-N7 | -2.01 | 108.18      | 110.62   |
| 81  | A3    | 1461 | OMG  | N2-C2-N1 | 2.00  | 120.98      | 116.71   |
| 81  | A3    | 1448 | OMC  | O2-C2-N3 | -2.00 | 119.07      | 122.33   |
| 81  | A3    | 296  | OMG  | C4-C5-N7 | -2.00 | 107.55      | 110.72   |
| 81  | A3    | 1857 | OMG  | N2-C2-N1 | 2.00  | 120.97      | 116.71   |

There are no chirality outliers.

All (139) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 82  | B3    | 78   | OMG  | O4'-C4'-C5'-O5' |
| 82  | B3    | 78   | OMG  | C3'-C4'-C5'-O5' |
| 82  | B3    | 96   | PSU  | C3'-C4'-C5'-O5' |
| 82  | B3    | 96   | PSU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 38   | OMC  | C3'-C4'-C5'-O5' |
| 3   | h1    | 123  | OMU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 140  | OMC  | C3'-C4'-C5'-O5' |
| 3   | h1    | 140  | OMC  | O4'-C4'-C5'-O5' |
| 3   | h1    | 392  | OMG  | O4'-C4'-C5'-O5' |
| 3   | h1    | 418  | OMC  | C1'-C2'-O2'-CM2 |
| 3   | h1    | 418  | OMC  | C3'-C2'-O2'-CM2 |
| 3   | h1    | 584  | PSU  | C2'-C1'-C5-C4   |
| 3   | h1    | 584  | PSU  | C2'-C1'-C5-C6   |
| 3   | h1    | 584  | PSU  | C3'-C4'-C5'-O5' |
| 3   | h1    | 598  | OMG  | O4'-C4'-C5'-O5' |
| 3   | h1    | 614  | OMU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 886  | OMU  | C1'-C2'-O2'-CM2 |
| 3   | h1    | 1194 | B8N  | N34-C33-C34-O35 |
| 3   | h1    | 1234 | OMU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1274 | OMG  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1274 | OMG  | C3'-C4'-C5'-O5' |
| 3   | h1    | 1308 | PSU  | C2'-C1'-C5-C4   |
| 3   | h1    | 1579 | A2M  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1787 | PSU  | C3'-C4'-C5'-O5' |
| 3   | h1    | 1787 | PSU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1790 | MA6  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1790 | MA6  | C3'-C4'-C5'-O5' |
| 81  | A3    | 40   | OMC  | C3'-C2'-O2'-CM2 |
| 81  | A3    | 296  | OMG  | O4'-C4'-C5'-O5' |
| 81  | A3    | 296  | OMG  | C3'-C4'-C5'-O5' |
| 81  | A3    | 660  | A2M  | C1'-C2'-O2'-CM' |
| 81  | A3    | 786  | PSU  | C2'-C1'-C5-C4   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 81  | A3    | 918  | OMG  | O4'-C4'-C5'-O5' |
| 81  | A3    | 918  | OMG  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2200 | OMC  | C2'-C1'-N1-C6   |
| 81  | A3    | 2259 | A2M  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2259 | A2M  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2284 | A2M  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2291 | OMG  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2291 | OMG  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2317 | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2368 | OMC  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2368 | OMC  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2804 | A2M  | C1'-C2'-O2'-CM' |
| 81  | A3    | 2804 | A2M  | C2'-C1'-N9-C8   |
| 81  | A3    | 2914 | A2M  | C2'-C1'-N9-C8   |
| 81  | A3    | 2956 | UR3  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2956 | UR3  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2200 | OMC  | C2'-C1'-N1-C2   |
| 3   | h1    | 38   | OMC  | O4'-C4'-C5'-O5' |
| 3   | h1    | 123  | OMU  | C3'-C4'-C5'-O5' |
| 3   | h1    | 392  | OMG  | C3'-C4'-C5'-O5' |
| 3   | h1    | 581  | OMU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 598  | OMG  | C3'-C4'-C5'-O5' |
| 3   | h1    | 614  | OMU  | C3'-C4'-C5'-O5' |
| 3   | h1    | 622  | A2M  | O4'-C4'-C5'-O5' |
| 3   | h1    | 622  | A2M  | C3'-C4'-C5'-O5' |
| 3   | h1    | 886  | OMU  | C3'-C4'-C5'-O5' |
| 3   | h1    | 1234 | OMU  | C3'-C4'-C5'-O5' |
| 3   | h1    | 1272 | OMU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1579 | A2M  | C3'-C4'-C5'-O5' |
| 81  | A3    | 399  | OMG  | O4'-C4'-C5'-O5' |
| 81  | A3    | 399  | OMG  | C3'-C4'-C5'-O5' |
| 81  | A3    | 1002 | PSU  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2914 | A2M  | C3'-C4'-C5'-O5' |
| 3   | h1    | 584  | PSU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 886  | OMU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 1002 | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2284 | A2M  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2317 | PSU  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2914 | A2M  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2804 | A2M  | C2'-C1'-N9-C4   |
| 81  | A3    | 2914 | A2M  | C2'-C1'-N9-C4   |
| 81  | A3    | 827  | A2M  | C3'-C2'-O2'-CM' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | h1    | 1194 | B8N  | N34-C33-C34-O36 |
| 81  | A3    | 1378 | A2M  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2873 | 5MC  | C2'-C1'-N1-C6   |
| 81  | A3    | 786  | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2269 | PSU  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2321 | PSU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1790 | MA6  | C5-C6-N6-C10    |
| 3   | h1    | 581  | OMU  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2413 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | h1    | 1790 | MA6  | C4'-C5'-O5'-P   |
| 3   | h1    | 544  | A2M  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2284 | A2M  | C2'-C1'-N9-C8   |
| 81  | A3    | 2200 | OMC  | O4'-C1'-N1-C2   |
| 81  | A3    | 2368 | OMC  | C3'-C2'-O2'-CM2 |
| 81  | A3    | 2413 | OMU  | C3'-C2'-O2'-CM2 |
| 81  | A3    | 2200 | OMC  | O4'-C1'-N1-C6   |
| 81  | A3    | 2873 | 5MC  | O4'-C1'-N1-C6   |
| 3   | h1    | 1433 | OMG  | C4'-C5'-O5'-P   |
| 81  | A3    | 228  | PSU  | C3'-C4'-C5'-O5' |
| 81  | A3    | 946  | A2M  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2926 | PSU  | C3'-C4'-C5'-O5' |
| 3   | h1    | 598  | OMG  | C4'-C5'-O5'-P   |
| 81  | A3    | 2317 | PSU  | C4'-C5'-O5'-P   |
| 81  | A3    | 2873 | 5MC  | O4'-C1'-N1-C2   |
| 81  | A3    | 2926 | PSU  | C4'-C5'-O5'-P   |
| 81  | A3    | 2269 | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2873 | 5MC  | C2'-C1'-N1-C2   |
| 3   | h1    | 622  | A2M  | C2'-C1'-N9-C8   |
| 81  | A3    | 827  | A2M  | C4'-C5'-O5'-P   |
| 81  | A3    | 656  | 1MA  | C2'-C1'-N9-C8   |
| 81  | A3    | 144  | OMU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 1448 | OMC  | C2'-C1'-N1-C6   |
| 81  | A3    | 656  | 1MA  | C2'-C1'-N9-C4   |
| 81  | A3    | 1461 | OMG  | C4'-C5'-O5'-P   |
| 81  | A3    | 2804 | A2M  | C4'-C5'-O5'-P   |
| 81  | A3    | 1378 | A2M  | C3'-C4'-C5'-O5' |
| 3   | h1    | 584  | PSU  | O4'-C1'-C5-C4   |
| 3   | h1    | 1194 | B8N  | O4'-C1'-C5-C4   |
| 3   | h1    | 1308 | PSU  | O4'-C1'-C5-C4   |
| 81  | A3    | 2947 | PSU  | O4'-C1'-C5-C4   |
| 81  | A3    | 2412 | OMG  | C3'-C2'-O2'-CM2 |
| 81  | A3    | 1448 | OMC  | C2'-C1'-N1-C2   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | h1    | 258  | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2261 | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2263 | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 817  | A2M  | O4'-C1'-N9-C8   |
| 81  | A3    | 786  | PSU  | C3'-C4'-C5'-O5' |
| 81  | A3    | 2321 | PSU  | C3'-C4'-C5'-O5' |
| 81  | A3    | 369  | A2M  | C1'-C2'-O2'-CM' |
| 3   | h1    | 622  | A2M  | O4'-C1'-N9-C8   |
| 81  | A3    | 946  | A2M  | O4'-C4'-C5'-O5' |
| 81  | A3    | 2926 | PSU  | O4'-C4'-C5'-O5' |
| 3   | h1    | 584  | PSU  | O4'-C1'-C5-C6   |
| 3   | h1    | 1524 | PSU  | O4'-C1'-C5-C6   |
| 81  | A3    | 970  | PSU  | O4'-C1'-C5-C6   |
| 81  | A3    | 2947 | PSU  | O4'-C1'-C5-C6   |
| 81  | A3    | 2914 | A2M  | O4'-C1'-N9-C8   |
| 81  | A3    | 827  | A2M  | O4'-C4'-C5'-O5' |
| 3   | h1    | 1524 | PSU  | O4'-C4'-C5'-O5' |
| 81  | A3    | 1448 | OMC  | O4'-C4'-C5'-O5' |
| 3   | h1    | 614  | OMU  | C2'-C1'-N1-C2   |
| 3   | h1    | 544  | A2M  | C4'-C5'-O5'-P   |
| 3   | h1    | 1027 | PSU  | C4'-C5'-O5'-P   |
| 3   | h1    | 1272 | OMU  | C4'-C5'-O5'-P   |
| 81  | A3    | 660  | A2M  | C4'-C5'-O5'-P   |

