



## Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 03:39 pm BST

PDB ID : 9RU9 / pdb\_00009ru9  
EMDB ID : EMD-54267  
Title : RPS26dC HEK mutant 80S ribosome bound to Kozak mRNA (RPS26dC-Kozak)  
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.  
Deposited on : 2025-07-03  
Resolution : 2.97 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:

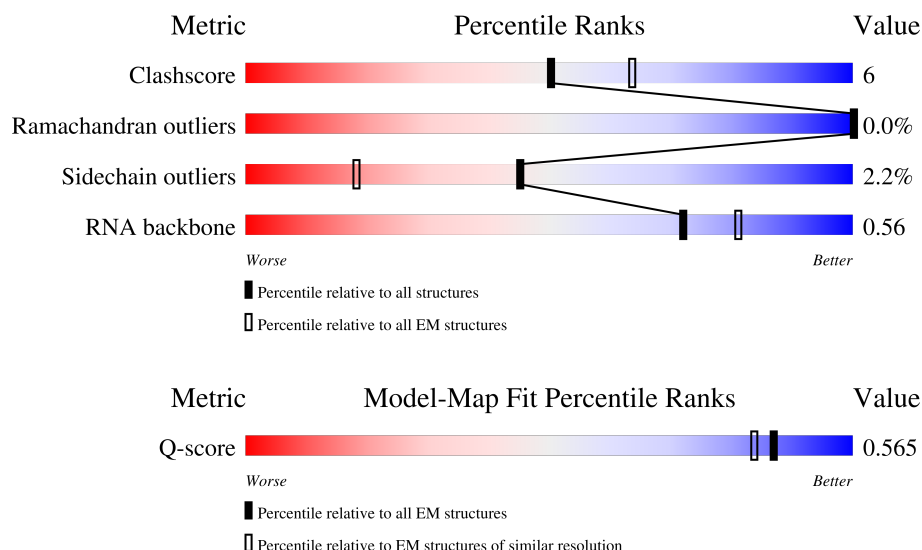
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 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                       | 13205 ( 2.47 - 3.47 )                                    |

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   | LA    | 257    |                  |
| 2   | SA    | 294    |                  |
| 3   | LB    | 403    |                  |

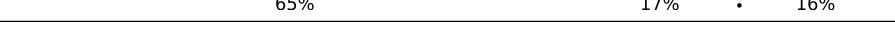
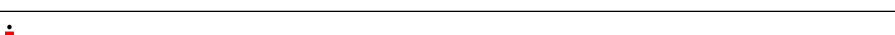
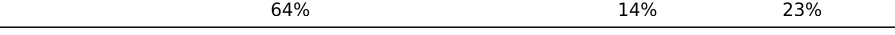
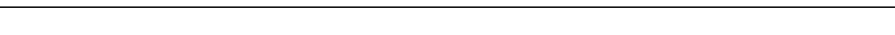
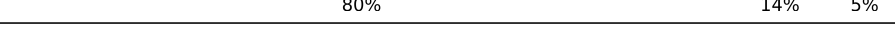
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | SB    | 264    |    |
| 5   | L8    | 156    |    |
| 6   | L7    | 120    |    |
| 7   | SD    | 243    |    |
| 8   | SJ    | 194    |    |
| 9   | SE    | 263    |    |
| 10  | SC    | 293    |    |
| 11  | SF    | 204    |    |
| 12  | SH    | 194    |    |
| 13  | SW    | 130    |    |
| 14  | SI    | 208    |    |
| 15  | SQ    | 146    |   |
| 16  | SU    | 119    |  |
| 17  | SK    | 165    |  |
| 18  | SO    | 151    |  |
| 19  | SX    | 143    |  |
| 20  | SM    | 132    |  |
| 21  | SS    | 152    |  |
| 22  | Sd    | 56     |  |
| 23  | SN    | 151    |  |
| 24  | SL    | 158    |  |
| 25  | SR    | 135    |  |
| 26  | SP    | 145    |  |
| 27  | ST    | 145    |  |
| 28  | SV    | 82     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | SY    | 133    |    |
| 30  | SZ    | 125    |    |
| 31  | Sa    | 115    |    |
| 32  | Sb    | 84     |    |
| 33  | Sc    | 69     |    |
| 34  | Se    | 133    |    |
| 35  | Sf    | 156    |    |
| 36  | Sg    | 317    |    |
| 37  | LC    | 427    |    |
| 38  | LJ    | 178    |    |
| 39  | LH    | 192    |   |
| 40  | LE    | 288    |  |
| 41  | LG    | 266    |  |
| 42  | LO    | 203    |  |
| 43  | LL    | 211    |  |
| 44  | LV    | 140    |  |
| 45  | LM    | 215    |  |
| 46  | La    | 148    |  |
| 47  | LN    | 204    |  |
| 48  | LI    | 214    |  |
| 49  | LD    | 297    |  |
| 50  | LQ    | 188    |  |
| 51  | LR    | 196    |  |
| 52  | LS    | 176    |  |
| 53  | LT    | 160    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | LP    | 184    |                  |
| 55  | LU    | 128    |                  |
| 56  | LX    | 156    |                  |
| 57  | LY    | 145    |                  |
| 58  | LZ    | 136    |                  |
| 59  | Lr    | 136    |                  |
| 60  | Lh    | 123    |                  |
| 61  | Lb    | 159    |                  |
| 62  | LF    | 248    |                  |
| 63  | Lc    | 115    |                  |
| 64  | Ld    | 125    |                  |
| 65  | Le    | 135    |                  |
| 66  | Lf    | 110    |                  |
| 67  | Lg    | 117    |                  |
| 68  | Li    | 105    |                  |
| 69  | Lj    | 97     |                  |
| 70  | Lk    | 70     |                  |
| 71  | Ll    | 51     |                  |
| 72  | Lm    | 128    |                  |
| 73  | Ln    | 25     |                  |
| 74  | Lo    | 106    |                  |
| 75  | Lp    | 92     |                  |
| 76  | Pt    | 77     |                  |
| 77  | mR    | 27     |                  |
| 78  | S2    | 1869   |                  |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 79  | L5    | 5069   | <br>44% 22% . 30% |
| 80  | Et    | 75     | <br>56% 36% 8%    |
| 81  | LW    | 157    | <br>35% . . 61%   |
| 82  | SG    | 249    | <br>71% 17% 12%   |

## 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 209052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | LA    | 250      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1921  | 1203 | 395 | 317 | 6 |         |       |

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | SA    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1692  | 1077 | 297 | 310 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| SA    | 2       | MET      | -      | initiating methionine | UNP P08865 |

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | LB    | 394      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3068  | 1956 | 583 | 515 | 14 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | SB    | 221      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1761  | 1118 | 319 | 310 | 14 |         |       |

- Molecule 5 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5   | L8    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3315  | 1481 | 585 | 1094 | 155 |         |       |

- Molecule 6 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 6   | L7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | SD    | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 1049 | 293 | 293 | 7 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | SJ    | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 944 | 298 | 233 | 2 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | SE    | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2044  | 1308 | 378 | 350 | 8 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | SC    | 220      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1685  | 1093 | 293 | 289 | 10 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | SF    | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1434  | 898 | 270 | 259 | 7 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | SH    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1409  | 903 | 262 | 243 | 1 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1030  | 657 | 193 | 174 | 6 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | SI    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1652  | 1036 | 328 | 283 | 5 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | SQ    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1109  | 707 | 210 | 189 | 3 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 16  | SU    | 101      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 519   | 313 | 101 | 105 |  |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | SK    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 678   | 437 | 122 | 114 | 5 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | SO    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 990   | 607 | 197 | 180 | 6 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | SX    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1088  | 687 | 215 | 183 | 3 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 20  | SM    | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 218   | 130 | 44 | 44 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| SM    | 105     | GLY      | GLN    | conflict | UNP P25398 |
| SM    | 106     | CYS      | ILE    | conflict | UNP P25398 |
| SM    | 107     | SER      | ASN    | conflict | UNP P25398 |
| SM    | 108     | CYS      | LEU    | conflict | UNP P25398 |
| SM    | 109     | VAL      | ILE    | conflict | UNP P25398 |
| SM    | 110     | VAL      | LYS    | conflict | UNP P25398 |

- Molecule 21 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | SS    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1184  | 746 | 244 | 193 | 1 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | Sd    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 458   | 286 | 94 | 73 | 5 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | SN    | 150      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1214  | 778 | 231 | 204 | 1 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | SL    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1148  | 731 | 215 | 196 | 6 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | SR    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1038  | 653 | 195 | 186 | 4 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | SP    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 665 | 198 | 179 | 7 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | ST    | 141      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1010  | 637 | 193 | 178 | 2 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | SV    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 628   | 388 | 116 | 120 | 4 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | SY    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 972   | 617 | 193 | 157 | 5 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | SZ    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 592   | 382 | 109 | 100 | 1 |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | Sa    | 98       | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 782   | 488 | 164 | 125 | 5 |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 403 | 118 | 114 | 7 |         |       |

- Molecule 33 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | Sc    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 274 | 86 | 87 | 2 |         |       |

- Molecule 34 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | Se    | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 373   | 227 | 84 | 61 | 1 |         |       |

- Molecule 35 is a protein called Ubiquitin.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | Sf    | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 194   | 116 | 37 | 38 | 3 |         |       |

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36  | Sg    | 311      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2387  | 1508 | 417 | 451 | 11 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | LC    | 366      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2914  | 1832 | 581 | 487 | 14 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | LJ    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1354  | 857 | 253 | 238 | 6 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | LE    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1786  | 1150 | 339 | 293 | 4 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | LG    | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1856  | 1182 | 359 | 311 | 4 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42  | LO    | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 1058 | 320 | 259 | 5 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43  | LL    | 206      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1662  | 1041 | 348 | 269 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| LL    | 112     | ALA      | THR    | conflict | UNP A0A6V7HLS0 |

- Molecule 44 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | LV    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 972   | 615 | 183 | 169 | 5 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | LM    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1116  | 716 | 214 | 179 | 7 |         |       |

- Molecule 46 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 729 | 235 | 185 | 3 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | LN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1700  | 1072 | 359 | 265 | 4 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | LI    | 203      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1645  | 1045 | 317 | 270 | 13 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | LD    | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2391  | 1513 | 436 | 428 | 14 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | LQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1512  | 944 | 314 | 249 | 5 |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | LR    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1476  | 914 | 317 | 236 | 9 |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 52  | LS    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1460  | 930 | 284 | 235 | 11 |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | LT    | 159      | Total | C   | N   | O   | S | 2       | 0     |
|     |       |          | 1311  | 833 | 256 | 216 | 6 |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | LP    | 153      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1249  | 781 | 243 | 216 | 9 |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | LU    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 804   | 515 | 140 | 147 | 2 |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | LX    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 966   | 618 | 181 | 166 | 1 |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | LY    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 691 | 223 | 185 | 3 |         |       |

- Molecule 58 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | LZ    | 135      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1115  | 719 | 211 | 182 | 3 |         |       |

- Molecule 59 is a protein called Large ribosomal subunit protein eL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | Lr    | 124      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1002  | 624 | 207 | 166 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| Lr    | 2       | MET      | -      | initiating methionine | UNP P46779 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1014  | 641 | 205 | 167 | 1 |         |       |

- Molecule 61 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | Lb    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 898   | 560 | 195 | 139 | 4 |         |       |

- Molecule 62 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 62  | LF    | 225      | Total | C    | N   | O   | S | 2       | 0     |
|     |       |          | 1885  | 1212 | 364 | 300 | 9 |         |       |

- Molecule 63 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | Lc    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 770   | 488 | 136 | 140 | 6 |         |       |

- Molecule 64 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | Ld    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 589   | 361 | 112 | 116 |   |         |       |

- Molecule 65 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | Le    | 128      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1061  | 672 | 219 | 165 | 5 |         |       |

- Molecule 66 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 555 | 174 | 143 | 3 |         |       |

- Molecule 67 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | Lg    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 548 | 180 | 141 | 6 |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | Li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 513 | 174 | 129 | 5 |         |       |

- Molecule 69 is a protein called Large ribosomal subunit protein eL37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | Lj    | 86       | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 712   | 439 | 157 | 111 | 5 |         |       |

- Molecule 70 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 70  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 568   | 366 | 103 | 98 | 1 |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 71  | Ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 437   | 278 | 95 | 63 | 1 |         |       |

- Molecule 72 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 72  | Lm    | 52       | Total | C   | N  | O  | S | 1       | 0     |
|     |       |          | 436   | 272 | 91 | 67 | 6 |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 73  | Ln    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 145 | 64 | 27 | 3 |         |       |

- Molecule 74 is a protein called Large ribosomal subunit protein eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | Lo    | 105      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 870   | 548 | 177 | 139 | 6 |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | Lp    | 91       | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 715   | 450 | 139 | 119 | 7 |         |       |

- Molecule 76 is a RNA chain called P site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 76  | Pt    | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1645  | 734 | 298 | 535 | 77 | 1 |         |       |

- Molecule 77 is a RNA chain called Kozak mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 77  | mR    | 7        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 156   | 69 | 32 | 48 | 7 |         |       |

- Molecule 78 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 78  | S2    | 1635     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 34940 | 15627 | 6260 | 11419 | 1634 |         |       |

- Molecule 79 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 79  | L5    | 3523     | Total | C     | N     | O     | P    | 1       | 0     |
|     |       |          | 75626 | 33716 | 13837 | 24550 | 3523 |         |       |

- Molecule 80 is a RNA chain called E site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 80  | Et    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 81 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 81  | LW    | 62       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 519   | 332 | 101 | 83 | 3 |         |       |

- Molecule 82 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 82  | SG    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1683  | 1053 | 337 | 286 | 7 |         |       |

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

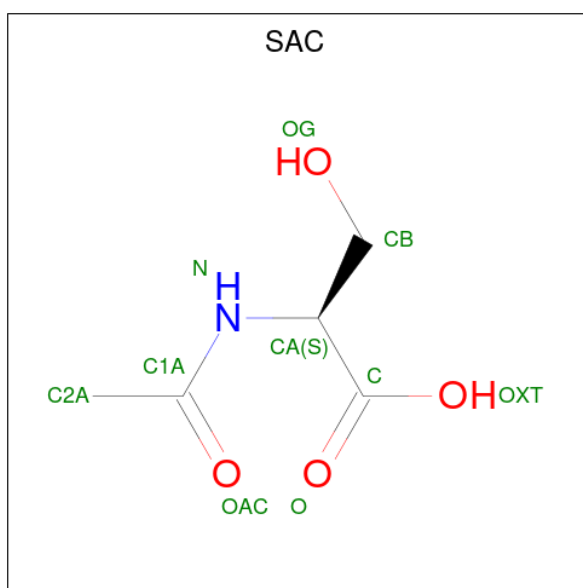
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 83  | LA    | 3        | Total | K | 0       |
|     |       |          | 3     | 3 |         |
| 83  | L8    | 3        | Total | K | 0       |
|     |       |          | 3     | 3 |         |
| 83  | L7    | 4        | Total | K | 0       |
|     |       |          | 4     | 4 |         |
| 83  | SO    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | SL    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | Sa    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | LH    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | LL    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | LN    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | LI    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | LQ    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 83  | Lb    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 83  | Le    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | Lf    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | Ll    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | mR    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | A     | 14       | Total | K  | 0       |
|     |       |          | 14    | 14 |         |

- Molecule 84 is N-ACETYL-SERINE (CCD ID: SAC) (formula:  $C_5H_9NO_4$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 84  | SA    | 1        | Total | C | N | O | 0       |
|     |       |          | 9     | 5 | 1 | 3 |         |
| 84  | Lr    | 1        | Total | C | N | O | 0       |
|     |       |          | 9     | 5 | 1 | 3 |         |

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 85  | LB    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 85  | L8    | 16       | Total | Mg | 0       |
|     |       |          | 16    | 16 |         |

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| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 85  | L7    | 15       | Total<br>15 | Mg<br>15 | 0       |
| 85  | SX    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | SS    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 85  | Sd    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | SN    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | ST    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LC    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LH    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LG    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LO    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 85  | LL    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LV    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | La    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LN    | 3        | Total<br>3  | Mg<br>3  | 0       |
| 85  | LD    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LQ    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 85  | LR    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LS    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | LP    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 85  | Lr    | 3        | Total<br>3  | Mg<br>3  | 0       |
| 85  | LF    | 1        | Total<br>1  | Mg<br>1  | 0       |

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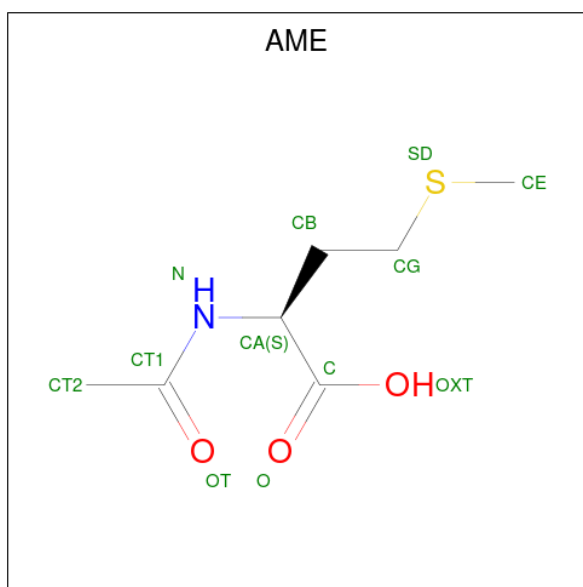
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| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 85  | Lc    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | Lf    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | Lg    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | Lj    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 85  | Lo    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | Lp    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 85  | Pt    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | Et    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 85  | D     | 12       | Total<br>12 | Mg<br>12 | 0       |

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

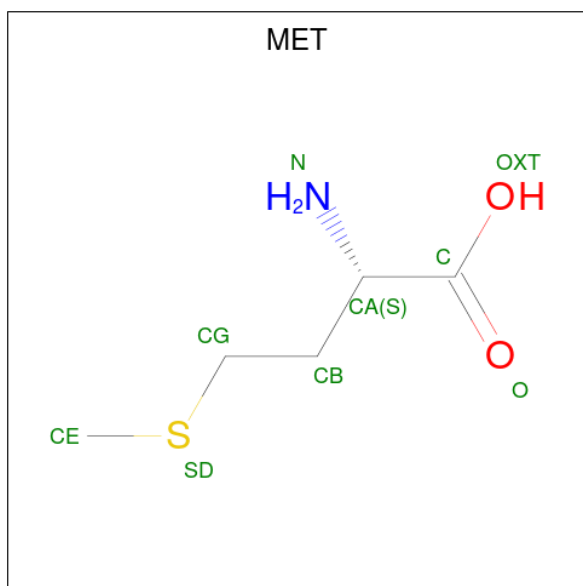
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 86  | Sd    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 86  | Sa    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 86  | Sf    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 86  | Lg    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 86  | Lj    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 86  | Lm    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 86  | Lo    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 86  | Lp    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 87 is N-ACETYLMETHIONINE (CCD ID: AME) (formula: C<sub>7</sub>H<sub>13</sub>NO<sub>3</sub>S).



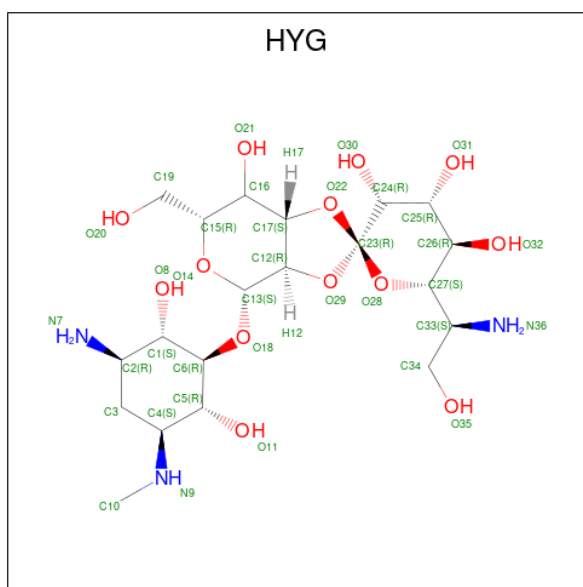
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 87  | SV    | 1        | Total | C | N | O | S | 0       |
|     |       |          | 11    | 7 | 1 | 2 | 1 |         |

- Molecule 88 is METHIONINE (CCD ID: MET) (formula:  $C_5H_{11}NO_2S$ ).



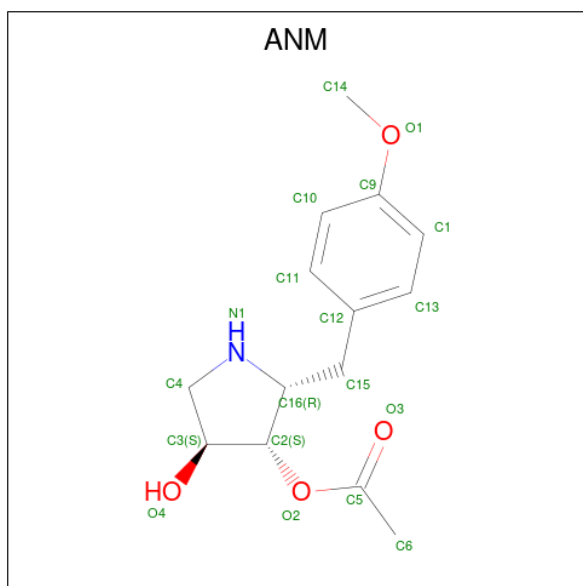
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 88  | Pt    | 1        | Total | C | N | O | S | 0       |
|     |       |          | 8     | 5 | 1 | 1 | 1 |         |

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula:  $C_{20}H_{37}N_3O_{13}$ ).



| Mol | Chain | Residues | Atoms |    |   |    | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 89  | S2    | 1        | Total | C  | N | O  | 0       |
|     |       |          | 36    | 20 | 3 | 13 |         |

- Molecule 90 is ANISOMYCIN (CCD ID: ANM) (formula:  $C_{14}H_{19}NO_4$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 90  | L5    | 1        | Total | C  | N | O | 0       |
|     |       |          | 19    | 14 | 1 | 4 |         |

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

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 91  | C     | 7        | Total | Na | 0       |
|     |       |          | 7     | 7  |         |

- Molecule 92 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 92  | LA    | 48       | Total | O  | 0       |
|     |       |          | 48    | 48 |         |
| 92  | LB    | 42       | Total | O  | 0       |
|     |       |          | 42    | 42 |         |
| 92  | L8    | 67       | Total | O  | 0       |
|     |       |          | 67    | 67 |         |
| 92  | L7    | 38       | Total | O  | 0       |
|     |       |          | 38    | 38 |         |
| 92  | SE    | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 92  | SO    | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |
| 92  | SN    | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 92  | SL    | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 92  | Sa    | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |
| 92  | LC    | 59       | Total | O  | 0       |
|     |       |          | 59    | 59 |         |
| 92  | LJ    | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 92  | LH    | 3        | Total | O  | 0       |
|     |       |          | 3     | 3  |         |
| 92  | LE    | 6        | Total | O  | 0       |
|     |       |          | 6     | 6  |         |
| 92  | LG    | 7        | Total | O  | 0       |
|     |       |          | 7     | 7  |         |
| 92  | LO    | 29       | Total | O  | 0       |
|     |       |          | 29    | 29 |         |
| 92  | LL    | 26       | Total | O  | 0       |
|     |       |          | 26    | 26 |         |
| 92  | LV    | 10       | Total | O  | 0       |
|     |       |          | 10    | 10 |         |
| 92  | LM    | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |
| 92  | La    | 26       | Total | O  | 0       |
|     |       |          | 26    | 26 |         |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 92  | LN    | 40       | Total<br>40 | O<br>40 | 0       |
| 92  | LI    | 11       | Total<br>11 | O<br>11 | 0       |
| 92  | LD    | 11       | Total<br>11 | O<br>11 | 0       |
| 92  | LQ    | 36       | Total<br>36 | O<br>36 | 0       |
| 92  | LR    | 17       | Total<br>17 | O<br>17 | 0       |
| 92  | LS    | 14       | Total<br>14 | O<br>14 | 0       |
| 92  | LT    | 18       | Total<br>18 | O<br>18 | 0       |
| 92  | LP    | 17       | Total<br>17 | O<br>17 | 0       |
| 92  | LU    | 1        | Total<br>1  | O<br>1  | 0       |
| 92  | LX    | 7        | Total<br>7  | O<br>7  | 0       |
| 92  | LY    | 10       | Total<br>10 | O<br>10 | 0       |
| 92  | LZ    | 5        | Total<br>5  | O<br>5  | 0       |
| 92  | Lr    | 12       | Total<br>12 | O<br>12 | 0       |
| 92  | Lh    | 5        | Total<br>5  | O<br>5  | 0       |
| 92  | Lb    | 10       | Total<br>10 | O<br>10 | 0       |
| 92  | LF    | 30       | Total<br>30 | O<br>30 | 0       |
| 92  | Lc    | 4        | Total<br>4  | O<br>4  | 0       |
| 92  | Ld    | 9        | Total<br>9  | O<br>9  | 0       |
| 92  | Le    | 28       | Total<br>28 | O<br>28 | 0       |
| 92  | Lf    | 16       | Total<br>16 | O<br>16 | 0       |
| 92  | Lg    | 22       | Total<br>22 | O<br>22 | 0       |

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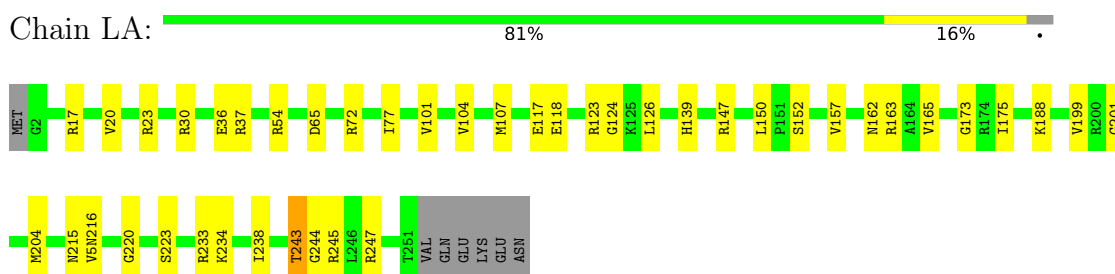
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 92  | Li    | 2        | Total<br>2  | O<br>2  | 0       |
| 92  | Lj    | 19       | Total<br>19 | O<br>19 | 0       |
| 92  | Lk    | 2        | Total<br>2  | O<br>2  | 0       |
| 92  | Ll    | 8        | Total<br>8  | O<br>8  | 0       |
| 92  | Lm    | 2        | Total<br>2  | O<br>2  | 0       |
| 92  | Ln    | 1        | Total<br>1  | O<br>1  | 0       |
| 92  | Lo    | 12       | Total<br>12 | O<br>12 | 0       |
| 92  | Lp    | 14       | Total<br>14 | O<br>14 | 0       |
| 92  | Pt    | 1        | Total<br>1  | O<br>1  | 0       |
| 92  | B     | 18       | Total<br>18 | O<br>18 | 0       |

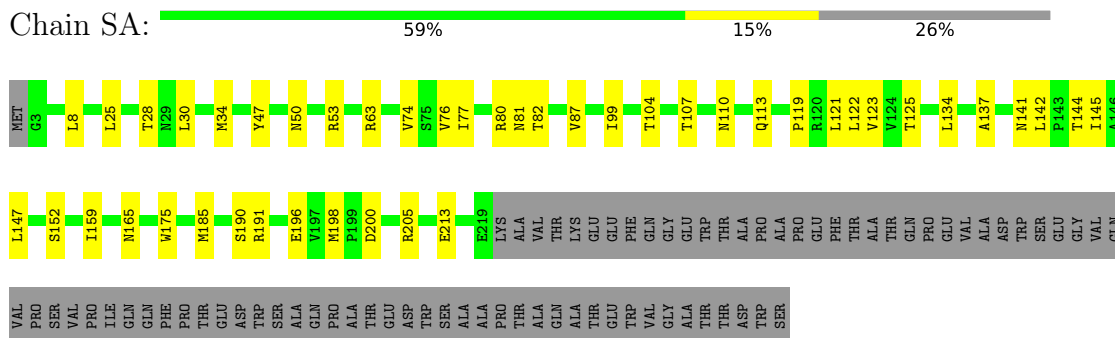
### 3 Residue-property plots

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

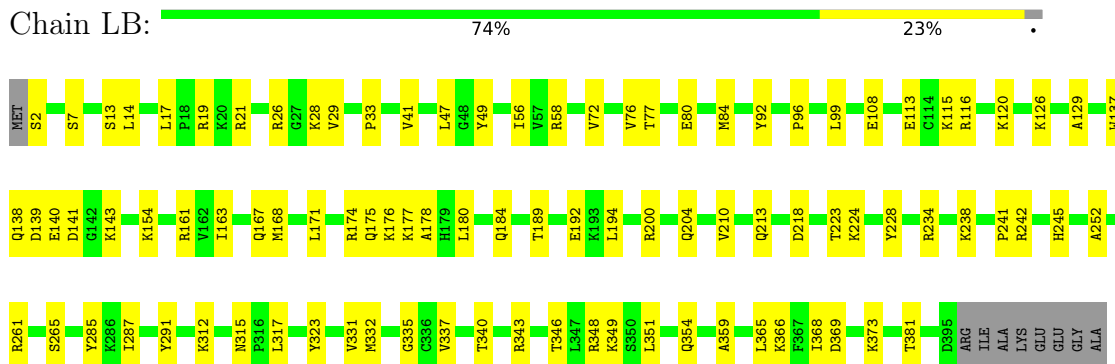
- Molecule 1: Large ribosomal subunit protein uL2



- Molecule 2: Small ribosomal subunit protein uS2

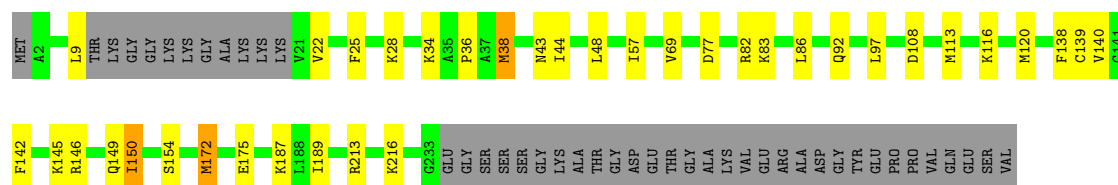


- Molecule 3: Large ribosomal subunit protein uL3



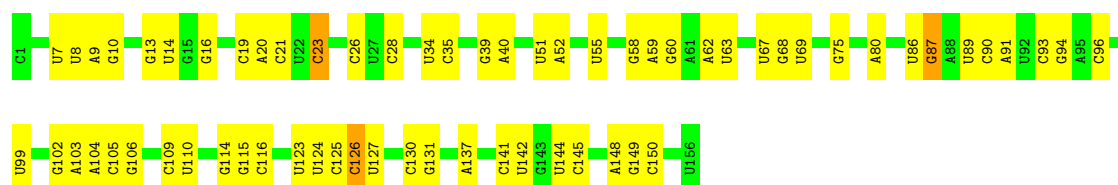
- Molecule 4: 40S ribosomal protein S3a

Chain SB:  70% 13% 16%



• Molecule 5: 5.8S rRNA

Chain L8:  59% 39%



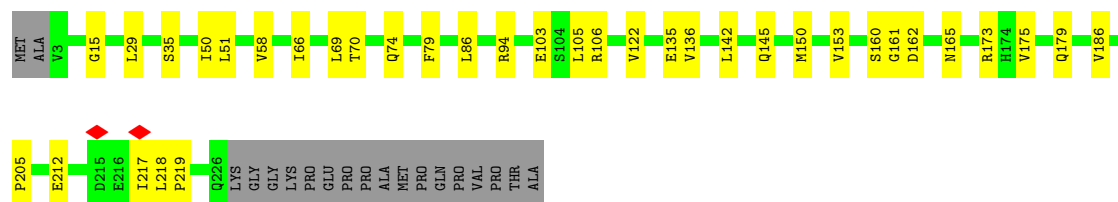
• Molecule 6: 5S rRNA

Chain L7:  63% 36%



• Molecule 7: 40S ribosomal protein S3

Chain SD:  77% 15% 8%



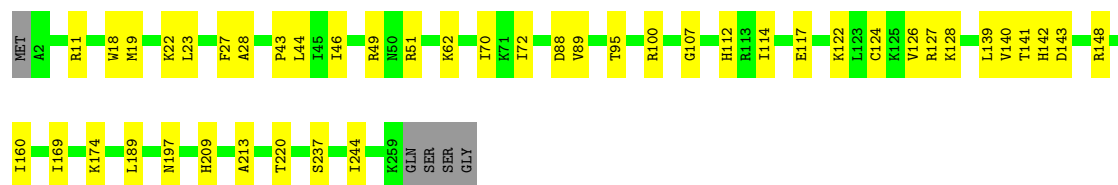
• Molecule 8: 40S ribosomal protein S9

Chain SJ:  83% 9% 8%



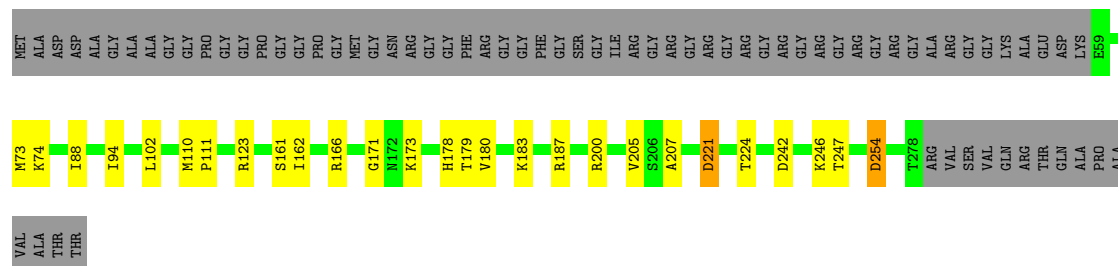
• Molecule 9: Small ribosomal subunit protein eS4, X isoform

Chain SE:  81% 17%



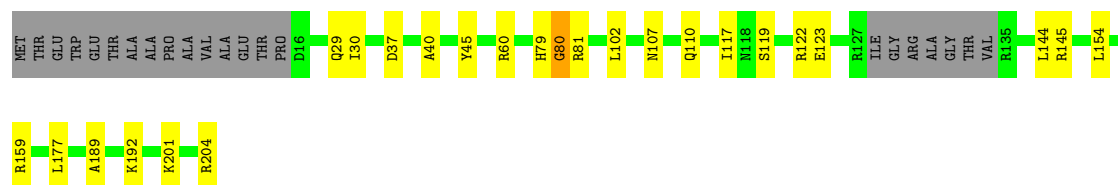
- Molecule 10: 40S ribosomal protein S2

Chain SC: 66% 9% 25%



- Molecule 11: 40S ribosomal protein S5

Chain SF: 77% 12% 11%



- Molecule 12: 40S ribosomal protein S7

Chain SH: 85% 9% 6%



- Molecule 13: 40S ribosomal protein S15a

Chain SW: 82% 17% 1%



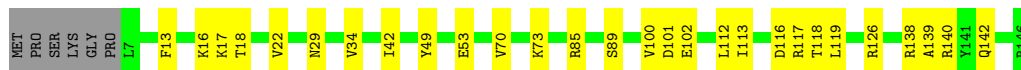
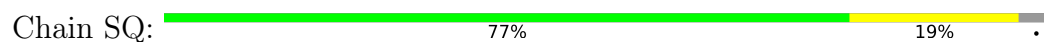
- Molecule 14: 40S ribosomal protein S8

Chain SI: 80% 19% 1%

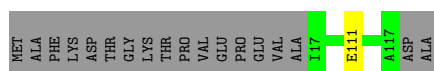




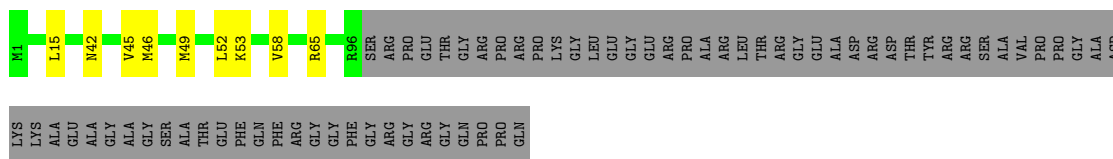
- Molecule 15: 40S ribosomal protein S16



- Molecule 16: 40S ribosomal protein S20



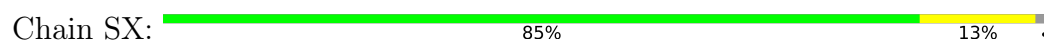
- Molecule 17: 40S ribosomal protein S10



- Molecule 18: 40S ribosomal protein S14

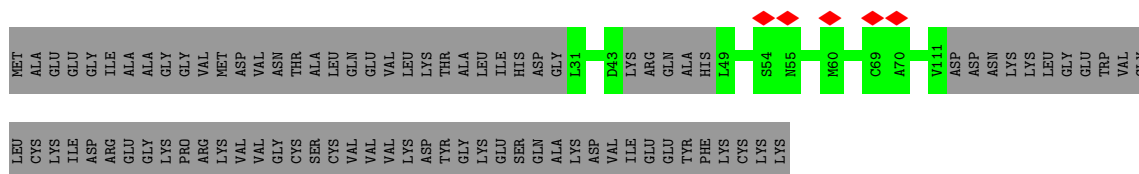


- Molecule 19: 40S ribosomal protein S23



- Molecule 20: Small ribosomal subunit protein eS12





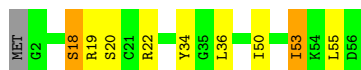
- Molecule 21: 40S ribosomal protein S18

Chain SS: 71% 26% .



- Molecule 22: 40S ribosomal protein S29

Chain Sd: 82% 12% . .



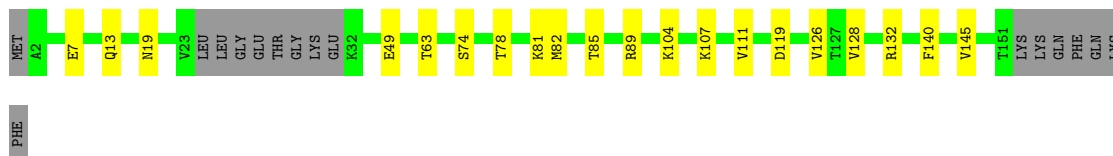
- Molecule 23: 40S ribosomal protein S13

Chain SN: 80% 19% .



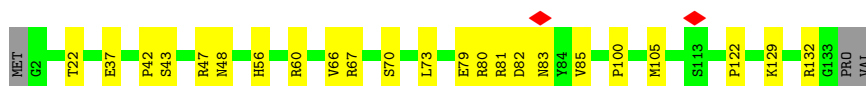
- Molecule 24: 40S ribosomal protein S11

Chain SL: 77% 13% 10%



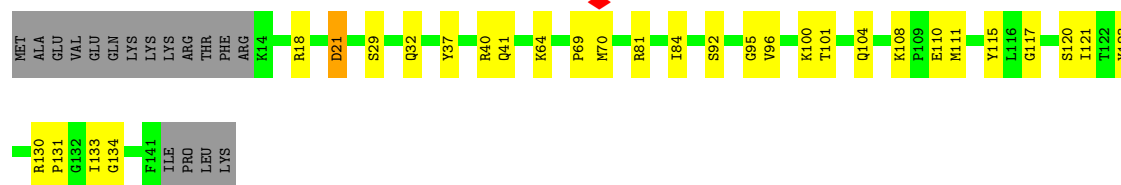
- Molecule 25: 40S ribosomal protein S17

Chain SR: 81% 17% .