There are no ring outliers.

57 monomers are involved in 74 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 81  | A3    | 2284 | A2M  | 2       | 0            |
| 3   | h1    | 1190 | PSU  | 1       | 0            |
| 81  | A3    | 369  | A2M  | 3       | 0            |
| 81  | A3    | 2653 | UY1  | 1       | 0            |
| 3   | h1    | 1283 | 4AC  | 1       | 0            |
| 3   | h1    | 1304 | PSU  | 1       | 0            |
| 3   | h1    | 1194 | B8N  | 3       | 0            |
| 81  | A3    | 2223 | A2M  | 2       | 0            |
| 81  | A3    | 1144 | A2M  | 1       | 0            |
| 3   | h1    | 1308 | PSU  | 1       | 0            |
| 81  | A3    | 674  | OMC  | 3       | 0            |
| 81  | A3    | 1460 | A2M  | 1       | 0            |
| 81  | A3    | 1482 | PSU  | 1       | 0            |
| 3   | h1    | 1447 | OMU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 81  | A3    | 2839 | OMC  | 1       | 0            |
| 81  | A3    | 2883 | PSU  | 1       | 0            |
| 81  | A3    | 918  | OMG  | 1       | 0            |
| 81  | A3    | 827  | A2M  | 1       | 0            |
| 81  | A3    | 2947 | PSU  | 1       | 0            |
| 81  | A3    | 2194 | PSU  | 1       | 0            |
| 81  | A3    | 464  | PSU  | 1       | 0            |
| 3   | h1    | 614  | OMU  | 1       | 0            |
| 81  | A3    | 399  | OMG  | 1       | 0            |
| 81  | A3    | 34   | PSU  | 1       | 0            |
| 3   | h1    | 1758 | A2M  | 1       | 0            |
| 81  | A3    | 3289 | OMU  | 2       | 0            |
| 3   | h1    | 1787 | PSU  | 1       | 0            |
| 3   | h1    | 28   | A2M  | 1       | 0            |
| 81  | A3    | 2398 | OMG  | 1       | 0            |
| 81  | A3    | 2732 | OMU  | 1       | 0            |
| 81  | A3    | 675  | OMU  | 1       | 0            |
| 81  | A3    | 970  | PSU  | 1       | 0            |
| 81  | A3    | 2261 | PSU  | 1       | 0            |
| 81  | A3    | 2317 | PSU  | 1       | 0            |
| 3   | h1    | 961  | PSU  | 1       | 0            |
| 3   | h1    | 1383 | OMU  | 1       | 0            |
| 3   | h1    | 1790 | MA6  | 2       | 0            |
| 81  | A3    | 2886 | OMU  | 3       | 0            |
| 81  | A3    | 2239 | OMG  | 1       | 0            |
| 3   | h1    | 1789 | MA6  | 3       | 0            |
| 3   | h1    | 1106 | PSU  | 1       | 0            |
| 3   | h1    | 762  | PSU  | 1       | 0            |
| 81  | A3    | 2412 | OMG  | 1       | 0            |
| 81  | A3    | 2804 | A2M  | 1       | 0            |
| 81  | A3    | 2368 | OMC  | 1       | 0            |
| 81  | A3    | 660  | A2M  | 2       | 0            |
| 81  | A3    | 2413 | OMU  | 1       | 0            |
| 3   | h1    | 392  | OMG  | 2       | 0            |
| 3   | h1    | 1645 | OMC  | 1       | 0            |
| 3   | h1    | 1781 | 4AC  | 2       | 0            |
| 3   | h1    | 977  | A2M  | 1       | 0            |
| 3   | h1    | 140  | OMC  | 1       | 0            |
| 81  | A3    | 2873 | 5MC  | 2       | 0            |
| 81  | A3    | 2962 | OMC  | 1       | 0            |
| 81  | A3    | 2747 | PSU  | 1       | 0            |
| 81  | A3    | 40   | OMC  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 81  | A3    | 2951 | OMC  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 290 ligands modelled in this entry, 283 are monoatomic - leaving 7 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 | $\# Z  > 2$ |
| 85  | SPD  | h1    | 2016 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 0.66 | 0           |
| 85  | SPD  | A3    | 3450 | -    | 9,9,9        | 0.31 | 0           | 8,8,8       | 0.51 | 0           |
| 86  | SPM  | A3    | 3451 | -    | 13,13,13     | 0.35 | 0           | 12,12,12    | 1.05 | 0           |
| 86  | SPM  | A3    | 3452 | -    | 13,13,13     | 0.37 | 0           | 12,12,12    | 1.03 | 0           |
| 86  | SPM  | h1    | 2017 | -    | 13,13,13     | 0.47 | 0           | 12,12,12    | 0.95 | 0           |
| 86  | SPM  | h1    | 2019 | -    | 13,13,13     | 0.42 | 0           | 12,12,12    | 1.03 | 0           |
| 86  | SPM  | h1    | 2018 | -    | 13,13,13     | 0.38 | 0           | 12,12,12    | 1.01 | 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 |
|-----|------|-------|------|------|---------|------------|-------|
| 85  | SPD  | h1    | 2016 | -    | -       | 4/7/7/7    | -     |
| 85  | SPD  | A3    | 3450 | -    | -       | 2/7/7/7    | -     |
| 86  | SPM  | A3    | 3451 | -    | -       | 5/11/11/11 | -     |
| 86  | SPM  | A3    | 3452 | -    | -       | 7/11/11/11 | -     |
| 86  | SPM  | h1    | 2017 | -    | -       | 5/11/11/11 | -     |
| 86  | SPM  | h1    | 2019 | -    | -       | 2/11/11/11 | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 86  | SPM  | h1    | 2018 | -    | -       | 3/11/11/11 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 86  | A3    | 3452 | SPM  | N10-C11-C12-C13 |
| 86  | A3    | 3452 | SPM  | C7-C8-C9-N10    |
| 86  | h1    | 2017 | SPM  | C7-C8-C9-N10    |
| 85  | h1    | 2016 | SPD  | C3-C4-C5-N6     |
| 85  | h1    | 2016 | SPD  | N6-C7-C8-C9     |
| 86  | h1    | 2017 | SPM  | N10-C11-C12-C13 |
| 85  | h1    | 2016 | SPD  | C4-C5-N6-C7     |
| 86  | A3    | 3452 | SPM  | N5-C6-C7-C8     |
| 86  | h1    | 2019 | SPM  | N5-C6-C7-C8     |
| 85  | h1    | 2016 | SPD  | C8-C7-N6-C5     |
| 86  | h1    | 2017 | SPM  | C8-C9-N10-C11   |
| 86  | A3    | 3451 | SPM  | C3-C4-N5-C6     |
| 86  | h1    | 2017 | SPM  | C11-C12-C13-N14 |
| 86  | A3    | 3451 | SPM  | N10-C11-C12-C13 |
| 85  | A3    | 3450 | SPD  | C2-C3-C4-C5     |
| 86  | h1    | 2018 | SPM  | C6-C7-C8-C9     |
| 86  | A3    | 3451 | SPM  | C7-C8-C9-N10    |
| 86  | A3    | 3452 | SPM  | C7-C6-N5-C4     |
| 86  | A3    | 3451 | SPM  | C8-C9-N10-C11   |
| 86  | h1    | 2019 | SPM  | C11-C12-C13-N14 |
| 86  | A3    | 3452 | SPM  | C2-C3-C4-N5     |
| 86  | h1    | 2017 | SPM  | C7-C6-N5-C4     |
| 86  | h1    | 2018 | SPM  | C7-C6-N5-C4     |
| 86  | A3    | 3452 | SPM  | C8-C9-N10-C11   |
| 86  | A3    | 3451 | SPM  | C11-C12-C13-N14 |
| 86  | A3    | 3452 | SPM  | C11-C12-C13-N14 |
| 86  | h1    | 2018 | SPM  | C8-C9-N10-C11   |
| 85  | A3    | 3450 | SPD  | C3-C4-C5-N6     |

There are no ring outliers.

5 monomers are involved in 12 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 85  | h1    | 2016 | SPD  | 2       | 0            |
| 85  | A3    | 3450 | SPD  | 6       | 0            |
| 86  | A3    | 3451 | SPM  | 1       | 0            |
| 86  | h1    | 2017 | SPM  | 2       | 0            |
| 86  | h1    | 2019 | SPM  | 1       | 0            |

## 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 |
|-----|-------|------------------|
| 81  | A3    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A3    | 2973:C    | O3'    | 2974:A    | P      | 4.08         |

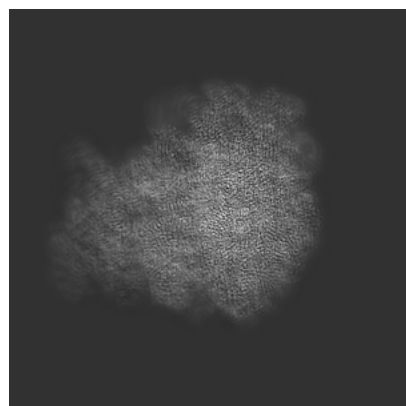
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15806. These allow visual inspection of the internal detail of the map and identification of artifacts.

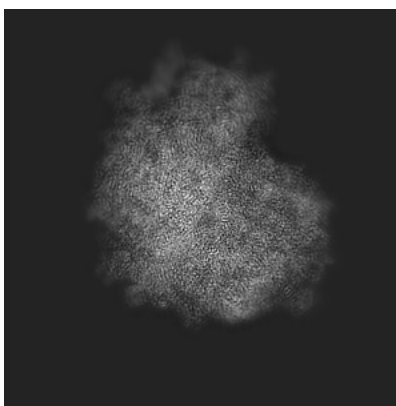
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

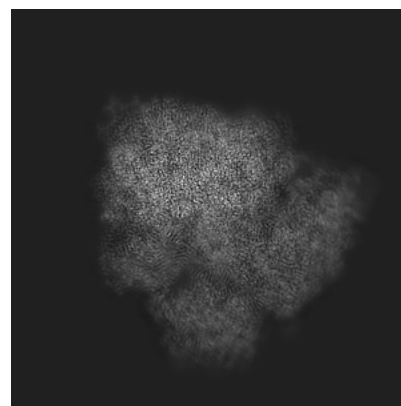
#### 6.1.1 Primary map



X

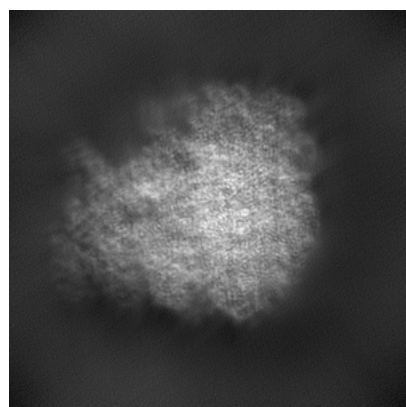


Y

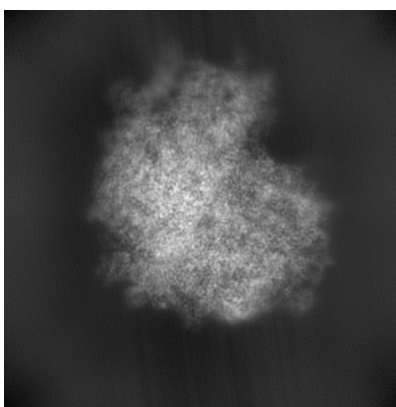


Z

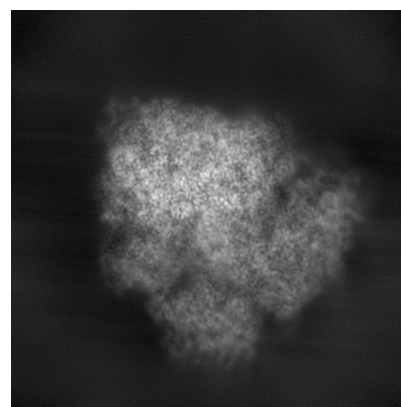
#### 6.1.2 Raw map



X



Y

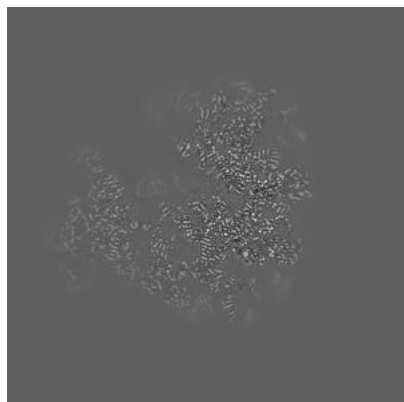


Z

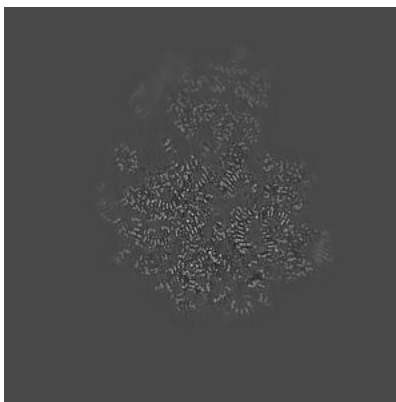
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