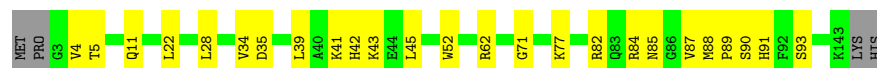
- Molecule 26: 40S ribosomal protein S15

Chain SP:  68% 20% 12%



- Molecule 27: 40S ribosomal protein S19

Chain ST:  80% 17%



- Molecule 28: Small ribosomal subunit protein eS21

Chain SV:  89% 11%



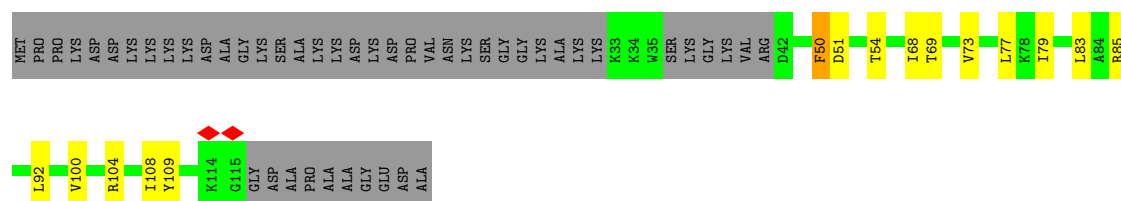
- Molecule 29: 40S ribosomal protein S24

Chain SY:  78% 14% 8%



- Molecule 30: 40S ribosomal protein S25

Chain SZ:  50% 11% 38%



- Molecule 31: 40S ribosomal protein S26

Chain Sa:  76% 10% 15%



- Molecule 32: 40S ribosomal protein S27

Chain Sb:  85% 14%



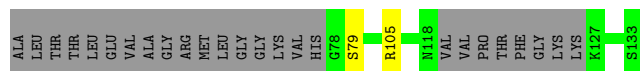
- Molecule 33: 40S ribosomal protein S28

Chain Sc:  65% 17% 16%



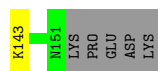
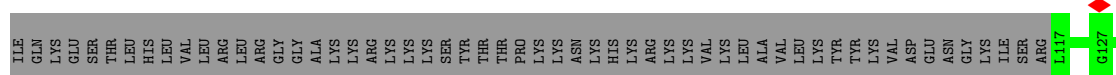
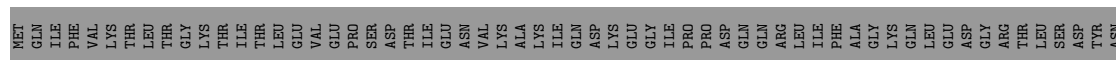
- Molecule 34: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:  35% 64%



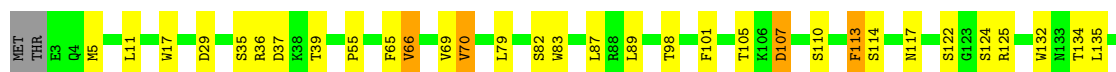
- Molecule 35: Ubiquitin

Chain Sf:  22% 78%

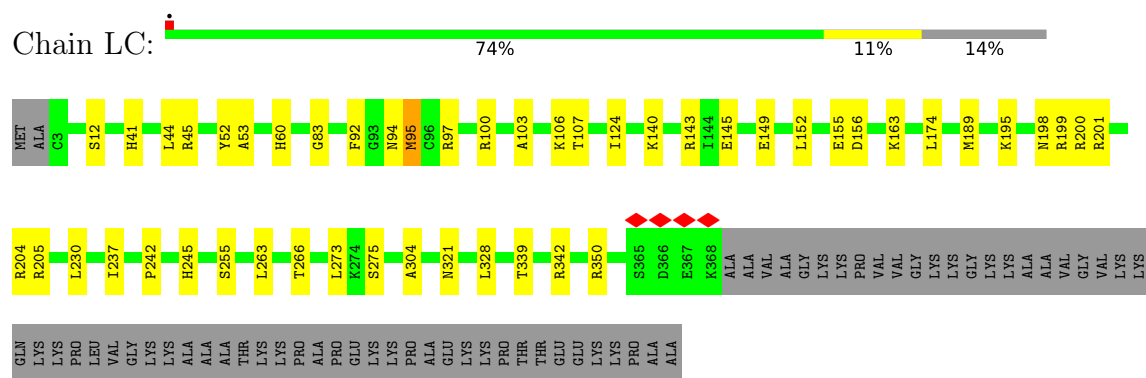


- Molecule 36: Receptor of activated protein C kinase 1

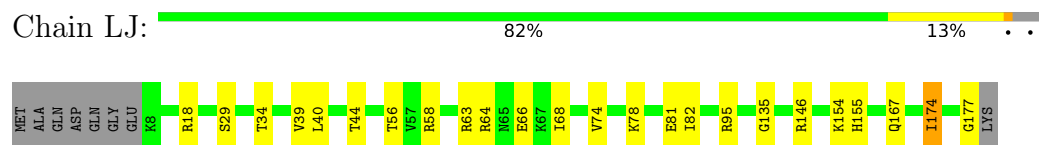
Chain Sg:  74% 23%



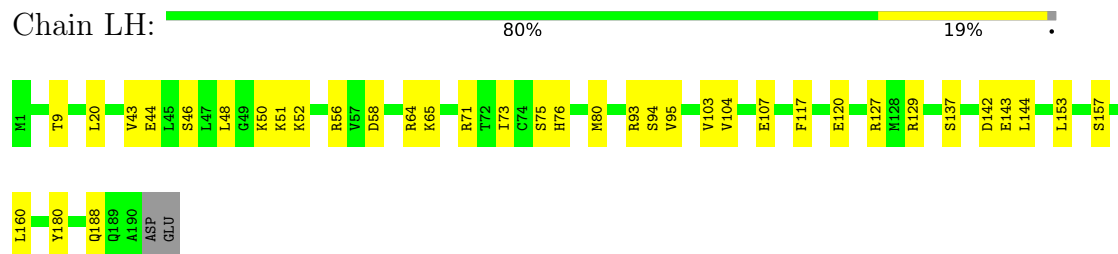
- Molecule 37: 60S ribosomal protein L4



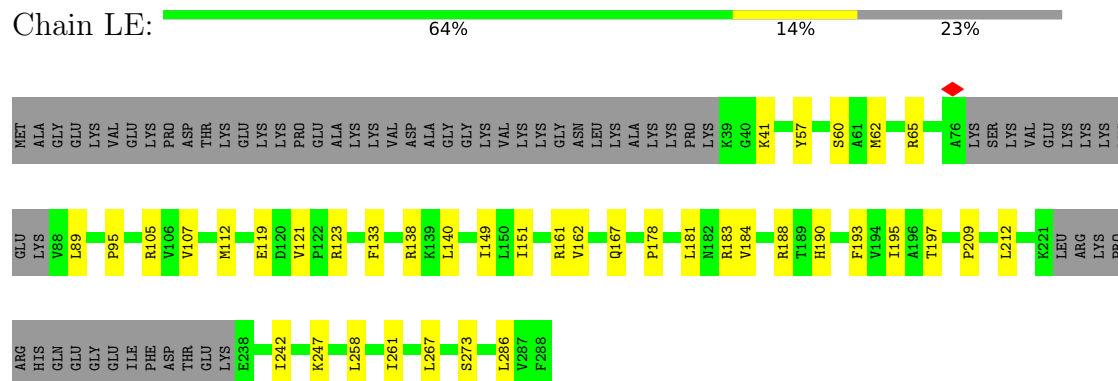
- Molecule 38: 60S ribosomal protein L11



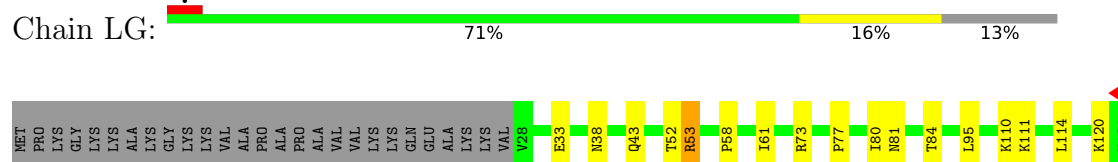
- Molecule 39: 60S ribosomal protein L9

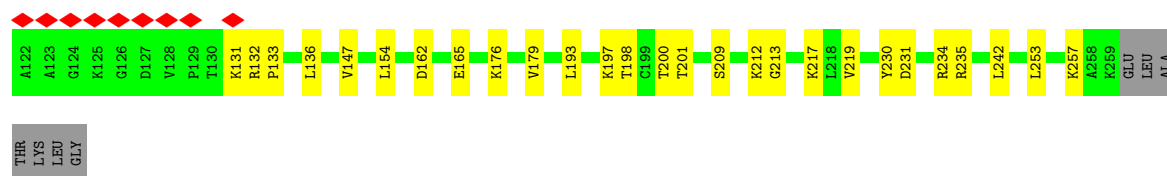


- Molecule 40: Large ribosomal subunit protein eL6



- Molecule 41: 60S ribosomal protein L7a





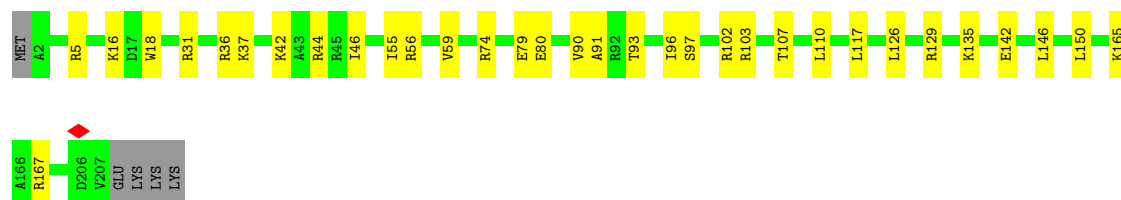
- Molecule 42: 60S ribosomal protein L13a

Chain LO:   80% 19%



- Molecule 43: 60S ribosomal protein L13

Chain LL:   82% 16%



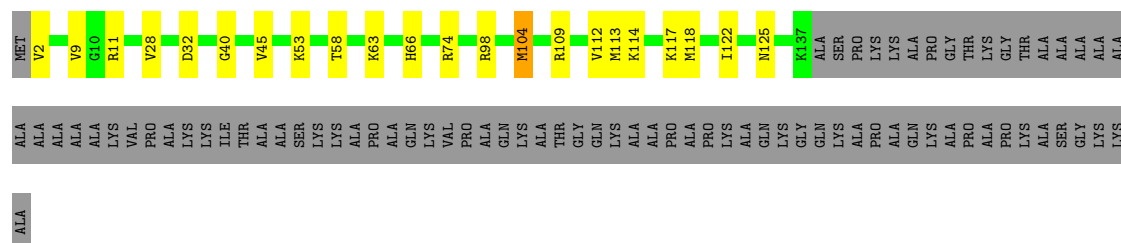
- Molecule 44: 60S ribosomal protein L23

Chain LV:    70% 22% 7%



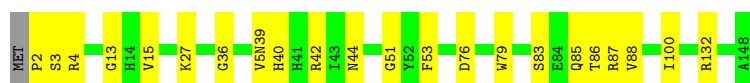
- Molecule 45: 60S ribosomal protein L14

Chain LM:    53% 10% 37%



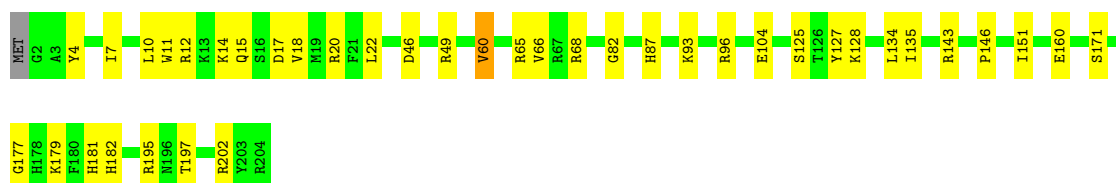
- Molecule 46: Large ribosomal subunit protein uL15

Chain La:  84% 15% .



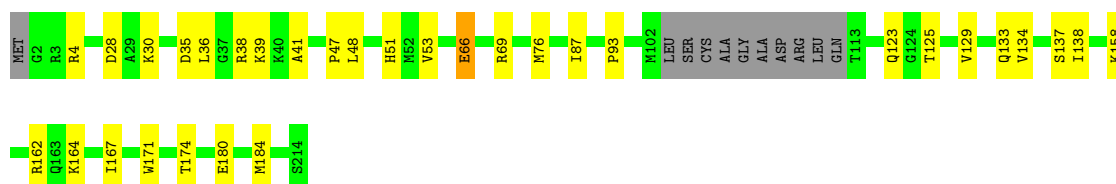
- Molecule 47: 60S ribosomal protein L15

Chain LN:  80% 19%



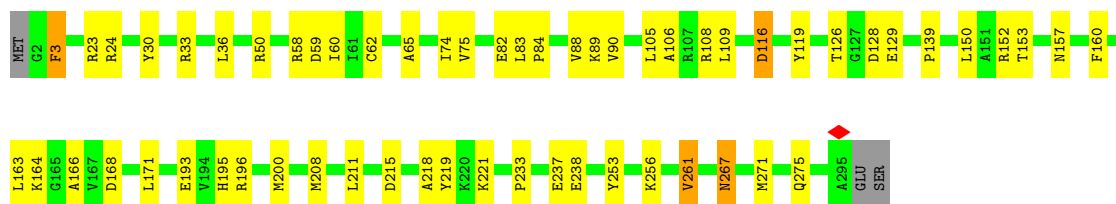
- Molecule 48: 60S ribosomal protein L10

Chain LI:  80% 14% 5%



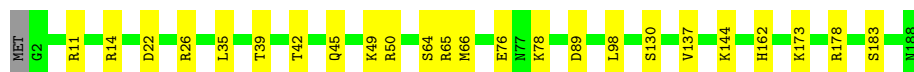
- Molecule 49: 60S ribosomal protein L5

Chain LD:  79% 19% ..



- Molecule 50: 60S ribosomal protein L18

Chain LQ:  87% 13% .

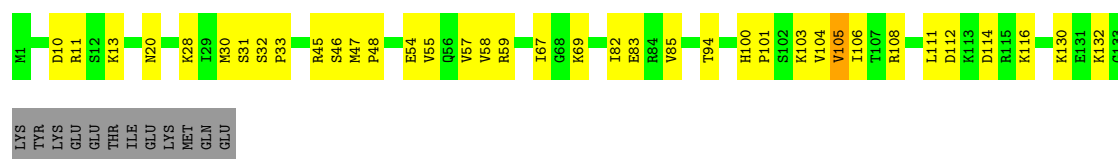


- Molecule 51: 60S ribosomal protein L19

Chain LR:  78% 17% 5%







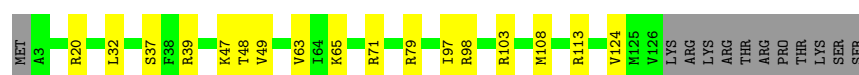
- Molecule 58: 60S ribosomal protein L27

Chain LZ: 82% 15% ..



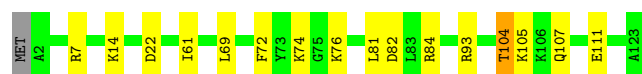
- Molecule 59: Large ribosomal subunit protein eL28

Chain Lr: 79% 12% 9%



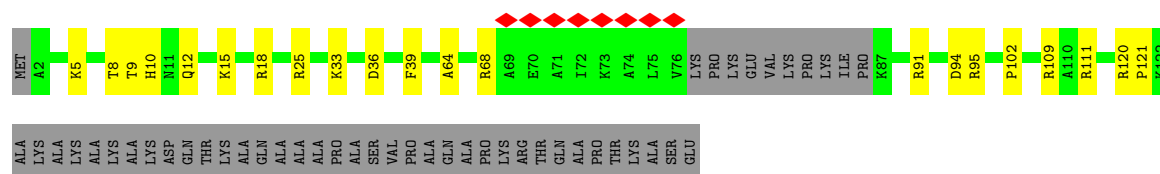
- Molecule 60: 60S ribosomal protein L35

Chain Lh: 86% 12% ..



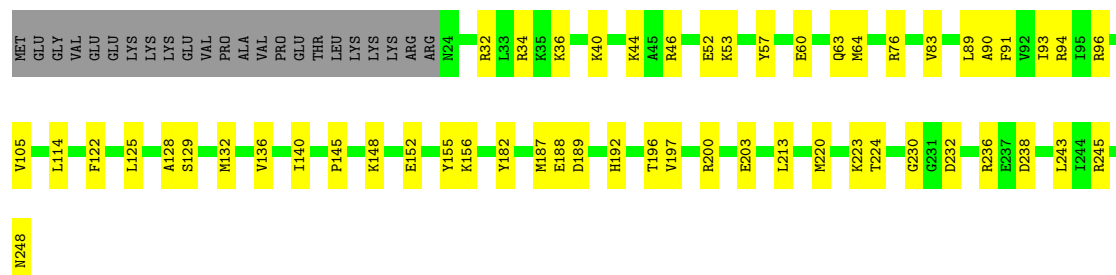
- Molecule 61: Large ribosomal subunit protein eL29

Chain Lb: 5% 57% 13% 30%



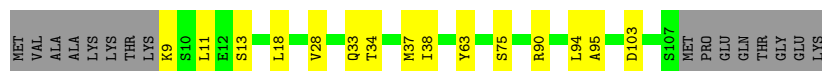
- Molecule 62: Large ribosomal subunit protein uL30

Chain LF: 69% 22% 9%



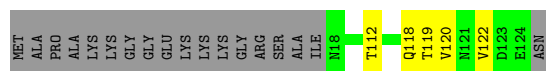
- Molecule 63: 60S ribosomal protein L30

Chain Lc:  73% 13% 14%



- Molecule 64: 60S ribosomal protein L31

Chain Ld:  82% 14%



- Molecule 65: 60S ribosomal protein L32

Chain Le:  77% 18% 5%



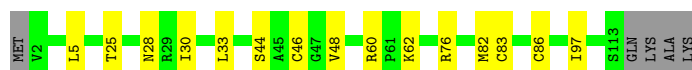
- Molecule 66: 60S ribosomal protein L35a

Chain Lf:  81% 18%



- Molecule 67: 60S ribosomal protein L34

Chain Lg:  83% 13%



- Molecule 68: 60S ribosomal protein L36

Chain Li:  86% 10%



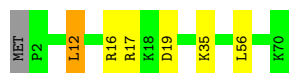
- Molecule 69: Large ribosomal subunit protein eL37

Chain Lj:  74% 14% 11%



- Molecule 70: 60S ribosomal protein L38

Chain Lk:  90% 7% ..



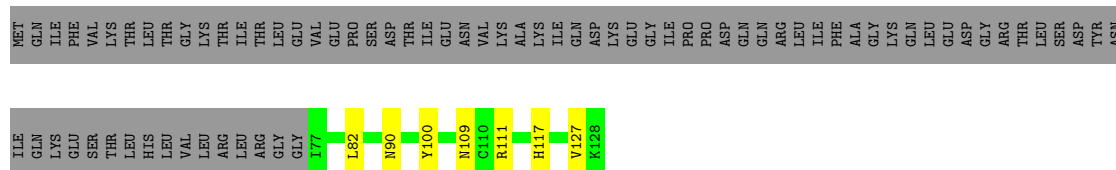
- Molecule 71: 60S ribosomal protein L39

Chain Ll:  76% 22% .



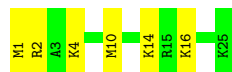
- Molecule 72: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  35% 5% 59%



- Molecule 73: 60S ribosomal protein L41

Chain Ln:  76% 24%

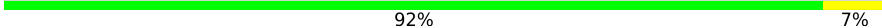


- Molecule 74: Large ribosomal subunit protein eL42

Chain Lo:  90% 9% .



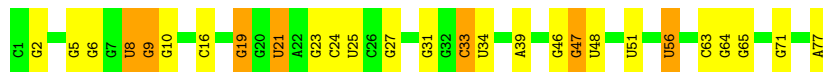
- Molecule 75: 60S ribosomal protein L37a

Chain Lp:  92% 7% .