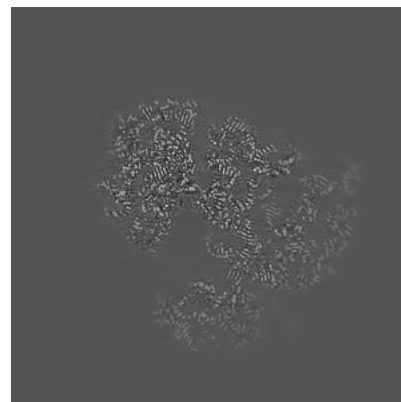
### 6.2.1 Primary map



X Index: 225

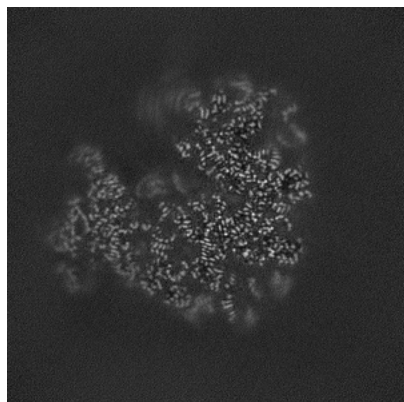


Y Index: 225

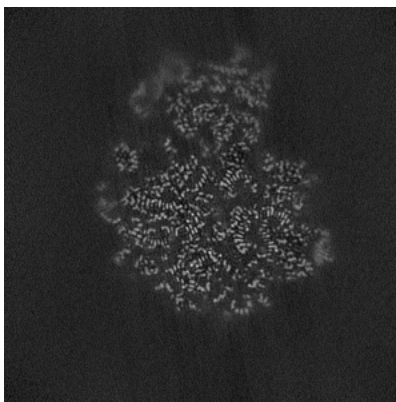


Z Index: 225

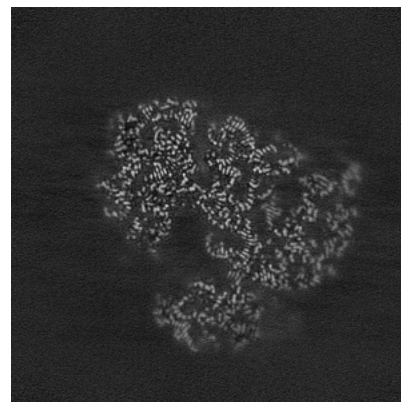
### 6.2.2 Raw map



X Index: 225



Y Index: 225

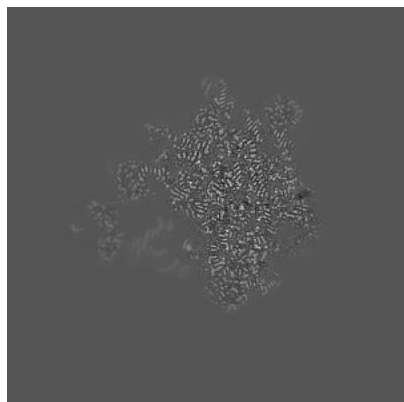


Z Index: 225

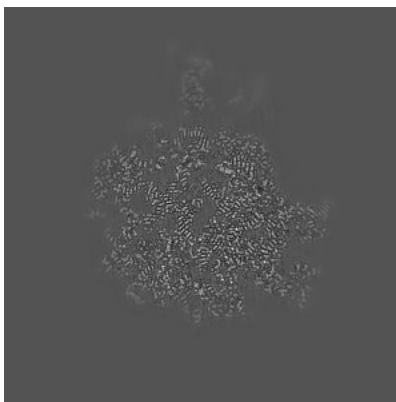
The images above show central slices of the map in three orthogonal directions.

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

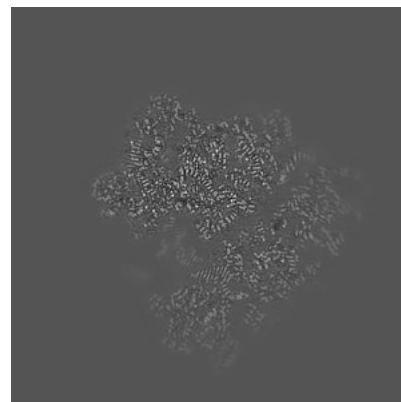
### 6.3.1 Primary map



X Index: 169

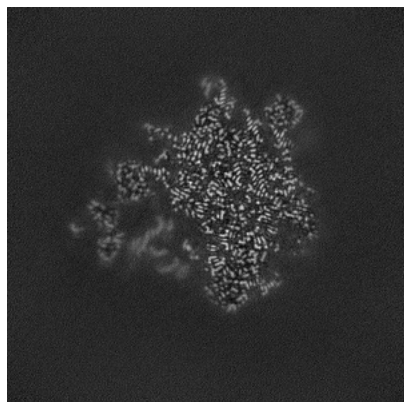


Y Index: 262

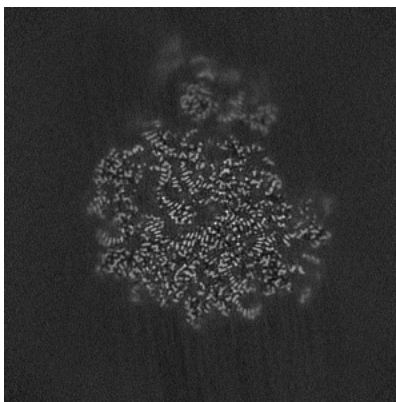


Z Index: 206

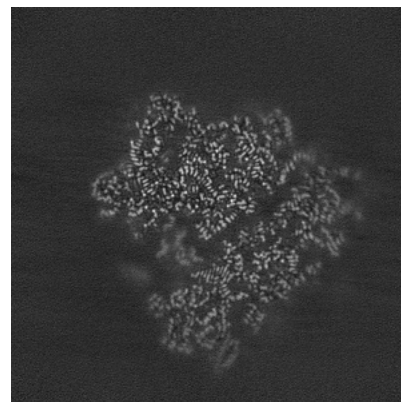
### 6.3.2 Raw map



X Index: 169



Y Index: 254

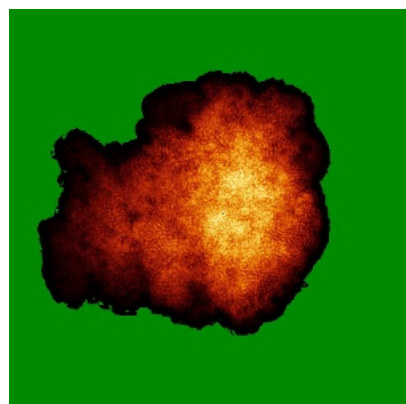


Z Index: 206

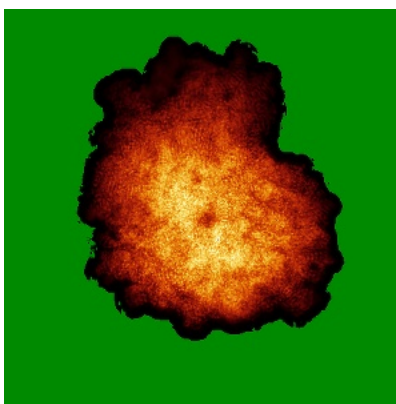
The images above show the largest variance slices of the map in three orthogonal directions.

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

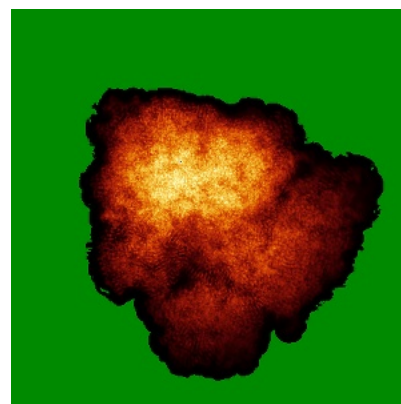
### 6.4.1 Primary map



X

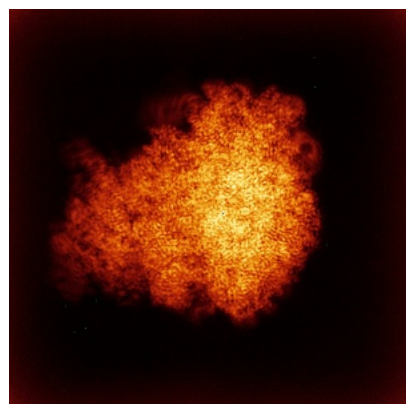


Y

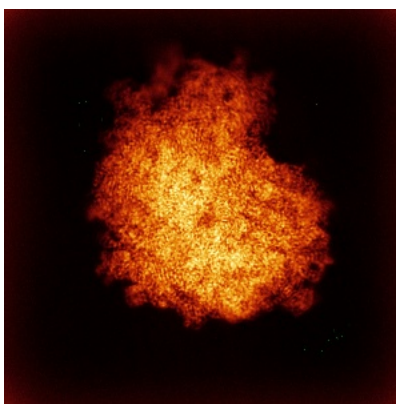


Z

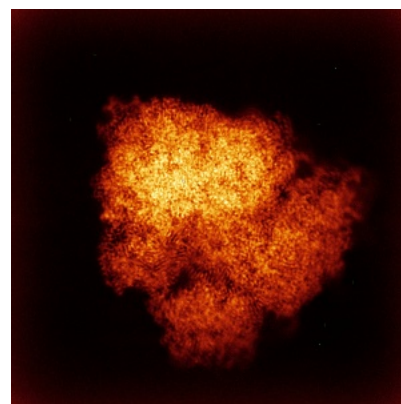
### 6.4.2 Raw map



X



Y

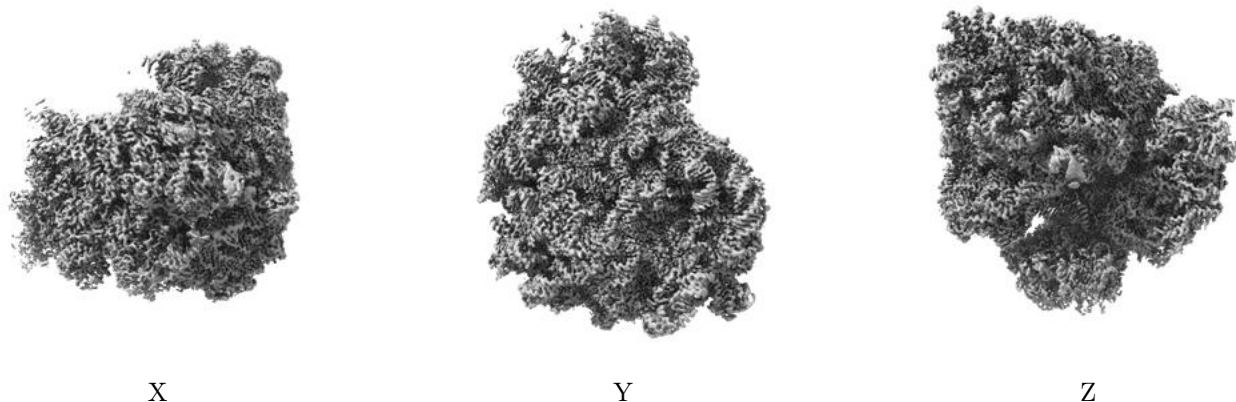


Z

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.

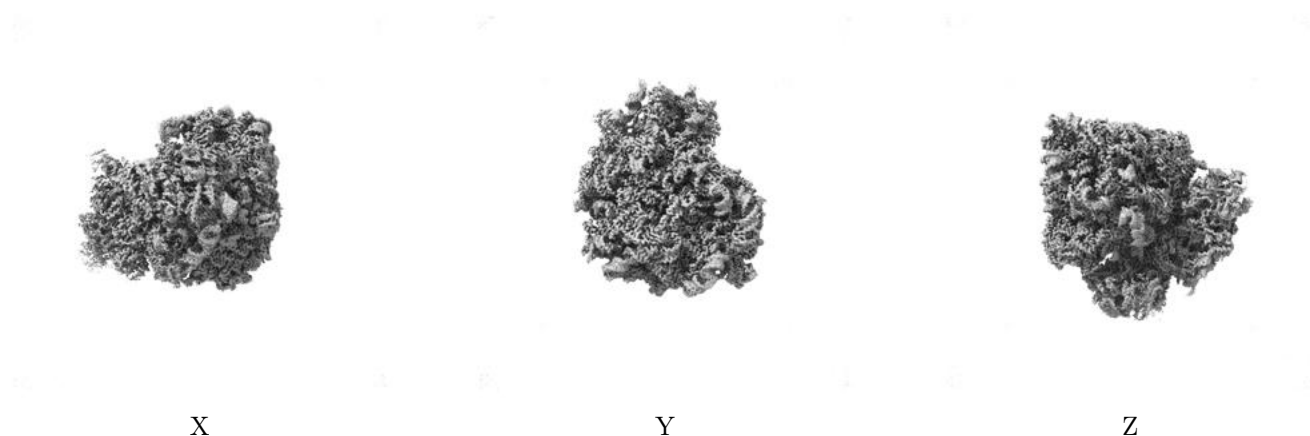
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

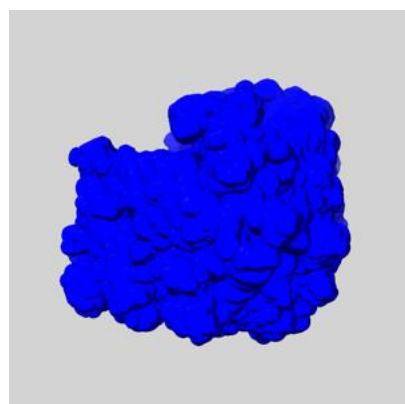
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

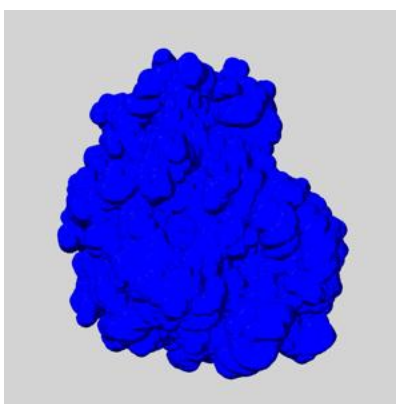
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

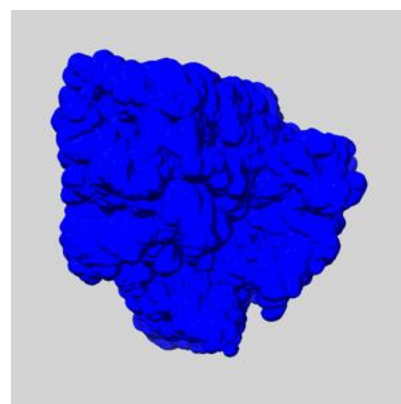
### 6.6.1 emd\_15806\_msk\_1.map [i](#)