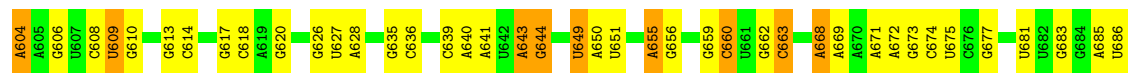
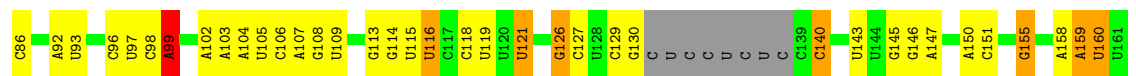
- Molecule 76: P site tRNA

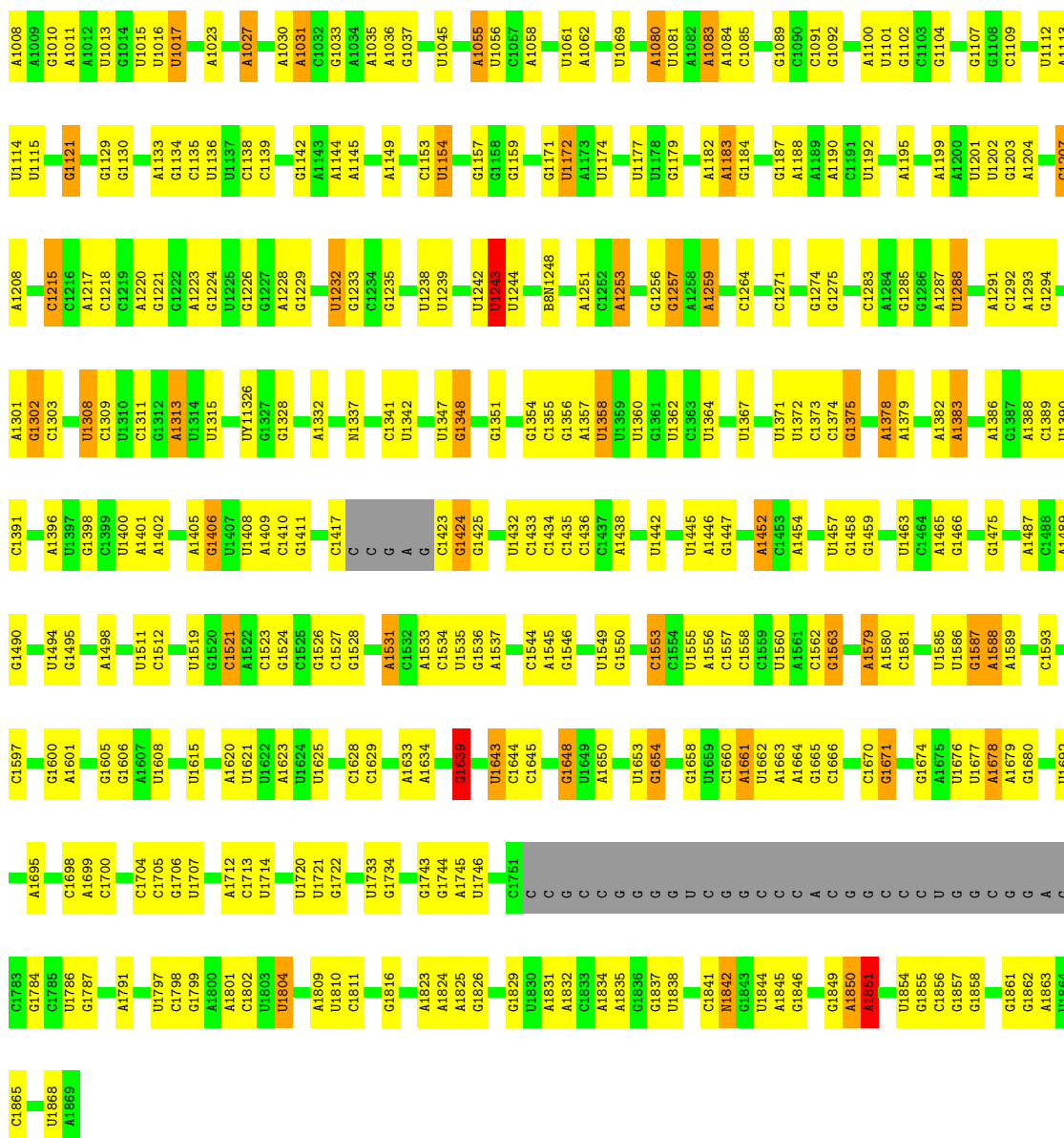
Chain Pt:  65% 26% 9%

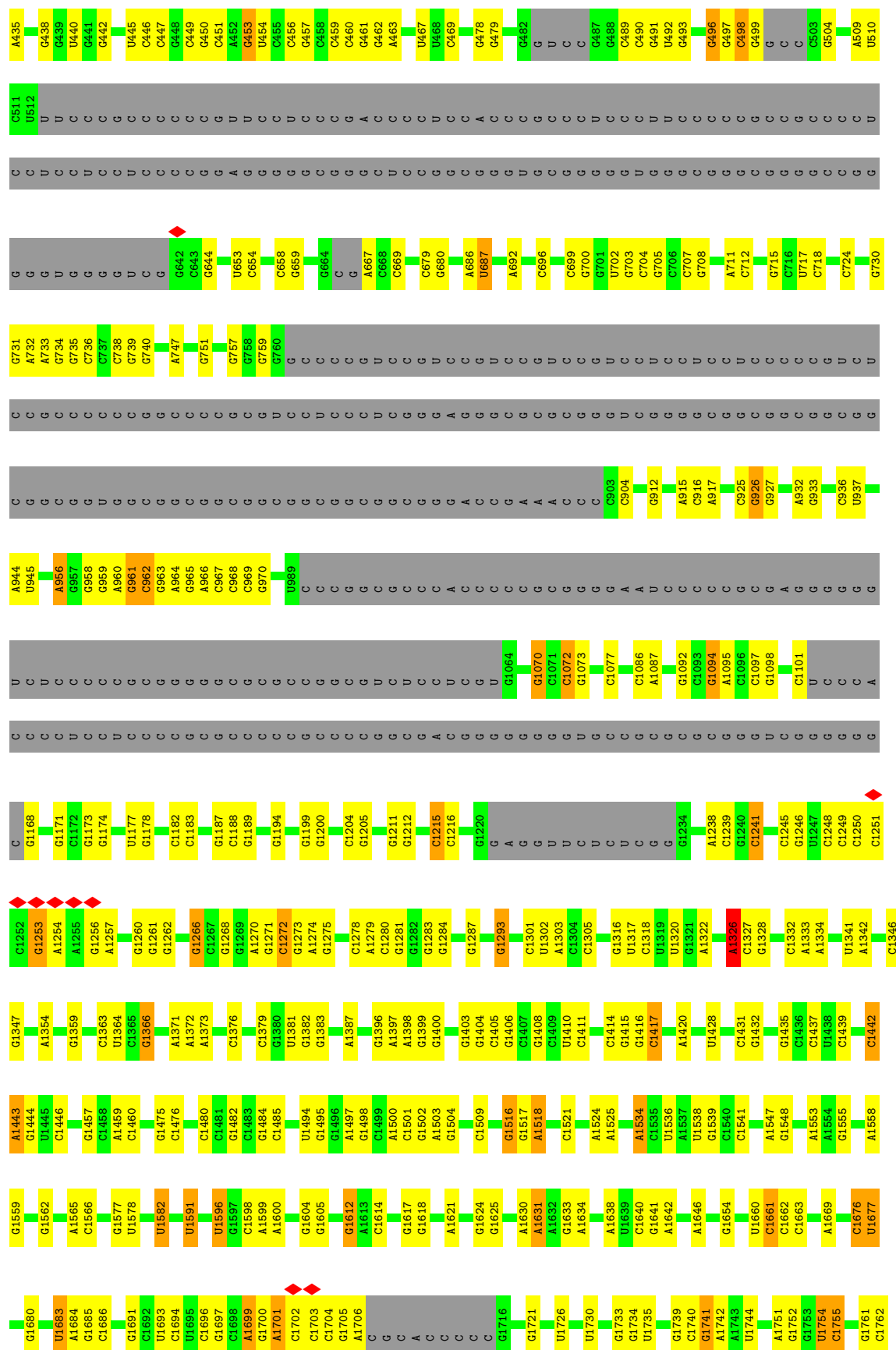


A G A U C C G C U A G C C G33 G34 G35 A36 A37 U38 G39 U G G A G A G A

| Category | Count |
|----------|-------|
| U1       | 10    |
| A2       | 10    |
| C3       | 10    |
| C4       | 10    |
| U5       | 10    |
| C6       | 10    |
| U12      | 10    |
| C13      | 10    |
| C14      | 10    |
| U15      | 10    |
| C16      | 10    |
| C17      | 10    |
| A27      | 10    |
| U28      | 10    |
| C29      | 10    |
| C30      | 10    |
| C33      | 10    |
| U34      | 10    |
| C35      | 10    |
| U36      | 10    |
| C37      | 10    |
| A38      | 10    |
| C41      | 10    |
| A42      | 10    |
| U43      | 10    |
| U44      | 10    |
| A45      | 10    |
| A46      | 10    |
| U51      | 10    |
| C52      | 10    |
| C56      | 10    |
| U57      | 10    |
| C58      | 10    |
| U59      | 10    |
| C62      | 10    |
| C63      | 10    |
| A64      | 10    |
| C65      | 10    |
| C66      | 10    |
| C67      | 10    |
| A68      | 10    |
| C73      | 10    |
| C74      | 0     |
| C75      | 0     |
| U76      | 10    |
| A77      | 10    |
| C78      | 10    |
| A79      | 10    |
| C80      | 10    |
| A84      | 10    |
| A85      | 10    |

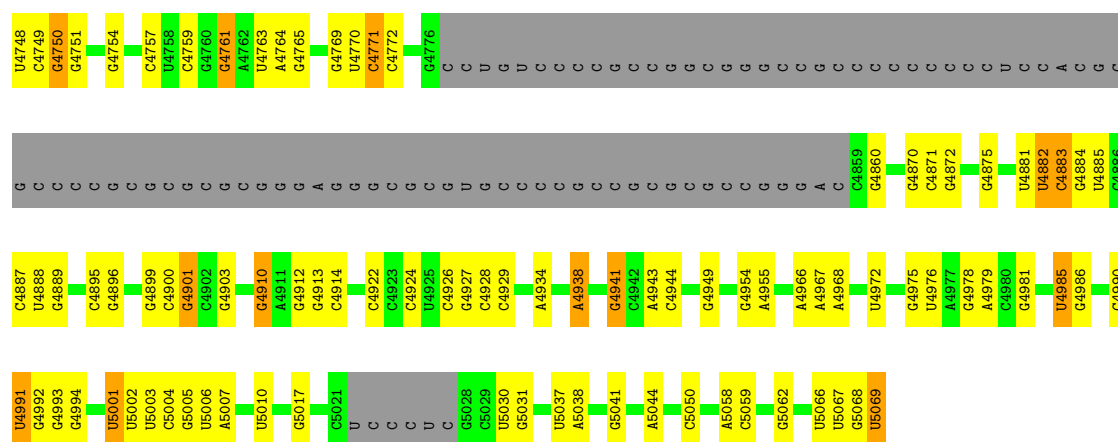




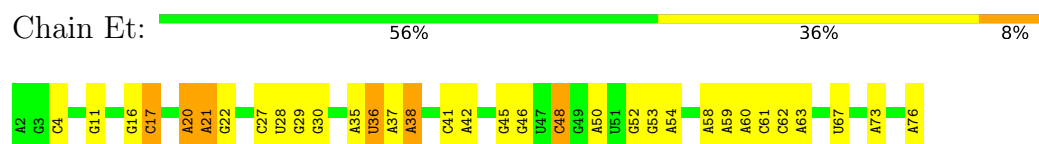




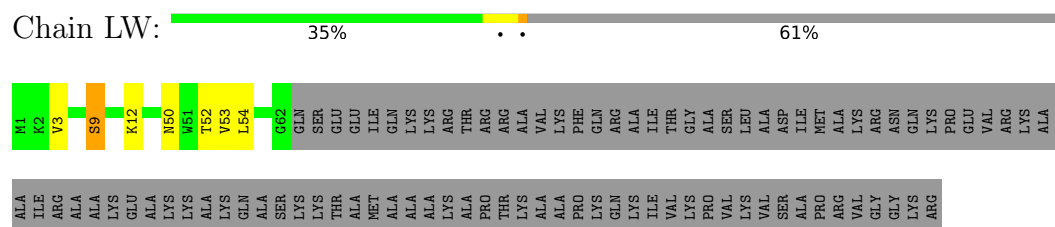




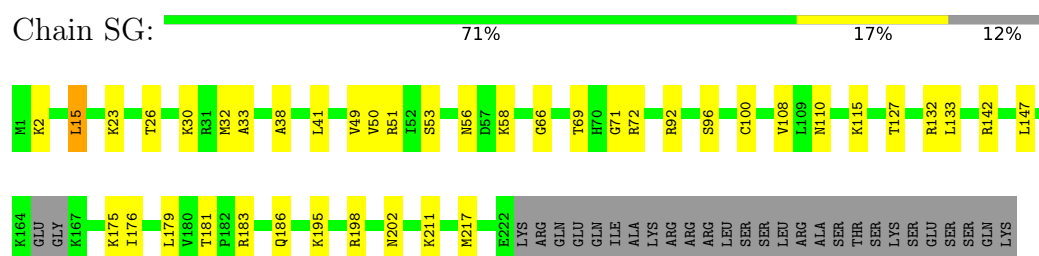
• Molecule 80: E site tRNA



• Molecule 81: 60S ribosomal protein L24



• Molecule 82: 40S ribosomal protein S6



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 59189                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1                                       | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.124                                   | Depositor |
| Minimum map value                    | -0.061                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.004                                   | Depositor |
| Recommended contour level            | 0.005                                   | Depositor |
| Map size (Å)                         | 395.52, 395.52, 395.52                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.824, 0.824, 0.824                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, PSU, HIC, A2M, HYG, ZN, 4SU, UR3, B8N, OMC, 4AC, UY1, MG, MA6, 6MZ, NA, V5N, ANM, H2U, 5MC, M3L, SAC, 1MA, K, HY3, AME, OMU, MLZ, G7M