X



Y

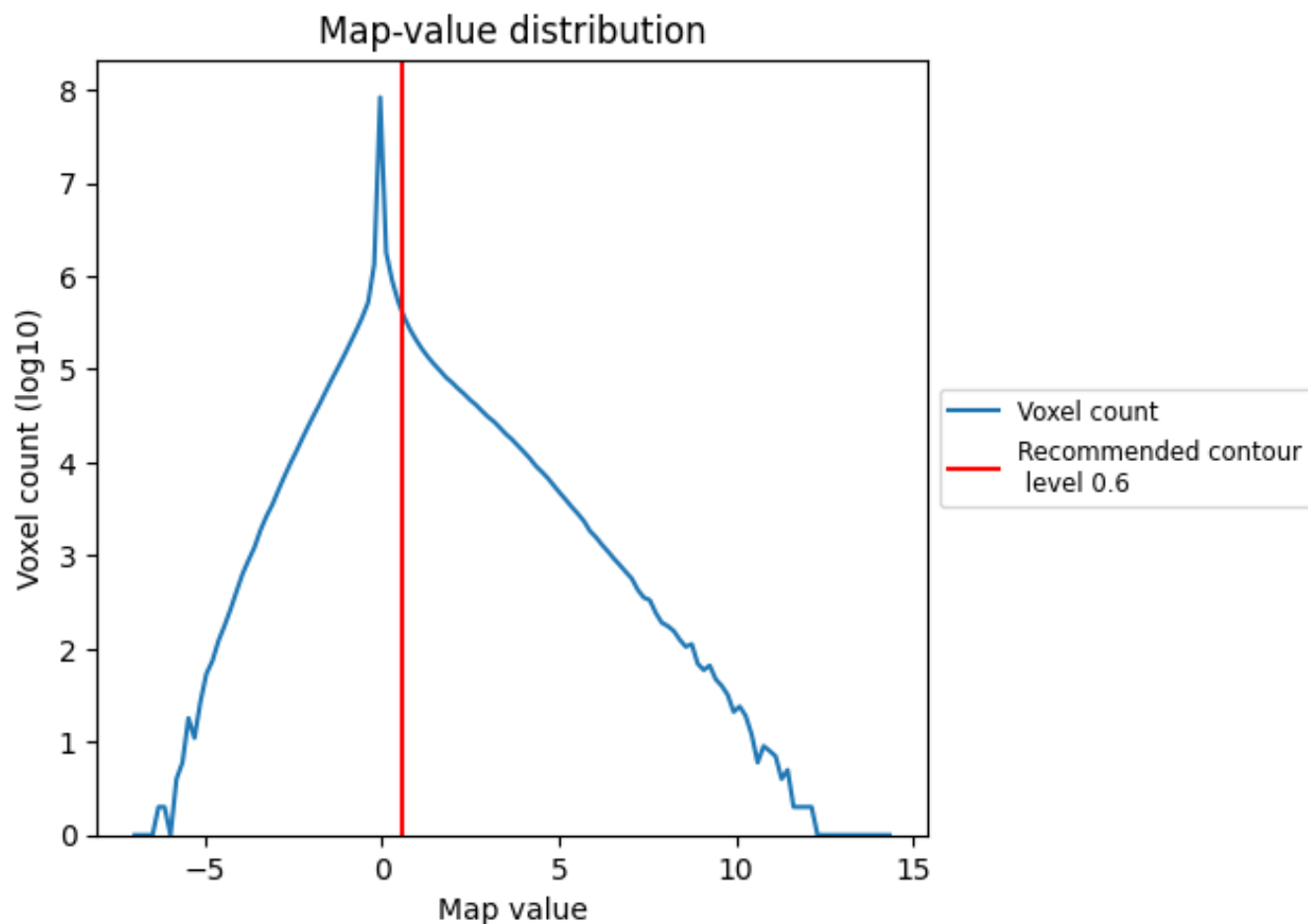


Z

## 7 Map analysis [i](#)

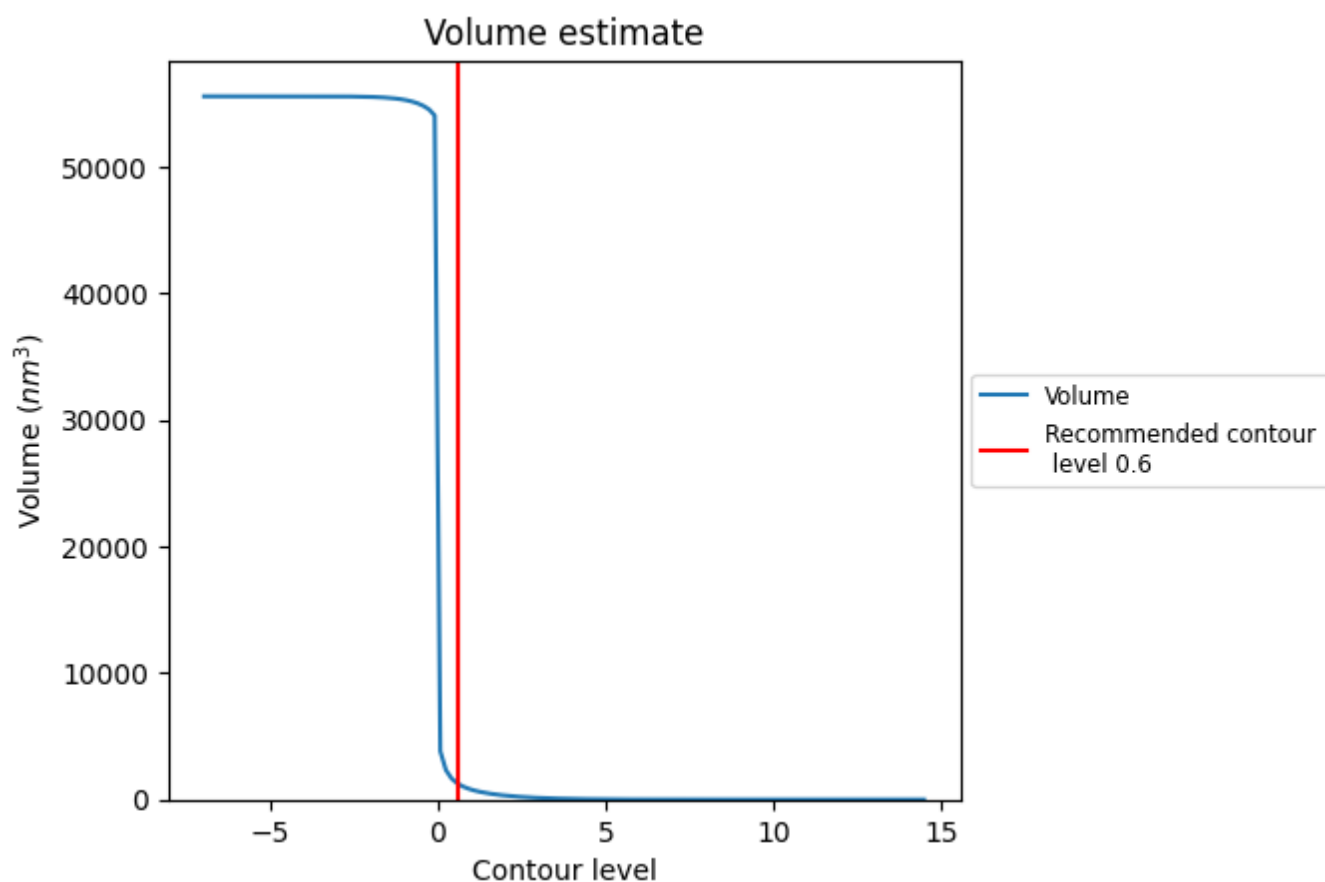
This section contains the results of statistical analysis of the map.

### 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.

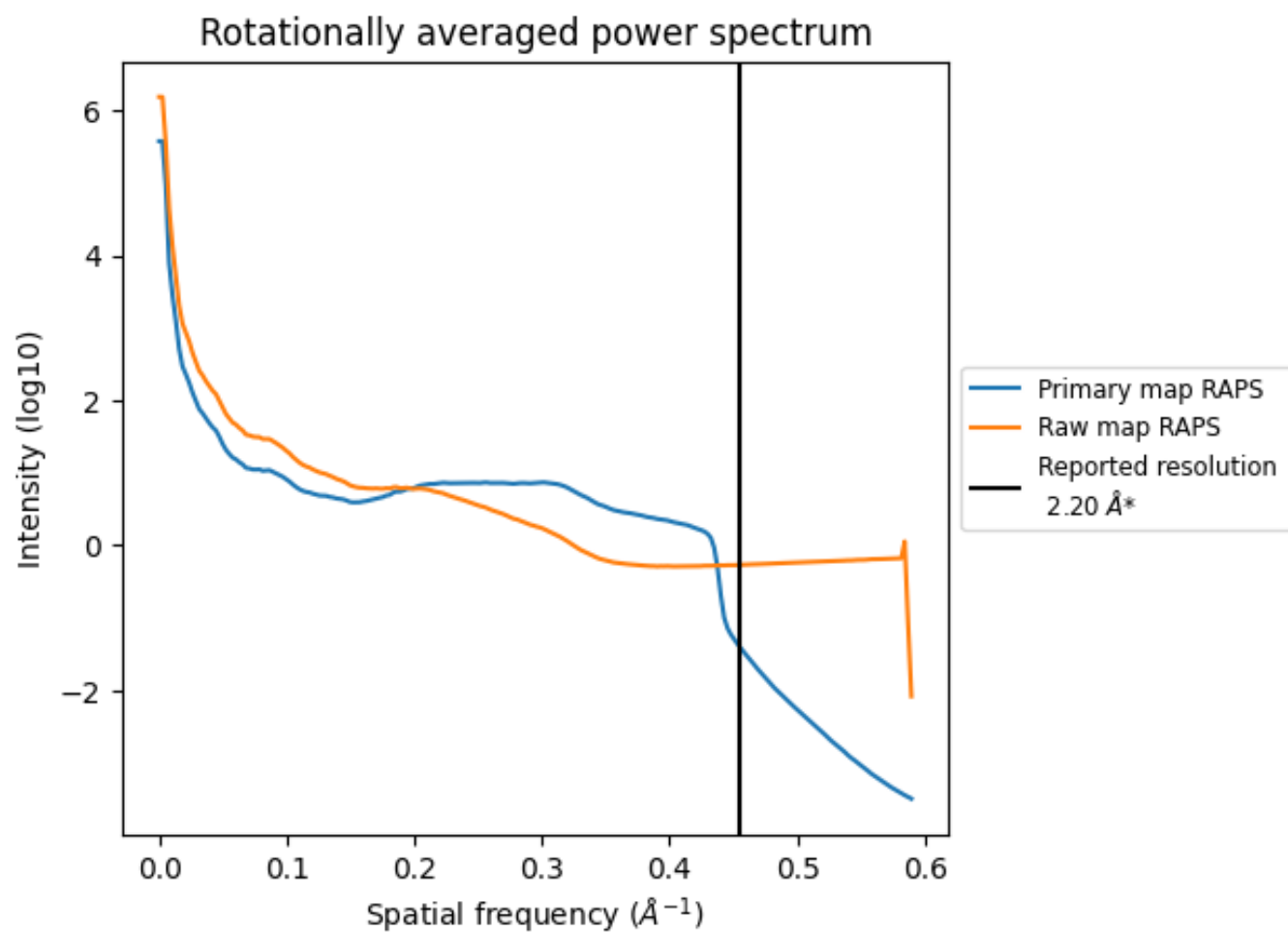
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1255  $\text{nm}^3$ ; this corresponds to an approximate mass of 1133 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 ⓘ