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   | LA    | 0.16         | 0/1949  | 0.29        | 0/2610        |
| 2   | SA    | 0.13         | 0/1728  | 0.27        | 0/2350        |
| 3   | LB    | 0.16         | 0/3122  | 0.30        | 0/4191        |
| 4   | SB    | 0.13         | 0/1787  | 0.31        | 1/2394 (0.0%) |
| 5   | L8    | 0.16         | 0/3631  | 0.28        | 0/5657        |
| 6   | L7    | 0.16         | 0/2858  | 0.25        | 0/4455        |
| 7   | SD    | 0.12         | 0/1667  | 0.31        | 0/2256        |
| 8   | SJ    | 0.13         | 0/1502  | 0.29        | 0/2008        |
| 9   | SE    | 0.13         | 0/2086  | 0.29        | 0/2809        |
| 10  | SC    | 0.13         | 0/1721  | 0.29        | 0/2329        |
| 11  | SF    | 0.12         | 0/1454  | 0.29        | 0/1956        |
| 12  | SH    | 0.15         | 0/1429  | 0.37        | 0/1920        |
| 13  | SW    | 0.15         | 0/1047  | 0.30        | 0/1401        |
| 14  | SI    | 0.14         | 0/1680  | 0.30        | 0/2244        |
| 15  | SQ    | 0.13         | 0/1126  | 0.30        | 0/1508        |
| 16  | SU    | 0.09         | 0/519   | 0.28        | 0/722         |
| 17  | SK    | 0.10         | 0/694   | 0.29        | 0/945         |
| 18  | SO    | 0.13         | 0/1003  | 0.29        | 0/1347        |
| 19  | SX    | 0.13         | 0/1096  | 0.28        | 0/1461        |
| 20  | SM    | 0.06         | 0/215   | 0.19        | 0/295         |
| 21  | SS    | 0.12         | 0/1202  | 0.30        | 0/1614        |
| 22  | Sd    | 0.14         | 0/469   | 0.28        | 0/623         |
| 23  | SN    | 0.13         | 0/1242  | 0.30        | 0/1671        |
| 24  | SL    | 0.15         | 0/1168  | 0.27        | 0/1565        |
| 25  | SR    | 0.13         | 0/1052  | 0.36        | 0/1413        |
| 26  | SP    | 0.15         | 0/1070  | 0.40        | 0/1430        |
| 27  | ST    | 0.15         | 0/1035  | 0.29        | 0/1402        |
| 28  | SV    | 0.12         | 0/635   | 0.27        | 0/850         |
| 29  | SY    | 0.13         | 0/988   | 0.28        | 0/1316        |
| 30  | SZ    | 0.12         | 0/599   | 0.30        | 0/808         |
| 31  | Sa    | 0.13         | 0/798   | 0.30        | 0/1070        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 32  | Sb    | 0.13         | 0/655   | 0.28        | 0/878         |
| 33  | Sc    | 0.13         | 0/451   | 0.28        | 0/604         |
| 34  | Se    | 0.11         | 0/375   | 0.26        | 0/491         |
| 35  | Sf    | 0.11         | 0/194   | 0.36        | 0/265         |
| 36  | Sg    | 0.15         | 0/2444  | 0.40        | 0/3332        |
| 37  | LC    | 0.16         | 0/2968  | 0.30        | 0/3985        |
| 38  | LJ    | 0.13         | 0/1377  | 0.28        | 0/1842        |
| 39  | LH    | 0.15         | 0/1537  | 0.30        | 0/2066        |
| 40  | LE    | 0.15         | 0/1820  | 0.31        | 0/2442        |
| 41  | LG    | 0.15         | 0/1889  | 0.32        | 0/2545        |
| 42  | LO    | 0.17         | 0/1674  | 0.32        | 0/2244        |
| 43  | LL    | 0.16         | 0/1696  | 0.34        | 0/2271        |
| 44  | LV    | 0.16         | 0/986   | 0.29        | 0/1324        |
| 45  | LM    | 0.15         | 0/1138  | 0.31        | 0/1523        |
| 46  | La    | 0.16         | 0/1168  | 0.30        | 0/1562        |
| 47  | LN    | 0.17         | 0/1745  | 0.30        | 0/2338        |
| 48  | LI    | 0.14         | 0/1683  | 0.27        | 0/2247        |
| 49  | LD    | 0.15         | 0/2437  | 0.33        | 0/3263        |
| 50  | LQ    | 0.16         | 0/1536  | 0.29        | 0/2052        |
| 51  | LR    | 0.15         | 0/1492  | 0.27        | 0/1985        |
| 52  | LS    | 0.16         | 0/1500  | 0.30        | 1/2013 (0.0%) |
| 53  | LT    | 0.17         | 0/1345  | 0.35        | 0/1795        |
| 54  | LP    | 0.16         | 0/1279  | 0.29        | 0/1716        |
| 55  | LU    | 0.15         | 0/818   | 0.36        | 0/1099        |
| 56  | LX    | 0.14         | 0/983   | 0.27        | 0/1323        |
| 57  | LY    | 0.14         | 0/1119  | 0.30        | 0/1489        |
| 58  | LZ    | 0.15         | 0/1141  | 0.29        | 0/1521        |
| 59  | Lr    | 0.14         | 0/1020  | 0.27        | 0/1367        |
| 60  | Lh    | 0.13         | 0/1022  | 0.27        | 0/1351        |
| 61  | Lb    | 0.13         | 0/900   | 0.30        | 0/1187        |
| 62  | LF    | 0.16         | 0/1926  | 0.32        | 0/2567        |
| 63  | Lc    | 0.14         | 0/780   | 0.27        | 0/1046        |
| 64  | Ld    | 0.12         | 0/591   | 0.29        | 0/822         |
| 65  | Le    | 0.16         | 0/1082  | 0.29        | 0/1443        |
| 66  | Lf    | 0.16         | 0/894   | 0.27        | 0/1198        |
| 67  | Lg    | 0.15         | 0/885   | 0.29        | 0/1182        |
| 68  | Li    | 0.12         | 0/832   | 0.32        | 0/1101        |
| 69  | Lj    | 0.16         | 0/731   | 0.31        | 0/967         |
| 70  | Lk    | 0.15         | 0/574   | 0.29        | 0/761         |
| 71  | Ll    | 0.13         | 0/447   | 0.24        | 0/592         |
| 72  | Lm    | 0.15         | 0/433   | 0.31        | 0/575         |
| 73  | Ln    | 0.18         | 0/240   | 0.36        | 0/305         |
| 74  | Lo    | 0.14         | 0/877   | 0.25        | 0/1156        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 75  | Lp    | 0.16         | 0/728           | 0.34        | 0/967           |
| 76  | Pt    | 0.20         | 1/1721 (0.1%)   | 0.23        | 0/2679          |
| 77  | mR    | 0.10         | 0/175           | 0.20        | 0/272           |
| 78  | S2    | 0.18         | 0/37093         | 0.26        | 0/57803         |
| 79  | L5    | 0.18         | 0/81582         | 0.27        | 0/127262        |
| 80  | Et    | 0.11         | 0/1795          | 0.23        | 0/2798          |
| 81  | LW    | 0.14         | 0/532           | 0.27        | 0/708           |
| 82  | SG    | 0.12         | 0/1703          | 0.31        | 0/2285          |
| All | All   | 0.17         | 1/218585 (0.0%) | 0.28        | 2/321229 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 76  | Pt    | 47  | G7M  | O3'-P | 5.04 | 1.61        | 1.56     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | SB    | 150 | ILE  | N-CA-C | -5.14 | 107.40      | 113.42   |
| 52  | LS    | 142 | VAL  | N-CA-C | -5.04 | 107.92      | 112.96   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | LA    | 1921  | 0        | 2014     | 32      | 0            |
| 2   | SA    | 1692  | 0        | 1689     | 27      | 0            |
| 3   | LB    | 3068  | 0        | 3103     | 63      | 0            |
| 4   | SB    | 1761  | 0        | 1816     | 25      | 0            |
| 5   | L8    | 3315  | 0        | 1685     | 38      | 0            |
| 6   | L7    | 2558  | 0        | 1294     | 31      | 0            |
| 7   | SD    | 1642  | 0        | 1635     | 21      | 0            |
| 8   | SJ    | 1477  | 0        | 1592     | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | SE    | 2044  | 0        | 2145     | 27      | 0            |
| 10  | SC    | 1685  | 0        | 1754     | 19      | 0            |
| 11  | SF    | 1434  | 0        | 1471     | 17      | 0            |
| 12  | SH    | 1409  | 0        | 1467     | 13      | 0            |
| 13  | SW    | 1030  | 0        | 1076     | 17      | 0            |
| 14  | SI    | 1652  | 0        | 1703     | 32      | 0            |
| 15  | SQ    | 1109  | 0        | 1177     | 19      | 0            |
| 16  | SU    | 519   | 0        | 254      | 0       | 0            |
| 17  | SK    | 678   | 0        | 569      | 6       | 0            |
| 18  | SO    | 990   | 0        | 1013     | 21      | 0            |
| 19  | SX    | 1088  | 0        | 1149     | 9       | 0            |
| 20  | SM    | 218   | 0        | 107      | 0       | 0            |
| 21  | SS    | 1184  | 0        | 1240     | 27      | 0            |
| 22  | Sd    | 458   | 0        | 448      | 8       | 0            |
| 23  | SN    | 1214  | 0        | 1301     | 20      | 0            |
| 24  | SL    | 1148  | 0        | 1194     | 13      | 0            |
| 25  | SR    | 1038  | 0        | 1065     | 16      | 0            |
| 26  | SP    | 1049  | 0        | 1092     | 22      | 0            |
| 27  | ST    | 1010  | 0        | 935      | 17      | 0            |
| 28  | SV    | 628   | 0        | 625      | 6       | 0            |
| 29  | SY    | 972   | 0        | 1019     | 15      | 0            |
| 30  | SZ    | 592   | 0        | 624      | 11      | 0            |
| 31  | Sa    | 782   | 0        | 835      | 8       | 0            |
| 32  | Sb    | 642   | 0        | 661      | 8       | 0            |
| 33  | Sc    | 449   | 0        | 470      | 6       | 0            |
| 34  | Se    | 373   | 0        | 401      | 1       | 0            |
| 35  | Sf    | 194   | 0        | 121      | 1       | 0            |
| 36  | Sg    | 2387  | 0        | 2316     | 45      | 0            |
| 37  | LC    | 2914  | 0        | 3087     | 38      | 0            |
| 38  | LJ    | 1354  | 0        | 1389     | 14      | 0            |
| 39  | LH    | 1518  | 0        | 1600     | 24      | 0            |
| 40  | LE    | 1786  | 0        | 1945     | 27      | 0            |
| 41  | LG    | 1856  | 0        | 1985     | 31      | 0            |
| 42  | LO    | 1642  | 0        | 1773     | 28      | 0            |
| 43  | LL    | 1662  | 0        | 1773     | 26      | 0            |
| 44  | LV    | 972   | 0        | 1034     | 18      | 0            |
| 45  | LM    | 1116  | 0        | 1176     | 15      | 0            |
| 46  | La    | 1152  | 0        | 1179     | 18      | 0            |
| 47  | LN    | 1700  | 0        | 1749     | 30      | 0            |
| 48  | LI    | 1645  | 0        | 1694     | 18      | 0            |
| 49  | LD    | 2391  | 0        | 2425     | 40      | 0            |
| 50  | LQ    | 1512  | 0        | 1628     | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 51  | LR    | 1476  | 0        | 1548     | 23      | 0            |
| 52  | LS    | 1460  | 0        | 1502     | 18      | 0            |
| 53  | LT    | 1311  | 0        | 1392     | 18      | 0            |
| 54  | LP    | 1249  | 0        | 1276     | 22      | 0            |
| 55  | LU    | 804   | 0        | 820      | 11      | 0            |
| 56  | LX    | 966   | 0        | 1040     | 7       | 0            |
| 57  | LY    | 1102  | 0        | 1181     | 23      | 0            |
| 58  | LZ    | 1115  | 0        | 1195     | 16      | 0            |
| 59  | Lr    | 1002  | 0        | 1076     | 13      | 0            |
| 60  | Lh    | 1014  | 0        | 1148     | 13      | 0            |
| 61  | Lb    | 898   | 0        | 983      | 15      | 0            |
| 62  | LF    | 1885  | 0        | 2022     | 39      | 0            |
| 63  | Lc    | 770   | 0        | 809      | 8       | 0            |
| 64  | Ld    | 589   | 0        | 356      | 0       | 0            |
| 65  | Le    | 1061  | 0        | 1160     | 18      | 0            |
| 66  | Lf    | 875   | 0        | 911      | 11      | 0            |
| 67  | Lg    | 875   | 0        | 951      | 10      | 0            |
| 68  | Li    | 821   | 0        | 890      | 9       | 0            |
| 69  | Lj    | 712   | 0        | 744      | 14      | 0            |
| 70  | Lk    | 568   | 0        | 637      | 6       | 0            |
| 71  | Ll    | 437   | 0        | 471      | 9       | 0            |
| 72  | Lm    | 436   | 0        | 476      | 5       | 0            |
| 73  | Ln    | 239   | 0        | 289      | 8       | 0            |
| 74  | Lo    | 870   | 0        | 936      | 6       | 0            |
| 75  | Lp    | 715   | 0        | 768      | 5       | 0            |
| 76  | Pt    | 1645  | 0        | 844      | 16      | 0            |
| 77  | mR    | 156   | 0        | 77       | 4       | 0            |
| 78  | S2    | 34940 | 0        | 17689    | 363     | 0            |
| 79  | L5    | 75626 | 0        | 38304    | 680     | 0            |
| 80  | Et    | 1604  | 0        | 815      | 18      | 0            |
| 81  | LW    | 519   | 0        | 533      | 4       | 0            |
| 82  | SG    | 1683  | 0        | 1735     | 32      | 0            |
| 83  | A     | 14    | 0        | 0        | 0       | 0            |
| 83  | L7    | 4     | 0        | 0        | 0       | 0            |
| 83  | L8    | 3     | 0        | 0        | 0       | 0            |
| 83  | LA    | 3     | 0        | 0        | 0       | 0            |
| 83  | LH    | 1     | 0        | 0        | 0       | 0            |
| 83  | LI    | 1     | 0        | 0        | 0       | 0            |
| 83  | LL    | 1     | 0        | 0        | 0       | 0            |
| 83  | LN    | 1     | 0        | 0        | 0       | 0            |
| 83  | LQ    | 1     | 0        | 0        | 0       | 0            |
| 83  | Lb    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 83  | Le    | 1     | 0        | 0        | 0       | 0            |
| 83  | Lf    | 1     | 0        | 0        | 0       | 0            |
| 83  | Ll    | 1     | 0        | 0        | 0       | 0            |
| 83  | SL    | 1     | 0        | 0        | 0       | 0            |
| 83  | SO    | 1     | 0        | 0        | 0       | 0            |
| 83  | Sa    | 1     | 0        | 0        | 0       | 0            |
| 83  | mR    | 1     | 0        | 0        | 0       | 0            |
| 84  | Lr    | 9     | 0        | 8        | 0       | 0            |
| 84  | SA    | 9     | 0        | 8        | 0       | 0            |
| 85  | D     | 12    | 0        | 0        | 0       | 0            |
| 85  | Et    | 1     | 0        | 0        | 0       | 0            |
| 85  | L7    | 15    | 0        | 0        | 0       | 0            |
| 85  | L8    | 16    | 0        | 0        | 0       | 0            |
| 85  | LB    | 1     | 0        | 0        | 0       | 0            |
| 85  | LC    | 1     | 0        | 0        | 0       | 0            |
| 85  | LD    | 1     | 0        | 0        | 0       | 0            |
| 85  | LF    | 1     | 0        | 0        | 0       | 0            |
| 85  | LG    | 1     | 0        | 0        | 0       | 0            |
| 85  | LH    | 1     | 0        | 0        | 0       | 0            |
| 85  | LL    | 1     | 0        | 0        | 0       | 0            |
| 85  | LN    | 3     | 0        | 0        | 0       | 0            |
| 85  | LO    | 2     | 0        | 0        | 0       | 0            |
| 85  | LP    | 2     | 0        | 0        | 0       | 0            |
| 85  | LQ    | 2     | 0        | 0        | 0       | 0            |
| 85  | LR    | 1     | 0        | 0        | 0       | 0            |
| 85  | LS    | 1     | 0        | 0        | 0       | 0            |
| 85  | LV    | 1     | 0        | 0        | 0       | 0            |
| 85  | La    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lc    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lf    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lg    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lj    | 2     | 0        | 0        | 0       | 0            |
| 85  | Lo    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lp    | 2     | 0        | 0        | 0       | 0            |
| 85  | Lr    | 3     | 0        | 0        | 0       | 0            |
| 85  | Pt    | 1     | 0        | 0        | 0       | 0            |
| 85  | SN    | 1     | 0        | 0        | 0       | 0            |
| 85  | SS    | 2     | 0        | 0        | 0       | 0            |
| 85  | ST    | 1     | 0        | 0        | 0       | 0            |
| 85  | SX    | 1     | 0        | 0        | 0       | 0            |
| 85  | Sd    | 1     | 0        | 0        | 0       | 0            |
| 86  | Lg    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86  | Lj    | 1     | 0        | 0        | 0       | 0            |
| 86  | Lm    | 1     | 0        | 0        | 0       | 0            |
| 86  | Lo    | 1     | 0        | 0        | 0       | 0            |
| 86  | Lp    | 1     | 0        | 0        | 0       | 0            |
| 86  | Sa    | 1     | 0        | 0        | 0       | 0            |
| 86  | Sd    | 1     | 0        | 0        | 0       | 0            |
| 86  | Sf    | 1     | 0        | 0        | 0       | 0            |
| 87  | SV    | 11    | 0        | 12       | 0       | 0            |
| 88  | Pt    | 8     | 0        | 8        | 0       | 0            |
| 89  | S2    | 36    | 0        | 37       | 0       | 0            |
| 90  | L5    | 19    | 0        | 18       | 1       | 0            |
| 91  | C     | 7     | 0        | 0        | 0       | 0            |
| 92  | B     | 18    | 0        | 0        | 0       | 0            |
| 92  | L7    | 38    | 0        | 0        | 1       | 0            |
| 92  | L8    | 67    | 0        | 0        | 1       | 0            |
| 92  | LA    | 48    | 0        | 0        | 0       | 0            |
| 92  | LB    | 42    | 0        | 0        | 2       | 0            |
| 92  | LC    | 59    | 0        | 0        | 3       | 0            |
| 92  | LD    | 11    | 0        | 0        | 0       | 0            |
| 92  | LE    | 6     | 0        | 0        | 0       | 0            |
| 92  | LF    | 30    | 0        | 0        | 1       | 0            |
| 92  | LG    | 7     | 0        | 0        | 0       | 0            |
| 92  | LH    | 3     | 0        | 0        | 0       | 0            |
| 92  | LI    | 11    | 0        | 0        | 0       | 0            |
| 92  | LJ    | 1     | 0        | 0        | 0       | 0            |
| 92  | LL    | 26    | 0        | 0        | 2       | 0            |
| 92  | LM    | 2     | 0        | 0        | 0       | 0            |
| 92  | LN    | 40    | 0        | 0        | 2       | 0            |
| 92  | LO    | 29    | 0        | 0        | 1       | 0            |
| 92  | LP    | 17    | 0        | 0        | 1       | 0            |
| 92  | LQ    | 36    | 0        | 0        | 1       | 0            |
| 92  | LR    | 17    | 0        | 0        | 1       | 0            |
| 92  | LS    | 14    | 0        | 0        | 0       | 0            |
| 92  | LT    | 18    | 0        | 0        | 0       | 0            |
| 92  | LU    | 1     | 0        | 0        | 0       | 0            |
| 92  | LV    | 10    | 0        | 0        | 0       | 0            |
| 92  | LX    | 7     | 0        | 0        | 1       | 0            |
| 92  | LY    | 10    | 0        | 0        | 0       | 0            |
| 92  | LZ    | 5     | 0        | 0        | 1       | 0            |
| 92  | La    | 26    | 0        | 0        | 1       | 0            |
| 92  | Lb    | 10    | 0        | 0        | 0       | 0            |
| 92  | Lc    | 4     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 92  | Ld    | 9      | 0        | 0        | 0       | 0            |
| 92  | Le    | 28     | 0        | 0        | 1       | 0            |
| 92  | Lf    | 16     | 0        | 0        | 1       | 0            |
| 92  | Lg    | 22     | 0        | 0        | 0       | 0            |
| 92  | Lh    | 5      | 0        | 0        | 0       | 0            |
| 92  | Li    | 2      | 0        | 0        | 0       | 0            |
| 92  | Lj    | 19     | 0        | 0        | 3       | 0            |
| 92  | Lk    | 2      | 0        | 0        | 0       | 0            |
| 92  | Ll    | 8      | 0        | 0        | 0       | 0            |
| 92  | Lm    | 2      | 0        | 0        | 0       | 0            |
| 92  | Ln    | 1      | 0        | 0        | 1       | 0            |
| 92  | Lo    | 12     | 0        | 0        | 0       | 0            |
| 92  | Lp    | 14     | 0        | 0        | 0       | 0            |
| 92  | Lr    | 12     | 0        | 0        | 1       | 0            |
| 92  | Pt    | 1      | 0        | 0        | 0       | 0            |
| 92  | SE    | 1      | 0        | 0        | 0       | 0            |
| 92  | SL    | 1      | 0        | 0        | 0       | 0            |
| 92  | SN    | 1      | 0        | 0        | 0       | 0            |
| 92  | SO    | 2      | 0        | 0        | 0       | 0            |
| 92  | Sa    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 209052 | 0        | 152166   | 2016    | 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 6.

All (2016) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:SP:29:SER:HB3  | 26:SP:32:GLN:HE22  | 1.46                     | 0.80              |
| 67:Lg:83:CYS:SG   | 67:Lg:86:CYS:HB2   | 2.22                     | 0.80              |
| 38:LJ:95:ARG:HE   | 38:LJ:177:GLY:HA2  | 1.49                     | 0.77              |
| 79:L5:2786:C:H5'' | 79:L5:2787:A:H5'   | 1.66                     | 0.77              |
| 36:Sg:217:MET:HG2 | 36:Sg:229:THR:HG23 | 1.66                     | 0.76              |
| 55:LU:23:LEU:HD21 | 55:LU:83:LEU:HB3   | 1.68                     | 0.76              |
| 79:L5:2520:C:O2   | 79:L5:2640:G:N2    | 2.20                     | 0.75              |
| 76:Pt:51:U:H3     | 76:Pt:65:G:H1      | 1.34                     | 0.72              |
| 43:LL:167:ARG:HE  | 46:La:100:ILE:HD11 | 1.54                     | 0.72              |
| 78:S2:191:A:H62   | 78:S2:208:G:H21    | 1.38                     | 0.72              |
| 22:Sd:22:ARG:HH21 | 78:S2:1553:C:H41   | 1.37                     | 0.72              |
| 36:Sg:153:CYS:HB2 | 36:Sg:168:CYS:H    | 1.55                     | 0.72              |
| 36:Sg:87:LEU:HB2  | 36:Sg:101:PHE:HB2  | 1.70                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 78:S2:851:C:H5''  | 78:S2:852:G:H5'   | 1.70                     | 0.71              |
| 21:SS:116:LYS:HA  | 79:L5:1766:A:H5'' | 1.73                     | 0.70              |
| 39:LH:137:SER:HB3 | 39:LH:143:GLU:HB3 | 1.74                     | 0.70              |
| 47:LN:60:VAL:HG22 | 47:LN:134:LEU:HB2 | 1.71                     | 0.70              |
| 27:ST:85:ASN:HB2  | 27:ST:88:MET:HB2  | 1.73                     | 0.70              |
| 63:Lc:34:THR:HG23 | 63:Lc:95:ALA:HB2  | 1.72                     | 0.70              |
| 79:L5:3663:A:N6   | 79:L5:4168:G:O2'  | 2.24                     | 0.70              |
| 79:L5:3717:A:H2'  | 79:L5:3718:A2M:H8 | 1.74                     | 0.70              |
| 39:LH:56:ARG:NH1  | 39:LH:58:ASP:OD2  | 2.25                     | 0.70              |
| 6:L7:72:U:O2      | 6:L7:103:A:N6     | 2.25                     | 0.69              |
| 5:L8:99:U:O4      | 69:Lj:65:ARG:NH2  | 2.25                     | 0.69              |
| 46:La:4:ARG:NH2   | 79:L5:2341:A:OP2  | 2.26                     | 0.69              |
| 43:LL:36:ARG:NH2  | 79:L5:1364:U:OP2  | 2.26                     | 0.69              |
| 59:Lr:98:ARG:NH1  | 79:L5:2262:G:N7   | 2.40                     | 0.68              |
| 7:SD:105:LEU:HB2  | 7:SD:122:VAL:HG21 | 1.75                     | 0.68              |
| 26:SP:40:ARG:NH2  | 78:S2:1615:U:O4   | 2.27                     | 0.68              |
| 74:Lo:98:LYS:HE3  | 79:L5:4233:A:H4'  | 1.73                     | 0.68              |
| 79:L5:4140:C:H2'  | 79:L5:4141:G:C4   | 2.29                     | 0.68              |
| 66:Lf:33:VAL:HG13 | 66:Lf:38:GLU:HB2  | 1.76                     | 0.68              |
| 44:LV:35:LYS:HD2  | 44:LV:67:LYS:HE2  | 1.76                     | 0.68              |
| 41:LG:58:PRO:HD2  | 41:LG:61:ILE:HD12 | 1.76                     | 0.67              |
| 52:LS:71:SER:O    | 52:LS:76:LYS:NZ   | 2.28                     | 0.67              |
| 25:SR:70:SER:HB3  | 25:SR:73:LEU:HB2  | 1.76                     | 0.67              |
| 39:LH:44:GLU:HG3  | 45:LM:2:VAL:HG12  | 1.77                     | 0.67              |
| 39:LH:93:ARG:HD2  | 39:LH:143:GLU:HG3 | 1.77                     | 0.66              |
| 79:L5:4573:G:N2   | 79:L5:4573:G:OP2  | 2.28                     | 0.66              |
| 3:LB:126:LYS:NZ   | 79:L5:4966:A:OP2  | 2.28                     | 0.66              |
| 43:LL:44:ARG:NH2  | 79:L5:186:G:OP2   | 2.28                     | 0.66              |
| 79:L5:704:C:N4    | 79:L5:707:C:OP2   | 2.29                     | 0.66              |
| 81:LW:52:THR:HG22 | 81:LW:54:LEU:H    | 1.61                     | 0.66              |
| 13:SW:3:ARG:HH12  | 13:SW:28:ARG:HH21 | 1.44                     | 0.66              |
| 49:LD:152:ARG:O   | 49:LD:157:ASN:ND2 | 2.29                     | 0.66              |
| 79:L5:2562:G:N2   | 79:L5:2565:A:OP2  | 2.29                     | 0.65              |
| 45:LM:74:ARG:NH2  | 79:L5:736:C:OP1   | 2.28                     | 0.65              |
| 78:S2:326:C:H5''  | 78:S2:327:G:H5'   | 1.79                     | 0.65              |
| 78:S2:99:A2M:N6   | 78:S2:433:A:N3    | 2.44                     | 0.65              |
| 54:LP:42:ARG:NH1  | 54:LP:110:ASP:OD1 | 2.30                     | 0.65              |
| 72:Lm:111:ARG:NH1 | 79:L5:4699:U:OP2  | 2.30                     | 0.65              |
| 13:SW:107:SER:HB2 | 78:S2:860:G:H21   | 1.61                     | 0.65              |
| 14:SI:98:LYS:HB3  | 78:S2:377:G:H5''  | 1.78                     | 0.65              |
| 79:L5:3765:G:O2'  | 79:L5:3767:C:N4   | 2.30                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 82:SG:69:THR:HG22  | 82:SG:71:GLY:H     | 1.61                     | 0.65              |
| 9:SE:44:LEU:HD13   | 9:SE:72:ILE:HD11   | 1.79                     | 0.65              |
| 13:SW:12:LYS:O     | 13:SW:16:ASN:ND2   | 2.30                     | 0.65              |
| 78:S2:126:G:H21    | 78:S2:180:G:H21    | 1.44                     | 0.65              |
| 49:LD:126:THR:HG23 | 49:LD:128:ASP:H    | 1.62                     | 0.65              |
| 7:SD:205:PRO:HA    | 25:SR:42:PRO:HG2   | 1.77                     | 0.64              |
| 26:SP:37:TYR:HB3   | 26:SP:41:GLN:HB2   | 1.79                     | 0.64              |
| 5:L8:40:A:N7       | 5:L8:104:A:N6      | 2.45                     | 0.64              |
| 80:Et:11:G:O6      | 80:Et:45:G:N2      | 2.30                     | 0.64              |
| 15:SQ:34:VAL:HG22  | 15:SQ:70:VAL:HB    | 1.80                     | 0.64              |
| 79:L5:3722:G:H2'   | 79:L5:3723:A2M:H8  | 1.78                     | 0.64              |
| 36:Sg:174:VAL:HB   | 36:Sg:188:HIS:HB2  | 1.79                     | 0.64              |
| 72:Lm:100:TYR:O    | 79:L5:4472:G:O2'   | 2.15                     | 0.64              |
| 7:SD:136:VAL:HG22  | 7:SD:186:VAL:HG22  | 1.78                     | 0.64              |
| 82:SG:32:MET:HB2   | 82:SG:100:CYS:HB2  | 1.79                     | 0.64              |
| 2:SA:80:ARG:NH2    | 2:SA:82:THR:OG1    | 2.30                     | 0.64              |
| 42:LO:106:ASP:O    | 79:L5:4910:G:N2    | 2.31                     | 0.64              |
| 78:S2:1139:C:H42   | 78:S2:1149:A:H62   | 1.43                     | 0.64              |
| 54:LP:42:ARG:NH2   | 54:LP:99:GLU:OE2   | 2.31                     | 0.63              |
| 62:LF:192:HIS:O    | 62:LF:196:THR:OG1  | 2.16                     | 0.63              |
| 41:LG:209:SER:HA   | 41:LG:212:LYS:HG3  | 1.80                     | 0.63              |
| 1:LA:215:ASN:ND2   | 79:L5:4546:A:N7    | 2.47                     | 0.63              |
| 13:SW:2:VAL:N      | 78:S2:1091:C:HO2'  | 1.96                     | 0.63              |
| 2:SA:77:ILE:HG12   | 2:SA:99:ILE:HB     | 1.81                     | 0.63              |
| 79:L5:3641:U:OP2   | 79:L5:3646:A:N6    | 2.28                     | 0.63              |
| 26:SP:100:LYS:HG2  | 26:SP:101:THR:HG23 | 1.81                     | 0.63              |
| 55:LU:100:LEU:HD13 | 55:LU:112:LEU:HD23 | 1.80                     | 0.63              |
| 1:LA:101:VAL:HG22  | 1:LA:165:VAL:HG22  | 1.81                     | 0.63              |
| 80:Et:16:G:H22     | 80:Et:48:C:H42     | 1.45                     | 0.63              |
| 47:LN:143:ARG:NH2  | 60:Lh:93:ARG:O     | 2.32                     | 0.63              |
| 79:L5:2020:U:H2'   | 79:L5:2021:G:H8    | 1.64                     | 0.63              |
| 11:SF:201:LYS:HG3  | 11:SF:204:ARG:HH21 | 1.63                     | 0.63              |
| 50:LQ:11:ARG:HG3   | 79:L5:2081:C:H5''  | 1.81                     | 0.63              |
| 18:SO:55:ARG:NH2   | 78:S2:953:C:O2     | 2.31                     | 0.62              |
| 79:L5:4594:U:H2'   | 79:L5:4595:G:H8    | 1.64                     | 0.62              |
| 3:LB:21:ARG:NH2    | 79:L5:4981:G:O6    | 2.32                     | 0.62              |
| 14:SI:162:LEU:HD11 | 14:SI:191:GLU:HG2  | 1.80                     | 0.62              |
| 22:Sd:18:SER:OG    | 78:S2:1556:A:N6    | 2.32                     | 0.62              |
| 76:Pt:25:U:O2'     | 79:L5:3770:PSU:OP1 | 2.17                     | 0.62              |
| 3:LB:261:ARG:NH2   | 92:LB:665:HOH:O    | 2.32                     | 0.62              |
| 30:SZ:104:ARG:NH2  | 78:S2:1593:C:OP2   | 2.31                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:LJ:18:ARG:HG3   | 38:LJ:135:GLY:HA3  | 1.81                     | 0.62              |
| 61:Lb:120:ARG:NH2  | 79:L5:1241:C:N3    | 2.44                     | 0.62              |
| 78:S2:43:U:OP2     | 78:S2:485:A:N6     | 2.33                     | 0.62              |
| 79:L5:2485:U:H2'   | 79:L5:2486:G:C8    | 2.33                     | 0.62              |
| 66:Lf:4:ARG:NH1    | 66:Lf:6:TRP:O      | 2.32                     | 0.62              |
| 36:Sg:11:LEU:HB2   | 36:Sg:307:VAL:HB   | 1.82                     | 0.62              |
| 79:L5:1332:C:H2'   | 79:L5:1333:A:H8    | 1.65                     | 0.62              |
| 47:LN:160:GLU:OE2  | 47:LN:160:GLU:N    | 2.23                     | 0.62              |
| 59:Lr:20:ARG:NH1   | 65:Le:78:LEU:O     | 2.33                     | 0.62              |
| 78:S2:928:G:H2'    | 78:S2:929:G:C8     | 2.35                     | 0.62              |
| 78:S2:1536:G:H2'   | 78:S2:1537:A:H8    | 1.64                     | 0.62              |
| 79:L5:2360:A:N6    | 79:L5:3861:A:N7    | 2.45                     | 0.62              |
| 51:LR:88:ARG:O     | 79:L5:2725:A:N6    | 2.32                     | 0.62              |
| 81:LW:9:SER:HA     | 81:LW:52:THR:HG23  | 1.81                     | 0.62              |
| 54:LP:17:SER:HB2   | 54:LP:98:ALA:HB2   | 1.81                     | 0.61              |
| 9:SE:100:ARG:HH12  | 9:SE:122:LYS:HA    | 1.64                     | 0.61              |
| 37:LC:189:MET:HE3  | 37:LC:200:ARG:HH21 | 1.64                     | 0.61              |
| 38:LJ:68:ILE:HD11  | 79:L5:4258:C:H5'   | 1.83                     | 0.61              |
| 41:LG:162:ASP:O    | 79:L5:150:U:N3     | 2.30                     | 0.61              |
| 50:LQ:144:LYS:HG3  | 79:L5:1460:C:H5''  | 1.82                     | 0.61              |
| 61:Lb:5:MLZ:HE3    | 61:Lb:8:THR:HB     | 1.83                     | 0.61              |
| 78:S2:1854:U:H2'   | 78:S2:1855:G:H8    | 1.66                     | 0.61              |
| 79:L5:1326:A2M:OP2 | 79:L5:4445:U:O2'   | 2.17                     | 0.61              |
| 37:LC:204:ARG:NH1  | 92:LC:615:HOH:O    | 2.33                     | 0.61              |
| 66:Lf:54:LYS:HE3   | 79:L5:4748:U:H5''  | 1.82                     | 0.61              |
| 79:L5:308:G:OP2    | 79:L5:308:G:N2     | 2.29                     | 0.61              |
| 44:LV:90:ARG:NH2   | 44:LV:140:ALA:O    | 2.33                     | 0.61              |
| 47:LN:202:ARG:NH2  | 79:L5:1372:A:OP1   | 2.26                     | 0.61              |
| 4:SB:216:LYS:NZ    | 78:S2:942:G:OP1    | 2.34                     | 0.61              |
| 41:LG:38:ASN:OD1   | 41:LG:43:GLN:NE2   | 2.34                     | 0.61              |
| 79:L5:62:A:N3      | 79:L5:77:U:O2'     | 2.29                     | 0.61              |
| 54:LP:97:ASN:ND2   | 79:L5:393:U:O2     | 2.33                     | 0.61              |
| 78:S2:958:G:N2     | 78:S2:965:U:O4     | 2.28                     | 0.61              |
| 79:L5:181:C:H2'    | 79:L5:182:G:H8     | 1.65                     | 0.61              |
| 79:L5:4620:OMU:OP2 | 79:L5:4670:C:N4    | 2.33                     | 0.61              |
| 76:Pt:9:G:O2'      | 76:Pt:10:G:N7      | 2.31                     | 0.61              |
| 3:LB:14:LEU:HD22   | 3:LB:17:LEU:HD11   | 1.82                     | 0.61              |
| 3:LB:174:ARG:NH1   | 79:L5:4985:U:O2    | 2.34                     | 0.61              |
| 11:SF:60:ARG:HD2   | 78:S2:1679:A:H2'   | 1.83                     | 0.61              |
| 25:SR:43:SER:OG    | 78:S2:1389:C:OP1   | 2.17                     | 0.60              |
| 39:LH:71:ARG:NH1   | 79:L5:4691:A:OP1   | 2.34                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:LZ:90:PRO:O     | 58:LZ:117:LYS:NZ   | 2.34                     | 0.60              |
| 66:Lf:43:LEU:O     | 66:Lf:109:ARG:NH2  | 2.33                     | 0.60              |
| 4:SB:138:PHE:O     | 4:SB:213:ARG:N     | 2.34                     | 0.60              |
| 79:L5:1245:C:H2'   | 79:L5:1246:G:H8    | 1.65                     | 0.60              |
| 79:L5:1562:G:N2    | 79:L5:1565:A:OP2   | 2.33                     | 0.60              |
| 55:LU:44:GLN:HG2   | 55:LU:63:ILE:HD12  | 1.84                     | 0.60              |
| 69:Lj:11:ARG:NH1   | 92:Lj:229:HOH:O    | 2.33                     | 0.60              |
| 3:LB:213:GLN:NE2   | 3:LB:285:TYR:O     | 2.34                     | 0.60              |
| 14:SI:57:ALA:HB2   | 14:SI:183:GLY:HA2  | 1.82                     | 0.60              |
| 29:SY:29:HIS:HE2   | 29:SY:69:THR:HG1   | 1.47                     | 0.60              |
| 43:LL:18:TRP:NE1   | 79:L5:1516:G:O2'   | 2.33                     | 0.60              |
| 7:SD:106:ARG:HG3   | 7:SD:175:VAL:HG22  | 1.82                     | 0.60              |
| 9:SE:19:MET:HG2    | 78:S2:846:G:H2'    | 1.83                     | 0.60              |
| 14:SI:103:LEU:HD22 | 14:SI:170:LYS:HB3  | 1.83                     | 0.60              |
| 52:LS:99:ASP:OD1   | 52:LS:108:GLN:NE2  | 2.34                     | 0.60              |
| 69:Lj:30:GLN:NE2   | 79:L5:1621:A:OP2   | 2.35                     | 0.60              |
| 71:Ll:2:SER:N      | 79:L5:2407:G:O6    | 2.34                     | 0.60              |
| 80:Et:16:G:H1'     | 80:Et:20:A:H61     | 1.66                     | 0.60              |
| 19:SX:127:ASN:O    | 19:SX:127:ASN:ND2  | 2.34                     | 0.60              |
| 53:LT:39:ILE:HD12  | 53:LT:102:ARG:HG2  | 1.83                     | 0.60              |
| 78:S2:1033:G:N1    | 78:S2:1080:A:O2'   | 2.26                     | 0.60              |
| 78:S2:1283:C:O2'   | 78:S2:1313:A:N1    | 2.35                     | 0.60              |
| 79:L5:453:G:N2     | 79:L5:1293:G:O6    | 2.33                     | 0.60              |
| 37:LC:149:GLU:OE2  | 59:Lr:71:ARG:NH1   | 2.34                     | 0.60              |
| 43:LL:31:ARG:NH2   | 92:LL:428:HOH:O    | 2.34                     | 0.60              |
| 49:LD:23:ARG:NH1   | 49:LD:23:ARG:O     | 2.34                     | 0.60              |
| 78:S2:1259:A:H1'   | 78:S2:1264:C:H42   | 1.65                     | 0.60              |
| 57:LY:54:GLU:HB2   | 57:LY:108:ARG:HB3  | 1.84                     | 0.60              |
| 21:SS:13:LEU:HB2   | 21:SS:20:ILE:HB    | 1.83                     | 0.59              |
| 18:SO:61:LYS:NZ    | 18:SO:80:ASP:OD2   | 2.29                     | 0.59              |
| 79:L5:1870:C:H2'   | 79:L5:1871:A2M:H8  | 1.84                     | 0.59              |
| 42:LO:185:VAL:O    | 42:LO:187:LYS:N    | 2.36                     | 0.59              |
| 61:Lb:36:ASP:OD1   | 79:L5:4314:C:O2'   | 2.20                     | 0.59              |
| 78:S2:165:G:OP2    | 78:S2:165:G:N2     | 2.34                     | 0.59              |
| 78:S2:1228:A:H2'   | 78:S2:1229:G:C8    | 2.37                     | 0.59              |
| 13:SW:51:GLU:HG2   | 32:Sb:8:LEU:HD21   | 1.83                     | 0.59              |
| 21:SS:22:GLY:HA2   | 21:SS:56:ALA:HB3   | 1.84                     | 0.59              |
| 37:LC:189:MET:SD   | 37:LC:201:ARG:NH1  | 2.75                     | 0.59              |
| 45:LM:53:LYS:NZ    | 79:L5:1924:C:OP1   | 2.29                     | 0.59              |
| 40:LE:178:PRO:HD2  | 40:LE:181:LEU:HD12 | 1.83                     | 0.59              |
| 42:LO:128:ARG:NH1  | 52:LS:162:GLN:OE1  | 2.35                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 78:S2:1720:U:HO2'  | 79:L5:3796:U:HO2' | 1.49                     | 0.59              |
| 82:SG:23:LYS:HB3   | 82:SG:41:LEU:HA   | 1.83                     | 0.59              |
| 8:SJ:38:ARG:NH1    | 78:S2:643:A:OP1   | 2.36                     | 0.59              |
| 11:SF:80:GLY:H     | 78:S2:1223:A:H5'' | 1.67                     | 0.59              |
| 57:LY:47:MET:HE3   | 57:LY:48:PRO:HD2  | 1.84                     | 0.59              |
| 63:Lc:11:LEU:HD13  | 63:Lc:75:SER:HB2  | 1.83                     | 0.59              |
| 1:LA:152:SER:OG    | 79:L5:3661:G:N7   | 2.35                     | 0.59              |
| 7:SD:103:GLU:OE2   | 7:SD:173:ARG:NE   | 2.32                     | 0.59              |
| 26:SP:40:ARG:NH1   | 78:S2:1620:A:O2'  | 2.36                     | 0.59              |
| 33:Sc:44:ARG:NH1   | 33:Sc:63:ARG:O    | 2.36                     | 0.59              |
| 40:LE:65:ARG:NH1   | 79:L5:1070:G:OP2  | 2.36                     | 0.59              |
| 78:S2:928:G:H1     | 78:S2:1013:U:H3   | 1.50                     | 0.59              |
| 78:S2:1400:U:O4    | 78:S2:1401:A:N6   | 2.35                     | 0.59              |
| 4:SB:28:LYS:HD3    | 4:SB:48:LEU:HD12  | 1.83                     | 0.59              |
| 41:LG:73:ARG:NE    | 79:L5:4076:G:OP1  | 2.32                     | 0.59              |
| 50:LQ:14:ARG:NH2   | 79:L5:2083:C:OP2  | 2.32                     | 0.59              |
| 73:Ln:4:LYS:NZ     | 92:Ln:102:HOH:O   | 2.35                     | 0.59              |
| 13:SW:55:ASP:O     | 13:SW:57:ARG:NH1  | 2.35                     | 0.59              |
| 18:SO:84:ARG:NH1   | 18:SO:87:GLU:OE2  | 2.36                     | 0.59              |
| 79:L5:1320:U:O2'   | 79:L5:1891:A:N1   | 2.29                     | 0.59              |
| 40:LE:161:ARG:NH1  | 40:LE:273:SER:OG  | 2.36                     | 0.58              |
| 79:L5:4140:C:O2    | 79:L5:4144:C:N4   | 2.36                     | 0.58              |
| 36:Sg:272:GLN:OE1  | 36:Sg:308:ARG:NH1 | 2.36                     | 0.58              |
| 46:La:76:ASP:N     | 46:La:76:ASP:OD1  | 2.35                     | 0.58              |