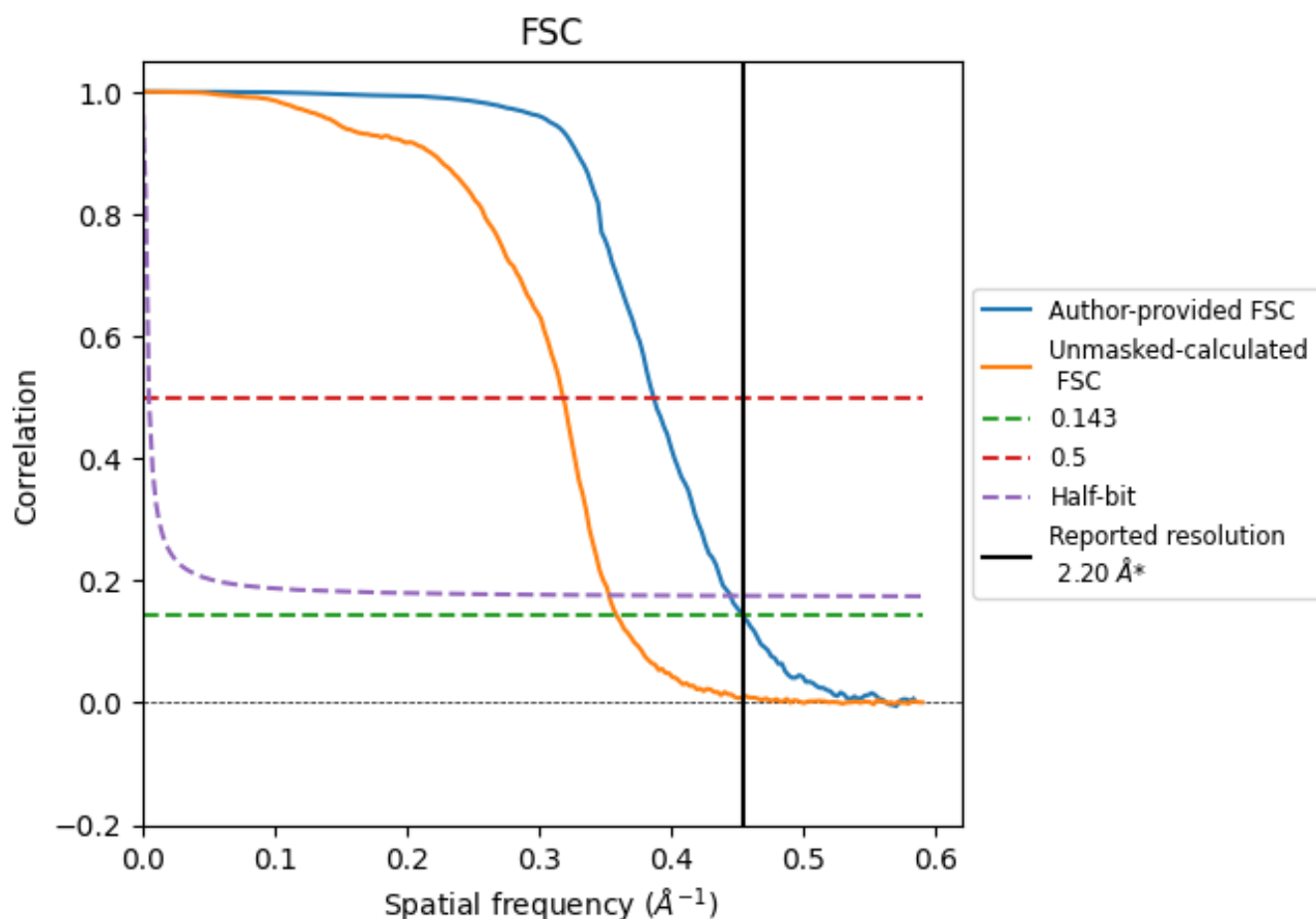


\*Reported resolution corresponds to spatial frequency of 0.455  $\text{\AA}^{-1}$

## 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 0.455  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

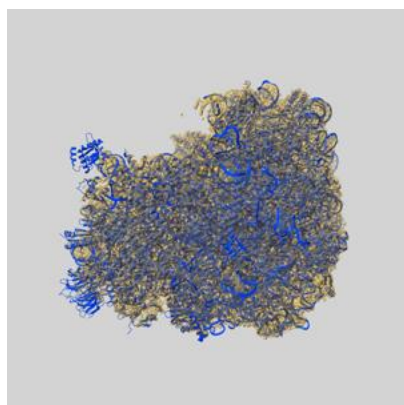
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.20                               | -    | -        |
| Author-provided FSC curve | 2.20                               | 2.59 | 2.25     |
| Unmasked-calculated*      | 2.79                               | 3.14 | 2.83     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.79 differs from the reported value 2.2 by more than 10 %

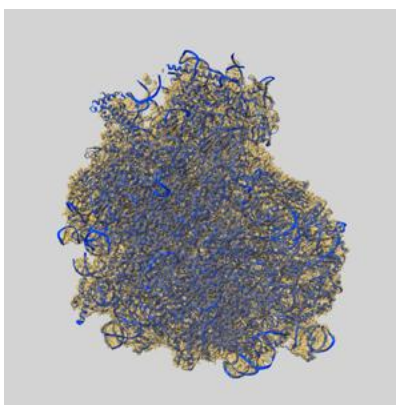
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15806 and PDB model 8B2L. Per-residue inclusion information can be found in section [3](#) on page [26](#).

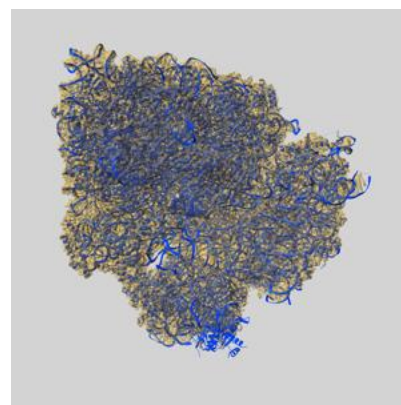
### 9.1 Map-model overlay [i](#)



X



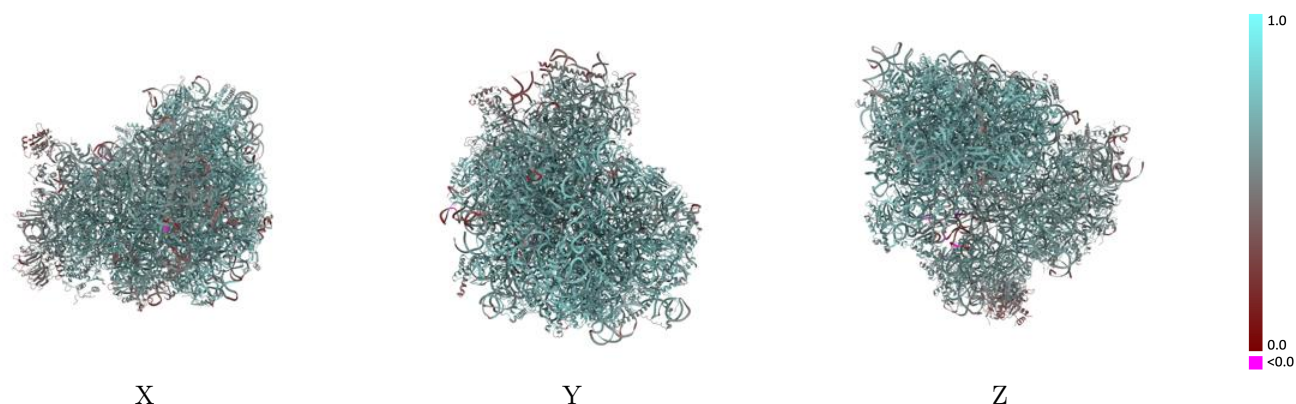
Y



Z

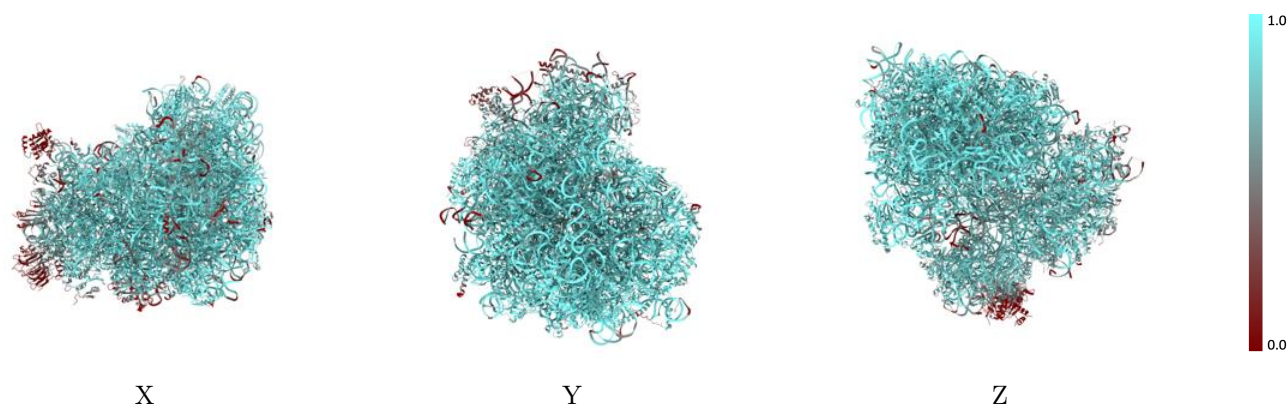
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