| 79:L5:4527:G:OP2   | 79:L5:4527:G:N2   | 2.34                     | 0.58              |
| 26:SP:21:ASP:N     | 26:SP:21:ASP:OD1  | 2.30                     | 0.58              |
| 45:LM:117:LYS:NZ   | 79:L5:4882:U:OP1  | 2.37                     | 0.58              |
| 50:LQ:66:MET:HE3   | 50:LQ:98:LEU:HD13 | 1.83                     | 0.58              |
| 56:LX:135:LYS:NZ   | 79:L5:2436:U:OP2  | 2.36                     | 0.58              |
| 58:LZ:100:VAL:HG22 | 58:LZ:106:LEU:HB3 | 1.86                     | 0.58              |
| 79:L5:2485:U:H2'   | 79:L5:2486:G:H8   | 1.68                     | 0.58              |
| 36:Sg:284:PRO:HB3  | 36:Sg:304:ASP:HB2 | 1.85                     | 0.58              |
| 42:LO:37:ARG:NH1   | 79:L5:4761:G:OP2  | 2.28                     | 0.58              |
| 18:SO:147:ARG:HG2  | 18:SO:150:ARG:HD3 | 1.83                     | 0.58              |
| 37:LC:321:ASN:ND2  | 79:L5:715:G:OP1   | 2.35                     | 0.58              |
| 41:LG:165:GLU:HG3  | 47:LN:10:LEU:HD23 | 1.85                     | 0.58              |
| 62:LF:155:TYR:OH   | 62:LF:188:GLU:OE2 | 2.19                     | 0.58              |
| 53:LT:4:THR:OG1    | 79:L5:4208:U:OP2  | 2.20                     | 0.58              |
| 79:L5:966:A:OP2    | 79:L5:2092:G:N2   | 2.36                     | 0.58              |
| 79:L5:1700:G:N7    | 79:L5:1704:C:N4   | 2.51                     | 0.58              |
| 79:L5:3718:A2M:H2  | 79:L5:3934:G:O4'  | 2.03                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:SJ:54:ARG:NH1    | 10:SC:200:ARG:O    | 2.36                     | 0.58              |
| 10:SC:178:HIS:ND1  | 10:SC:221:ASP:OD2  | 2.36                     | 0.58              |
| 43:LL:16:LYS:NZ    | 79:L5:48:G:OP1     | 2.36                     | 0.58              |
| 71:L1:44:TRP:O     | 71:L1:48:LYS:NZ    | 2.37                     | 0.58              |
| 18:SO:34:PHE:HB3   | 18:SO:41:PHE:HB2   | 1.85                     | 0.58              |
| 19:SX:119:ARG:NH2  | 78:S2:1192:U:OP2   | 2.36                     | 0.58              |
| 46:La:44:ASN:ND2   | 79:L5:1683:PSU:OP1 | 2.37                     | 0.58              |
| 49:LD:84:PRO:O     | 49:LD:89:LYS:NZ    | 2.35                     | 0.58              |
| 4:SB:113:MET:HE3   | 4:SB:142:PHE:HE1   | 1.69                     | 0.58              |
| 37:LC:304:ALA:HB1  | 79:L5:2096:G:H21   | 1.67                     | 0.58              |
| 69:Lj:20:ARG:NH2   | 69:Lj:39:TYR:OH    | 2.34                     | 0.58              |
| 78:S2:126:G:OP1    | 82:SG:198:ARG:NH1  | 2.33                     | 0.58              |
| 79:L5:1697:G:N2    | 79:L5:2084:C:OP1   | 2.32                     | 0.58              |
| 43:LL:5:ARG:NH2    | 79:L5:1850:A:OP2   | 2.36                     | 0.58              |
| 59:Lr:37:SER:OG    | 79:L5:2267:U:OP1   | 2.19                     | 0.58              |
| 78:S2:1662:U:O4    | 78:S2:1663:A:N6    | 2.37                     | 0.58              |
| 79:L5:3723:A2M:H2' | 79:L5:3724:A2M:H8  | 1.86                     | 0.58              |
| 78:S2:155:G:H4'    | 82:SG:15:LEU:HD13  | 1.84                     | 0.57              |
| 78:S2:1546:G:N2    | 78:S2:1670:C:O2    | 2.34                     | 0.57              |
| 79:L5:1548:G:O2'   | 79:L5:2812:A:N3    | 2.35                     | 0.57              |
| 79:L5:3823:G:OP2   | 79:L5:3823:G:N2    | 2.27                     | 0.57              |
| 5:L8:67:U:H2'      | 5:L8:68:G:H8       | 1.69                     | 0.57              |
| 69:Lj:55:ARG:NH2   | 79:L5:364:G:O6     | 2.37                     | 0.57              |
| 3:LB:137:TRP:O     | 3:LB:143:LYS:NZ    | 2.37                     | 0.57              |
| 12:SH:46:THR:HG21  | 12:SH:97:GLN:HG2   | 1.86                     | 0.57              |
| 61:Lb:36:ASP:HB3   | 61:Lb:39:PHE:HB3   | 1.86                     | 0.57              |
| 62:LF:105:VAL:HG13 | 62:LF:136:VAL:HG12 | 1.85                     | 0.57              |
| 14:SI:64:ASN:ND2   | 78:S2:302:A:N3     | 2.53                     | 0.57              |
| 18:SO:135:ILE:O    | 78:S2:943:U:O2'    | 2.22                     | 0.57              |
| 73:Ln:10:MET:HE2   | 78:S2:1172:U:H5''  | 1.85                     | 0.57              |
| 79:L5:307:A:N3     | 79:L5:310:G:O2'    | 2.35                     | 0.57              |
| 7:SD:135:GLU:HG3   | 7:SD:153:VAL:HG22  | 1.85                     | 0.57              |
| 22:Sd:18:SER:HG    | 78:S2:1556:A:N6    | 2.03                     | 0.57              |
| 27:ST:82:ARG:HB2   | 78:S2:1589:A:H4'   | 1.86                     | 0.57              |
| 66:Lf:29:LYS:NZ    | 92:Lf:308:HOH:O    | 2.36                     | 0.57              |
| 78:S2:1745:A:H1'   | 82:SG:66:GLY:HA2   | 1.86                     | 0.57              |
| 5:L8:126:C:H42     | 79:L5:2543:A:H4'   | 1.69                     | 0.57              |
| 30:SZ:68:ILE:HB    | 30:SZ:109:TYR:HB2  | 1.86                     | 0.57              |
| 40:LE:105:ARG:NH1  | 79:L5:469:C:O2     | 2.37                     | 0.57              |
| 47:LN:49:ARG:NH1   | 92:LN:413:HOH:O    | 2.37                     | 0.57              |
| 47:LN:182:HIS:NE2  | 79:L5:291:U:O2'    | 2.29                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:LR:116:ASP:OD1  | 51:LR:116:ASP:N    | 2.36                     | 0.57              |
| 9:SE:43:PRO:HG2    | 9:SE:46:ILE:HG13   | 1.87                     | 0.57              |
| 14:SI:6:ASP:OD1    | 14:SI:9:HIS:ND1    | 2.37                     | 0.57              |
| 47:LN:17:ASP:OD2   | 47:LN:20:ARG:NH2   | 2.37                     | 0.57              |
| 53:LT:87:LYS:NZ    | 79:L5:4305:G:N7    | 2.50                     | 0.57              |
| 79:L5:1591:U:OP2   | 79:L5:2856:C:O2'   | 2.23                     | 0.57              |
| 79:L5:4115:G:N2    | 79:L5:4115:G:OP2   | 2.36                     | 0.57              |
| 80:Et:53:G:H2'     | 80:Et:54:A:H8      | 1.70                     | 0.57              |
| 5:L8:93:C:OP1      | 69:Lj:76:HIS:NE2   | 2.31                     | 0.57              |
| 78:S2:46:A:N6      | 78:S2:97:U:O2      | 2.37                     | 0.57              |
| 78:S2:317:C:OP2    | 82:SG:183:ARG:NH2  | 2.32                     | 0.57              |
| 79:L5:4474:A:OP2   | 79:L5:4476:C:N4    | 2.38                     | 0.57              |
| 41:LG:154:LEU:HD13 | 41:LG:219:VAL:HG12 | 1.87                     | 0.56              |
| 62:LF:52:GLU:OE2   | 79:L5:1238:A:O2'   | 2.22                     | 0.56              |
| 78:S2:925:G:H1     | 78:S2:1017:U:H3    | 1.52                     | 0.56              |
| 6:L7:6:C:N4        | 92:L7:424:HOH:O    | 2.39                     | 0.56              |
| 18:SO:142:ARG:NH1  | 31:Sa:23:CYS:O     | 2.37                     | 0.56              |
| 29:SY:29:HIS:NE2   | 29:SY:69:THR:OG1   | 2.33                     | 0.56              |
| 78:S2:1536:G:H2'   | 78:S2:1537:A:C8    | 2.40                     | 0.56              |
| 79:L5:1895:G:O2'   | 79:L5:1907:A:N3    | 2.33                     | 0.56              |
| 79:L5:2335:C:H2'   | 79:L5:2336:G:H8    | 1.68                     | 0.56              |
| 2:SA:104:THR:O     | 2:SA:107:THR:OG1   | 2.21                     | 0.56              |
| 10:SC:254:ASP:N    | 10:SC:254:ASP:OD1  | 2.38                     | 0.56              |
| 11:SF:102:LEU:HD21 | 30:SZ:100:VAL:HG21 | 1.86                     | 0.56              |
| 15:SQ:142:GLN:NE2  | 78:S2:1527:C:OP1   | 2.36                     | 0.56              |
| 48:LI:30:LYS:HG3   | 48:LI:66:GLU:HG3   | 1.86                     | 0.56              |
| 69:Lj:49:TRP:O     | 79:L5:1646:A:O2'   | 2.21                     | 0.56              |
| 78:S2:512:A2M:H4'  | 78:S2:576:A2M:H2   | 1.86                     | 0.56              |
| 78:S2:1658:G:OP2   | 78:S2:1660:C:N4    | 2.38                     | 0.56              |
| 79:L5:2848:G:O2'   | 79:L5:3838:U:O4    | 2.18                     | 0.56              |
| 79:L5:4353:PSU:H5' | 79:L5:4354:U:H5'   | 1.86                     | 0.56              |
| 10:SC:179:THR:OG1  | 10:SC:180:VAL:N    | 2.39                     | 0.56              |
| 36:Sg:149:GLU:HG2  | 36:Sg:171:ASP:HB3  | 1.87                     | 0.56              |
| 77:mR:39:G:OP1     | 78:S2:1704:C:N4    | 2.37                     | 0.56              |
| 78:S2:151:C:O2'    | 82:SG:132:ARG:NH2  | 2.38                     | 0.56              |
| 79:L5:961:G:O2'    | 79:L5:963:G:N7     | 2.39                     | 0.56              |
| 40:LE:119:GLU:HB3  | 65:Le:7:LEU:HD22   | 1.88                     | 0.56              |
| 42:LO:176:ARG:HD2  | 79:L5:4769:G:H5''  | 1.88                     | 0.56              |
| 52:LS:3:ALA:O      | 52:LS:111:ARG:NH2  | 2.39                     | 0.56              |
| 78:S2:613:G:N2     | 78:S2:626:G:OP1    | 2.38                     | 0.56              |
| 78:S2:1259:A:N6    | 78:S2:1519:U:OP1   | 2.36                     | 0.56              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 79:L5:67:C:OP2       | 79:L5:312:G:N2     | 2.37                     | 0.56              |
| 2:SA:205:ARG:NH2     | 2:SA:213:GLU:OE1   | 2.29                     | 0.56              |
| 25:SR:79:GLU:O       | 25:SR:83:ASN:ND2   | 2.38                     | 0.56              |
| 50:LQ:173:LYS:NZ     | 79:L5:88:A:N7      | 2.53                     | 0.56              |
| 78:S2:84:A:N3        | 78:S2:150:A:O2'    | 2.38                     | 0.56              |
| 79:L5:2809:G:O2'     | 79:L5:4644:G:OP1   | 2.23                     | 0.56              |
| 4:SB:25:PHE:HA       | 4:SB:28:LYS:HD2    | 1.87                     | 0.56              |
| 36:Sg:114:SER:O      | 36:Sg:117:ASN:ND2  | 2.39                     | 0.56              |
| 42:LO:60:LYS:NZ      | 79:L5:2046:G:OP1   | 2.36                     | 0.56              |
| 44:LV:107:ASN:HD21   | 44:LV:111:GLU:HB2  | 1.71                     | 0.56              |
| 45:LM:118:MET:HE3    | 45:LM:122:ILE:HD11 | 1.88                     | 0.56              |
| 52:LS:174:THR:HG1    | 79:L5:4763:U:HO2'  | 1.52                     | 0.56              |
| 78:S2:106:C:OP1      | 78:S2:431:G:O2'    | 2.23                     | 0.56              |
| 78:S2:1101:U:H2'     | 78:S2:1102:G:H8    | 1.71                     | 0.56              |
| 79:L5:4589:A:N1      | 79:L5:4621:C:O2'   | 2.37                     | 0.56              |
| 14:SI:3:ILE:O        | 14:SI:30:GLY:N     | 2.36                     | 0.56              |
| 57:LY:28:LYS:NZ      | 79:L5:241:G:OP1    | 2.36                     | 0.56              |
| 67:Lg:5:LEU:HD21     | 67:Lg:30:ILE:HG22  | 1.88                     | 0.56              |
| 10:SC:187[B]:ARG:NH2 | 78:S2:1154:U:OP2   | 2.36                     | 0.56              |
| 21:SS:145:THR:HA     | 78:S2:1523:C:H4'   | 1.87                     | 0.56              |
| 23:SN:87:ASP:OD2     | 23:SN:87:ASP:N     | 2.37                     | 0.56              |
| 43:LL:55:ILE:O       | 43:LL:97:SER:OG    | 2.21                     | 0.56              |
| 50:LQ:65:ARG:NH1     | 79:L5:1459:A:OP1   | 2.38                     | 0.56              |
| 78:S2:587:A:H5'      | 78:S2:592:C:H41    | 1.70                     | 0.56              |
| 5:L8:102:G:OP2       | 5:L8:104:A:O2'     | 2.22                     | 0.56              |
| 9:SE:88:ASP:OD2      | 9:SE:122:LYS:NZ    | 2.38                     | 0.56              |
| 11:SF:145:ARG:HH12   | 78:S2:1220:A:H4'   | 1.71                     | 0.56              |
| 82:SG:49:VAL:HG12    | 82:SG:115:LYS:HB3  | 1.88                     | 0.56              |
| 3:LB:312:LYS:NZ      | 3:LB:368:ILE:O     | 2.38                     | 0.55              |
| 6:L7:19:C:OP2        | 38:LJ:154:LYS:NZ   | 2.37                     | 0.55              |
| 14:SI:101:ILE:HD12   | 14:SI:190:LEU:HD11 | 1.88                     | 0.55              |
| 65:Le:9:LYS:HB3      | 79:L5:703:G:H5''   | 1.86                     | 0.55              |
| 78:S2:562:U:H2'      | 78:S2:563:G:C8     | 2.41                     | 0.55              |
| 78:S2:874:G:H2'      | 78:S2:875:A:H8     | 1.71                     | 0.55              |
| 1:LA:223:SER:OG      | 79:L5:3748:A:O2'   | 2.20                     | 0.55              |
| 3:LB:168:MET:HA      | 3:LB:171:LEU:HD12  | 1.88                     | 0.55              |
| 24:SL:119:ASP:OD1    | 24:SL:119:ASP:N    | 2.37                     | 0.55              |
| 78:S2:436:OMG:OP2    | 78:S2:471:G:O2'    | 2.24                     | 0.55              |
| 78:S2:532:C:H2'      | 78:S2:533:A:C8     | 2.41                     | 0.55              |
| 78:S2:1424:G:H2'     | 78:S2:1425:G:H8    | 1.71                     | 0.55              |
| 79:L5:1332:C:H2'     | 79:L5:1333:A:C8    | 2.42                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:L5:4274:A:H2'  | 79:L5:4275:G:C8    | 2.41                     | 0.55              |
| 79:L5:4993:G:H22  | 79:L5:5058:A:H2    | 1.55                     | 0.55              |
| 36:Sg:213:ASP:OD1 | 36:Sg:213:ASP:N    | 2.37                     | 0.55              |
| 56:LX:64:SER:HB2  | 60:Lh:69:LEU:HD22  | 1.89                     | 0.55              |
| 79:L5:1705:G:H2'  | 79:L5:1706:A:C8    | 2.41                     | 0.55              |
| 12:SH:20:GLU:HB2  | 12:SH:48:ALA:HB3   | 1.88                     | 0.55              |
| 23:SN:5:HIS:HB3   | 23:SN:117:LEU:HD13 | 1.89                     | 0.55              |
| 32:Sb:11:SER:OG   | 32:Sb:13:GLU:OE1   | 2.25                     | 0.55              |
| 44:LV:84:GLN:HE21 | 44:LV:86:LYS:HB3   | 1.70                     | 0.55              |
| 45:LM:9:VAL:HG11  | 45:LM:66:HIS:HA    | 1.89                     | 0.55              |
| 79:L5:751:G:O6    | 79:L5:912:G:N2     | 2.33                     | 0.55              |
| 79:L5:4537:C:H2'  | 79:L5:4538:G:H8    | 1.72                     | 0.55              |
| 79:L5:4541:G:N2   | 79:L5:4544:A:OP2   | 2.32                     | 0.55              |
| 3:LB:113:GLU:HA   | 3:LB:116:ARG:HD2   | 1.88                     | 0.55              |
| 14:SI:142:SER:HB3 | 14:SI:145:ILE:HG22 | 1.87                     | 0.55              |
| 41:LG:81:ASN:O    | 41:LG:84:THR:OG1   | 2.24                     | 0.55              |
| 78:S2:165:G:H1'   | 82:SG:110:ASN:HD22 | 1.71                     | 0.55              |
| 78:S2:420:G:O2'   | 78:S2:660:C:N3     | 2.40                     | 0.55              |
| 78:S2:1550:G:O2'  | 78:S2:1558:C:O2    | 2.23                     | 0.55              |
| 79:L5:5068:G:N2   | 79:L5:5069:U:O4    | 2.37                     | 0.55              |
| 18:SO:101:GLY:HA3 | 18:SO:134:PRO:HD2  | 1.88                     | 0.55              |
| 58:LZ:29:ILE:HG22 | 58:LZ:32:GLY:H     | 1.70                     | 0.55              |
| 79:L5:1558:A:H2'  | 79:L5:1559:G:H8    | 1.71                     | 0.55              |
| 79:L5:2407:G:OP2  | 79:L5:2407:G:N2    | 2.36                     | 0.55              |
| 42:LO:125:LYS:HG3 | 42:LO:129:LEU:HD12 | 1.89                     | 0.55              |
| 54:LP:116:HIS:HB3 | 54:LP:149:ILE:HB   | 1.87                     | 0.55              |
| 60:Lh:81:LEU:HA   | 60:Lh:84:ARG:HD2   | 1.89                     | 0.55              |
| 76:Pt:63:C:H2'    | 76:Pt:64:G:H8      | 1.71                     | 0.55              |
| 79:L5:2045:G:O6   | 79:L5:3870:C:O2'   | 2.24                     | 0.55              |
| 1:LA:234:LYS:HG2  | 1:LA:238:ILE:HG12  | 1.89                     | 0.55              |
| 54:LP:82:ARG:NH1  | 92:LP:327:HOH:O    | 2.39                     | 0.55              |
| 2:SA:191:ARG:NH2  | 28:SV:44:GLY:O     | 2.40                     | 0.55              |
| 3:LB:26:ARG:NH1   | 92:LB:634:HOH:O    | 2.40                     | 0.55              |
| 4:SB:44:ILE:HD11  | 4:SB:86:LEU:HD12   | 1.89                     | 0.55              |
| 36:Sg:110:SER:HB3 | 36:Sg:154:VAL:HG22 | 1.89                     | 0.55              |
| 49:LD:196:ARG:NH2 | 49:LD:237:GLU:OE2  | 2.32                     | 0.55              |
| 51:LR:37:SER:OG   | 51:LR:40:GLN:NE2   | 2.38                     | 0.55              |
| 65:Le:108:ARG:NH1 | 79:L5:2326:G:OP1   | 2.38                     | 0.55              |
| 79:L5:4077:A:N1   | 79:L5:4171:C:N4    | 2.54                     | 0.55              |
| 81:LW:3:VAL:HG11  | 81:LW:12:LYS:HE3   | 1.88                     | 0.55              |
| 6:L7:99:G:N7      | 52:LS:55:LYS:NZ    | 2.54                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:SO:56:VAL:HG13  | 18:SO:60:MET:HE2   | 1.89                     | 0.55              |
| 23:SN:103:GLU:HG3  | 23:SN:104:ARG:HD2  | 1.89                     | 0.55              |
| 63:Lc:38:ILE:HG21  | 63:Lc:63:TYR:HB3   | 1.88                     | 0.55              |
| 78:S2:1396:A:O2'   | 78:S2:1398:G:N7    | 2.37                     | 0.55              |
| 5:L8:150:C:N4      | 41:LG:52:THR:O     | 2.39                     | 0.54              |
| 42:LO:49:ARG:NH1   | 79:L5:1930:U:OP2   | 2.36                     | 0.54              |
| 79:L5:4309:G:H5'   | 79:L5:4338:G:H5''  | 1.88                     | 0.54              |
| 6:L7:29:C:O2       | 6:L7:50:A:N6       | 2.38                     | 0.54              |
| 21:SS:117:ILE:HD12 | 26:SP:111:MET:HG2  | 1.89                     | 0.54              |
| 48:LI:76:MET:HE2   | 48:LI:138:ILE:HG21 | 1.89                     | 0.54              |
| 79:L5:4519:C:H5''  | 79:L5:4520:G:H5''  | 1.89                     | 0.54              |
| 79:L5:4734:A:H2'   | 79:L5:4735:G:C8    | 2.42                     | 0.54              |
| 79:L5:4927:G:OP2   | 79:L5:4927:G:N2    | 2.39                     | 0.54              |
| 14:SI:181:GLN:NE2  | 78:S2:380:G:OP2    | 2.40                     | 0.54              |
| 39:LH:94:SER:HB2   | 39:LH:142:ASP:HB3  | 1.88                     | 0.54              |
| 45:LM:11:ARG:NH1   | 45:LM:58:THR:O     | 2.41                     | 0.54              |
| 47:LN:181:HIS:O    | 47:LN:195:ARG:NH2  | 2.29                     | 0.54              |
| 48:LI:66:GLU:OE1   | 48:LI:69:ARG:NH2   | 2.35                     | 0.54              |
| 54:LP:64:ASN:ND2   | 54:LP:80:GLN:OE1   | 2.33                     | 0.54              |