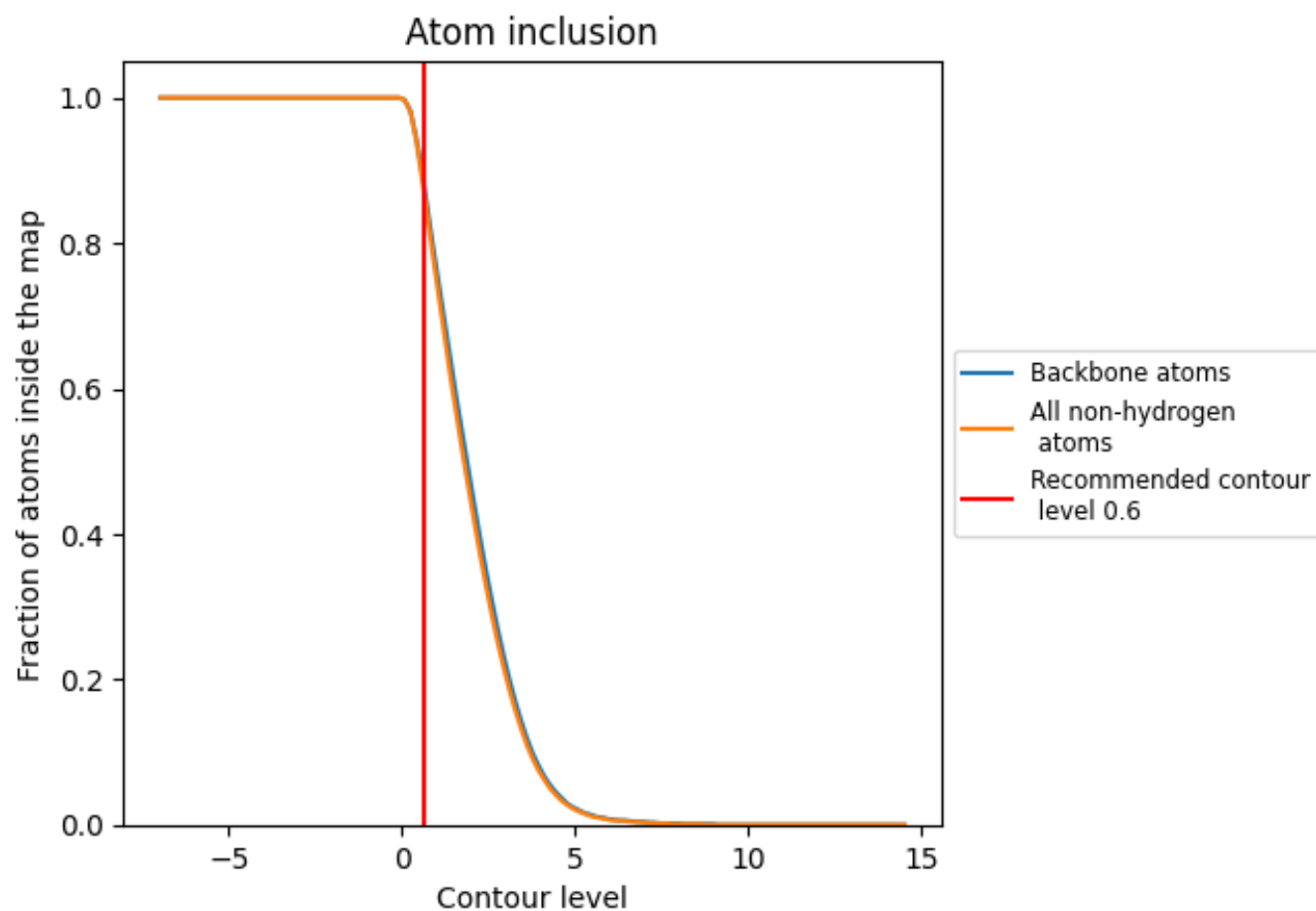
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8810   |  0.6390   |
| A1    |  0.8190   |  0.5960   |
| A3    |  0.9420   |  0.6580   |
| B1    |  0.8630   |  0.5920   |
| B3    |  0.9250   |  0.6540   |
| C1    |  0.0330   |  0.3580   |
| C3    |  0.9920   |  0.6690   |
| D1    |  0.5440   |  0.5170   |
| D3    |  0.9470   |  0.6870   |
| E1    |  0.7930   |  0.5800   |
| E3    |  0.9330   |  0.6720   |
| F1    |  0.8900   |  0.6410   |
| F3    |  0.9950   |  0.7280   |
| G1    |  0.8220   |  0.6030   |
| G3    |  0.9850  |  0.7180  |
| H1    |  0.6990 |  0.5590 |
| H3    |  0.8540 |  0.6410 |
| I1    |  0.6890 |  0.5490 |
| I3    |  0.9690 |  0.6980 |
| J1    |  0.9250 |  0.6660 |
| J3    |  0.9700 |  0.6940 |
| K1    |  0.7610 |  0.5970 |
| K3    |  0.7590 |  0.5600 |
| L1    |  0.7270 |  0.5640 |
| L3    |  0.9570 |  0.6940 |
| M1    |  0.7750 |  0.6010 |
| M3    |  0.9300 |  0.6620 |
| N1    |  0.1380 |  0.4170 |
| N3    |  0.9490 |  0.6890 |
| O1    |  0.5500 |  0.5350 |
| O3    |  0.9770 |  0.7160 |
| P1    |  0.8080 |  0.5880 |
| P3    |  0.9180 |  0.6510 |
| Q1    |  0.1780 |  0.4430 |
| Q3    |  0.8990 |  0.6680 |



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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| R1    | 0.5160         | 0.5290  |
| R3    | 0.9800         | 0.7230  |
| S1    | 0.9260         | 0.6540  |
| S3    | 0.9820         | 0.7150  |
| T1    | 0.9500         | 0.6840  |
| T3    | 0.9280         | 0.6820  |
| U1    | 0.8230         | 0.6030  |
| U3    | 0.9420         | 0.6640  |
| V1    | 0.8900         | 0.6270  |
| V3    | 0.9940         | 0.7270  |
| W1    | 0.8970         | 0.6440  |
| W2    | 0.7580         | 0.4970  |
| W3    | 0.8320         | 0.6110  |
| X1    | 0.8990         | 0.6400  |
| X3    | 0.9840         | 0.7200  |
| Y1    | 0.7710         | 0.5880  |
| Y3    | 0.9610         | 0.6930  |
| Z1    | 0.8330         | 0.6130  |
| Z3    | 0.9730         | 0.7140  |
| a1    | 0.6660         | 0.5540  |
| a3    | 0.9650         | 0.7040  |
| b1    | 0.8110         | 0.5990  |
| b3    | 0.8580         | 0.6320  |
| c1    | 0.8940         | 0.6520  |
| c3    | 0.8650         | 0.6390  |
| d1    | 0.7620         | 0.5730  |
| d3    | 0.9680         | 0.7060  |
| e1    | 0.9660         | 0.6780  |
| e3    | 0.9690         | 0.7020  |
| f1    | 0.7230         | 0.5770  |
| f3    | 0.9620         | 0.7020  |
| g3    | 0.9640         | 0.6900  |
| h1    | 0.9020         | 0.6130  |
| h3    | 0.8880         | 0.6410  |
| i2    | 0.6690         | 0.5070  |
| j3    | 0.9670         | 0.7050  |
| k1    | 0.6380         | 0.5290  |
| k3    | 0.9520         | 0.6830  |
| l1    | 0.5510         | 0.5210  |
| l3    | 0.3670         | 0.3350  |
| m3    | 0.9560         | 0.6860  |
| n3    | 0.9210         | 0.6620  |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| o3    |  0.9910 |  0.7270 |
| p3    |  0.9360 |  0.6640 |
| q3    |  0.9460 |  0.6940 |
| r3    |  0.9710 |  0.7100 |
| s3    |  0.9290 |  0.6870 |
| t3    |  0.8750 |  0.6240 |
| u3    |  0.9090 |  0.6590 |