| 57:LY:111:LEU:HB3  | 57:LY:116:LYS:HE3  | 1.89                     | 0.54              |
| 78:S2:568:C:H2'    | 78:S2:569:A:C8     | 2.43                     | 0.54              |
| 78:S2:1228:A:H2'   | 78:S2:1229:G:H8    | 1.73                     | 0.54              |
| 1:LA:147:ARG:HG2   | 1:LA:157:VAL:HG22  | 1.89                     | 0.54              |
| 2:SA:141:ASN:ND2   | 28:SV:31:SER:O     | 2.39                     | 0.54              |
| 3:LB:242:ARG:NH2   | 79:L5:2856:C:O2    | 2.32                     | 0.54              |
| 15:SQ:100:VAL:HG12 | 15:SQ:101:ASP:H    | 1.73                     | 0.54              |
| 48:LI:4:ARG:NH1    | 79:L5:1866:U:OP1   | 2.29                     | 0.54              |
| 78:S2:640:A:H2'    | 78:S2:641:A:C8     | 2.43                     | 0.54              |
| 78:S2:1220:A:N3    | 78:S2:1677:U:O2'   | 2.35                     | 0.54              |
| 79:L5:2579:G:N2    | 79:L5:2582:A:OP2   | 2.34                     | 0.54              |
| 79:L5:2777:G:H5''  | 79:L5:2778:G:H5'   | 1.89                     | 0.54              |
| 3:LB:77:THR:OG1    | 3:LB:335:GLY:O     | 2.23                     | 0.54              |
| 40:LE:181:LEU:O    | 79:L5:4883:C:N4    | 2.35                     | 0.54              |
| 51:LR:108:ARG:NH2  | 79:L5:2899:C:OP1   | 2.29                     | 0.54              |
| 55:LU:80:LYS:N     | 79:L5:2620:G:OP1   | 2.27                     | 0.54              |
| 3:LB:369:ASP:OD2   | 3:LB:373:LYS:NZ    | 2.40                     | 0.54              |
| 4:SB:150:ILE:HD13  | 25:SR:129:LYS:HB2  | 1.89                     | 0.54              |
| 5:L8:14:U:O2       | 79:L5:420:A:N6     | 2.41                     | 0.54              |
| 8:SJ:18:ARG:NH1    | 78:S2:3:C:O2       | 2.40                     | 0.54              |
| 21:SS:45:LEU:HD22  | 21:SS:50:ILE:HD11  | 1.89                     | 0.54              |
| 62:LF:46:ARG:HH22  | 79:L5:1704:C:HO2'  | 1.50                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 78:S2:44:U:O4      | 78:S2:485:A:N6     | 2.41                     | 0.54              |
| 79:L5:1283:G:N1    | 79:L5:2076:G:OP1   | 2.36                     | 0.54              |
| 79:L5:1739:G:N3    | 79:L5:1742:A:N6    | 2.55                     | 0.54              |
| 79:L5:2758:G:O2'   | 79:L5:2765:A:N3    | 2.35                     | 0.54              |
| 1:LA:247:ARG:HB3   | 78:S2:1069:U:H4'   | 1.89                     | 0.54              |
| 3:LB:139:ASP:OD2   | 3:LB:141:ASP:N     | 2.40                     | 0.54              |
| 5:L8:20:A:O2'      | 79:L5:2333:G:OP1   | 2.25                     | 0.54              |
| 57:LY:45:ARG:NH2   | 79:L5:238:C:OP2    | 2.41                     | 0.54              |
| 58:LZ:31:ASP:OD1   | 58:LZ:31:ASP:N     | 2.40                     | 0.54              |
| 78:S2:491:C:O2     | 78:S2:493:A:N6     | 2.38                     | 0.54              |
| 79:L5:3620:G:OP1   | 79:L5:3622:C:N4    | 2.41                     | 0.54              |
| 80:Et:62:C:H2'     | 80:Et:63:A:C8      | 2.43                     | 0.54              |
| 21:SS:88:LYS:O     | 26:SP:18:ARG:NH1   | 2.41                     | 0.54              |
| 41:LG:234:ARG:HH11 | 41:LG:235:ARG:HH21 | 1.55                     | 0.54              |
| 23:SN:83:ASP:N     | 23:SN:83:ASP:OD1   | 2.40                     | 0.54              |
| 42:LO:87:MET:SD    | 79:L5:1912:G:N2    | 2.81                     | 0.54              |
| 22:Sd:19:ARG:NH2   | 78:S2:1661:A:OP1   | 2.41                     | 0.53              |
| 22:Sd:34:TYR:OH    | 78:S2:1549:U:OP1   | 2.24                     | 0.53              |
| 25:SR:100:PRO:HG3  | 25:SR:122:PRO:HG3  | 1.89                     | 0.53              |
| 78:S2:1030:A:H2'   | 78:S2:1031:A2M:H8  | 1.89                     | 0.53              |
| 40:LE:190:HIS:HB3  | 40:LE:193:PHE:HD2  | 1.74                     | 0.53              |
| 45:LM:40:GLY:HA3   | 45:LM:45:VAL:HB    | 1.91                     | 0.53              |
| 65:Le:39:ARG:NH2   | 92:Le:311:HOH:O    | 2.36                     | 0.53              |
| 73:Ln:4:LYS:NZ     | 78:S2:1844:U:O4    | 2.33                     | 0.53              |
| 76:Pt:47:G7M:H2'   | 76:Pt:48:U:H5''    | 1.90                     | 0.53              |
| 4:SB:175:GLU:OE2   | 4:SB:187:LYS:NZ    | 2.37                     | 0.53              |
| 26:SP:69:PRO:O     | 26:SP:70:MET:HG2   | 2.08                     | 0.53              |
| 37:LC:140:LYS:HE3  | 37:LC:245:HIS:HB2  | 1.90                     | 0.53              |
| 59:Lr:32:LEU:O     | 59:Lr:113:ARG:NH1  | 2.41                     | 0.53              |
| 67:Lg:76:ARG:NH2   | 79:L5:2583:C:OP2   | 2.40                     | 0.53              |
| 79:L5:2416:G:N2    | 79:L5:2427:G:O6    | 2.40                     | 0.53              |
| 82:SG:26:THR:O     | 82:SG:30:LYS:NZ    | 2.41                     | 0.53              |
| 8:SJ:40:LYS:NZ     | 78:S2:641:A:OP1    | 2.40                     | 0.53              |
| 36:Sg:5:MET:HA     | 36:Sg:312:VAL:HA   | 1.89                     | 0.53              |
| 37:LC:103:ALA:HA   | 79:L5:1517:G:H22   | 1.72                     | 0.53              |
| 41:LG:200:THR:OG1  | 79:L5:150:U:OP2    | 2.23                     | 0.53              |
| 76:Pt:10:G:O6      | 76:Pt:46:G:N2      | 2.41                     | 0.53              |
| 78:S2:106:C:H2'    | 78:S2:107:A:H8     | 1.72                     | 0.53              |
| 78:S2:165:G:H4'    | 82:SG:53:SER:HB3   | 1.90                     | 0.53              |
| 79:L5:1500:A:H5''  | 79:L5:1501:C:H5''  | 1.91                     | 0.53              |
| 79:L5:2745:A:H2'   | 79:L5:2746:A:H8    | 1.73                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:SI:99:ASN:HB2   | 78:S2:377:G:H5'    | 1.91                     | 0.53              |
| 23:SN:2:GLY:N      | 78:S2:1092:G:OP1   | 2.42                     | 0.53              |
| 7:SD:142:LEU:HD13  | 7:SD:150:MET:HE2   | 1.91                     | 0.53              |
| 27:ST:85:ASN:ND2   | 27:ST:89:PRO:O     | 2.41                     | 0.53              |
| 35:Sf:143:LYS:NZ   | 78:S2:1311:C:OP1   | 2.39                     | 0.53              |
| 79:L5:3700:C:O2'   | 79:L5:3774:A:N3    | 2.37                     | 0.53              |
| 80:Et:41:C:H2'     | 80:Et:42:A:H8      | 1.73                     | 0.53              |
| 82:SG:142:ARG:HA   | 82:SG:147:LEU:HB3  | 1.90                     | 0.53              |
| 1:LA:117:GLU:HG2   | 1:LA:124:GLY:H     | 1.73                     | 0.53              |
| 7:SD:35:SER:HB2    | 7:SD:51:LEU:HD23   | 1.91                     | 0.53              |
| 7:SD:212:GLU:H     | 7:SD:212:GLU:CD    | 2.17                     | 0.53              |
| 48:LI:87:ILE:HG12  | 48:LI:138:ILE:HG23 | 1.89                     | 0.53              |
| 62:LF:40:LYS:HE3   | 62:LF:44:LYS:HE2   | 1.89                     | 0.53              |
| 79:L5:1503:A:H4'   | 79:L5:1504:G:H5'   | 1.91                     | 0.53              |
| 14:SI:2:GLY:N      | 78:S2:441:C:OP2    | 2.41                     | 0.53              |
| 37:LC:106:LYS:NZ   | 92:LC:619:HOH:O    | 2.33                     | 0.53              |
| 61:Lb:33:LYS:NZ    | 79:L5:4299:PSU:OP1 | 2.42                     | 0.53              |
| 2:SA:134:LEU:HD21  | 2:SA:144:THR:HG21  | 1.90                     | 0.53              |
| 36:Sg:164:ILE:HG22 | 36:Sg:178:ASN:HA   | 1.91                     | 0.53              |
| 49:LD:166:ALA:HB1  | 49:LD:171:LEU:HD12 | 1.91                     | 0.53              |
| 58:LZ:21:ARG:NH1   | 92:LZ:201:HOH:O    | 2.39                     | 0.53              |
| 78:S2:107:A:H2'    | 78:S2:108:G:C8     | 2.44                     | 0.53              |
| 79:L5:489:C:O2     | 79:L5:667:A:N6     | 2.42                     | 0.53              |
| 79:L5:2589:C:HO2'  | 79:L5:2767:U:HO2'  | 1.54                     | 0.53              |
| 79:L5:4537:C:H2'   | 79:L5:4538:G:C8    | 2.44                     | 0.53              |
| 30:SZ:79:ILE:HB    | 30:SZ:83:LEU:HD23  | 1.90                     | 0.53              |
| 38:LJ:81:GLU:HG3   | 38:LJ:82:ILE:HD13  | 1.91                     | 0.53              |
| 49:LD:108:ARG:HE   | 49:LD:253:TYR:HB2  | 1.73                     | 0.53              |
| 55:LU:111:GLU:HG2  | 55:LU:113:ARG:HG3  | 1.91                     | 0.53              |
| 74:Lo:34:TYR:O     | 74:Lo:39:ARG:NH1   | 2.41                     | 0.53              |
| 79:L5:4750:G:H2'   | 79:L5:4751:G:H8    | 1.73                     | 0.53              |
| 2:SA:50:ASN:HB3    | 2:SA:53:ARG:HG3    | 1.90                     | 0.52              |
| 12:SH:83:LEU:HD13  | 12:SH:92:VAL:HG11  | 1.91                     | 0.52              |
| 21:SS:88:LYS:HG2   | 26:SP:18:ARG:HD2   | 1.90                     | 0.52              |
| 42:LO:130:LYS:HB2  | 42:LO:133:ARG:HG2  | 1.92                     | 0.52              |
| 65:Le:89:LEU:HD13  | 65:Le:118:LEU:HD22 | 1.91                     | 0.52              |
| 79:L5:4274:A:H2'   | 79:L5:4275:G:H8    | 1.73                     | 0.52              |
| 3:LB:108:GLU:OE2   | 3:LB:138:GLN:NE2   | 2.32                     | 0.52              |
| 45:LM:98:ARG:NH1   | 79:L5:4872:G:O6    | 2.43                     | 0.52              |
| 52:LS:15:ARG:HB3   | 52:LS:27:LEU:HD23  | 1.90                     | 0.52              |
| 79:L5:1414:C:H2'   | 79:L5:1415:G:C8    | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:Et:62:C:H2'     | 80:Et:63:A:H8      | 1.72                     | 0.52              |
| 13:SW:55:ASP:OD1   | 13:SW:55:ASP:N     | 2.41                     | 0.52              |
| 23:SN:64:ARG:NH1   | 78:S2:919:A:OP2    | 2.31                     | 0.52              |
| 40:LE:123:ARG:NH2  | 79:L5:961:G:O6     | 2.37                     | 0.52              |
| 43:LL:135:LYS:NZ   | 79:L5:170:C:O2'    | 2.42                     | 0.52              |
| 49:LD:160:PHE:HA   | 49:LD:163:LEU:HB3  | 1.91                     | 0.52              |
| 55:LU:101:ARG:HE   | 55:LU:103:VAL:HG22 | 1.75                     | 0.52              |
| 62:LF:128:ALA:O    | 79:L5:1726:U:O2'   | 2.26                     | 0.52              |
| 79:L5:1320:U:O2    | 79:L5:1891:A:N6    | 2.43                     | 0.52              |
| 79:L5:2520:C:H2'   | 79:L5:2521:G:H8    | 1.74                     | 0.52              |
| 79:L5:2640:G:H2'   | 79:L5:2641:A:C8    | 2.45                     | 0.52              |
| 6:L7:11:A:N1       | 6:L7:66:G:O2'      | 2.40                     | 0.52              |
| 15:SQ:89:SER:HB3   | 15:SQ:112:LEU:HD13 | 1.90                     | 0.52              |
| 66:Lf:35:ALA:HB3   | 66:Lf:38:GLU:HG3   | 1.91                     | 0.52              |
| 78:S2:1171:G:O2'   | 78:S2:1187:G:O6    | 2.22                     | 0.52              |
| 79:L5:4598:C:O2    | 79:L5:4612:C:N4    | 2.36                     | 0.52              |
| 82:SG:2:LYS:HB2    | 82:SG:108:VAL:HG23 | 1.91                     | 0.52              |
| 1:LA:107:MET:O     | 1:LA:139:HIS:NE2   | 2.35                     | 0.52              |
| 17:SK:15:LEU:HD22  | 17:SK:49:MET:HE1   | 1.92                     | 0.52              |
| 23:SN:40:LEU:HB3   | 23:SN:45:LEU:HD12  | 1.92                     | 0.52              |
| 63:Lc:28:VAL:HG21  | 63:Lc:37:MET:HG3   | 1.91                     | 0.52              |
| 3:LB:154:LYS:HG3   | 3:LB:194:LEU:HD12  | 1.92                     | 0.52              |
| 4:SB:77:ASP:OD1    | 4:SB:77:ASP:N      | 2.43                     | 0.52              |
| 38:LJ:146:ARG:HG3  | 49:LD:150:LEU:HD12 | 1.91                     | 0.52              |
| 79:L5:496:G:H2'    | 79:L5:497:G:C8     | 2.44                     | 0.52              |
| 79:L5:2568:C:H2'   | 79:L5:2569:G:H8    | 1.73                     | 0.52              |
| 50:LQ:42:THR:HB    | 79:L5:1428:U:H5''  | 1.90                     | 0.52              |
| 56:LX:83:THR:HG22  | 79:L5:2434:G:H5''  | 1.91                     | 0.52              |
| 78:S2:848:U:H2'    | 78:S2:849:A:H8     | 1.75                     | 0.52              |
| 3:LB:167:GLN:NE2   | 3:LB:204:GLN:OE1   | 2.37                     | 0.52              |
| 13:SW:11:LEU:HD22  | 13:SW:72:CYS:HB2   | 1.92                     | 0.52              |
| 18:SO:98:ARG:HB3   | 18:SO:132:VAL:HG23 | 1.92                     | 0.52              |
| 26:SP:81:ARG:NH2   | 26:SP:117:GLY:O    | 2.43                     | 0.52              |
| 33:Sc:21:THR:OG1   | 33:Sc:22:GLY:N     | 2.43                     | 0.52              |
| 42:LO:166:ILE:HG13 | 42:LO:169:ARG:HH21 | 1.74                     | 0.52              |
| 70:Lk:19:ASP:OD2   | 70:Lk:19:ASP:N     | 2.36                     | 0.52              |
| 79:L5:3861:A:H2'   | 79:L5:3862:A:H8    | 1.75                     | 0.52              |
| 79:L5:4141:G:N2    | 79:L5:4143:G:O6    | 2.43                     | 0.52              |
| 1:LA:36:GLU:OE2    | 1:LA:163:ARG:NH1   | 2.43                     | 0.52              |
| 2:SA:147:LEU:O     | 2:SA:165:ASN:ND2   | 2.41                     | 0.52              |
| 9:SE:27:PHE:O      | 78:S2:495:U:O2'    | 2.28                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:SY:108:LYS:NZ   | 78:S2:506:G:OP1    | 2.43                     | 0.52              |
| 49:LD:267:ASN:N    | 49:LD:267:ASN:OD1  | 2.42                     | 0.52              |
| 78:S2:140:C:H42    | 78:S2:313:A:H61    | 1.57                     | 0.52              |
| 78:S2:981:A:H2'    | 78:S2:982:G:C8     | 2.44                     | 0.52              |
| 79:L5:369:G:N2     | 79:L5:372:A:OP2    | 2.35                     | 0.52              |
| 79:L5:1942:A:H2'   | 79:L5:1943:A:C8    | 2.45                     | 0.52              |
| 1:LA:220:GLY:O     | 79:L5:3749:C:O2'   | 2.28                     | 0.51              |
| 10:SC:161:SER:O    | 10:SC:161:SER:OG   | 2.26                     | 0.51              |
| 53:LT:130:ARG:NE   | 79:L5:1837:A:OP2   | 2.40                     | 0.51              |
| 55:LU:61:VAL:HG22  | 55:LU:74:SER:HB2   | 1.90                     | 0.51              |
| 65:Le:16:ARG:NH1   | 79:L5:438:G:OP1    | 2.29                     | 0.51              |
| 79:L5:2415:OMU:H2' | 79:L5:2416:G:O4'   | 2.10                     | 0.51              |
| 79:L5:3946:G:H1    | 79:L5:4067:U:H3    | 1.58                     | 0.51              |
| 3:LB:140:GLU:N     | 3:LB:140:GLU:OE2   | 2.42                     | 0.51              |
| 4:SB:139:CYS:SG    | 4:SB:172:MET:HE1   | 2.49                     | 0.51              |
| 21:SS:134:GLN:NE2  | 78:S2:1608:U:OP1   | 2.44                     | 0.51              |
| 27:ST:90:SER:O     | 27:ST:91:HIS:ND1   | 2.43                     | 0.51              |
| 42:LO:9:LEU:HD23   | 42:LO:118:MET:HB2  | 1.91                     | 0.51              |
| 92:Lj:205:HOH:O    | 79:L5:1600:A:OP1   | 2.19                     | 0.51              |
| 79:L5:1480:C:O2'   | 79:L5:1482:G:OP2   | 2.24                     | 0.51              |
| 79:L5:2745:A:H2'   | 79:L5:2746:A:C8    | 2.45                     | 0.51              |
| 79:L5:3893:C:O2'   | 79:L5:4979:A:N1    | 2.41                     | 0.51              |
| 3:LB:291:TYR:OH    | 3:LB:315:ASN:ND2   | 2.42                     | 0.51              |
| 6:L7:35:U:O2       | 6:L7:45:U:O2'      | 2.27                     | 0.51              |
| 10:SC:183:LYS:NZ   | 13:SW:91:ASN:O     | 2.42                     | 0.51              |
| 21:SS:121:ARG:HG3  | 21:SS:131:VAL:HB   | 1.92                     | 0.51              |
| 37:LC:205:ARG:HG2  | 79:L5:2297:G:H5'   | 1.91                     | 0.51              |
| 51:LR:124:TYR:OH   | 79:L5:2666:U:OP2   | 2.20                     | 0.51              |
| 62:LF:76:ARG:NE    | 79:L5:730:G:OP2    | 2.41                     | 0.51              |
| 79:L5:158:A:H5''   | 79:L5:159:C:H2'    | 1.91                     | 0.51              |
| 79:L5:3788:C:N4    | 79:L5:3812:C:OP2   | 2.41                     | 0.51              |
| 79:L5:4670:C:O2'   | 79:L5:4672:A:OP2   | 2.25                     | 0.51              |
| 79:L5:4967:A:H2'   | 79:L5:4968:A:H8    | 1.75                     | 0.51              |
| 25:SR:129:LYS:NZ   | 78:S2:1100:A:OP1   | 2.35                     | 0.51              |
| 29:SY:103:SER:HB3  | 29:SY:106:GLN:HG3  | 1.93                     | 0.51              |
| 36:Sg:154:VAL:O    | 36:Sg:155:ARG:NE   | 2.43                     | 0.51              |
| 36:Sg:249:CYS:HB3  | 36:Sg:289:LEU:HD13 | 1.93                     | 0.51              |
| 53:LT:70:HIS:ND1   | 79:L5:4314:C:OP1   | 2.43                     | 0.51              |
| 66:Lf:23:GLU:OE1   | 79:L5:438:G:N2     | 2.34                     | 0.51              |
| 5:L8:26:C:O2'      | 37:LC:53:ALA:O     | 2.24                     | 0.51              |
| 7:SD:29:LEU:HD21   | 7:SD:69:LEU:HD11   | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:SD:162:ASP:OD1   | 7:SD:165:ASN:ND2   | 2.42                     | 0.51              |
| 11:SF:123:GLU:OE2  | 11:SF:204:ARG:NH1  | 2.43                     | 0.51              |
| 11:SF:144:LEU:HD23 | 33:Sc:49:PRO:HG2   | 1.91                     | 0.51              |
| 24:SL:81:LYS:HB3   | 78:S2:394:G:H5'    | 1.92                     | 0.51              |
| 36:Sg:66:VAL:HA    | 36:Sg:82:SER:HA    | 1.93                     | 0.51              |
| 43:LL:74:ARG:NH2   | 79:L5:109:G:OP2    | 2.44                     | 0.51              |
| 78:S2:388:U:H2'    | 78:S2:389:A:H8     | 1.75                     | 0.51              |
| 80:Et:41:C:H2'     | 80:Et:42:A:C8      | 2.45                     | 0.51              |
| 3:LB:2:SER:N       | 79:L5:4517:A:OP2   | 2.44                     | 0.51              |
| 9:SE:11:ARG:HA     | 9:SE:28:ALA:HB2    | 1.92                     | 0.51              |
| 43:LL:80:GLU:HG3   | 43:LL:110:LEU:HD12 | 1.90                     | 0.51              |
| 47:LN:96:ARG:NH2   | 47:LN:104:GLU:OE1  | 2.43                     | 0.51              |
| 51:LR:105:LEU:HD13 | 51:LR:135:LYS:HE3  | 1.93                     | 0.51              |
| 78:S2:1204:A:O2'   | 78:S2:1700:C:OP2   | 2.22                     | 0.51              |
| 79:L5:300:A:H2'    | 79:L5:301:G:H8     | 1.75                     | 0.51              |
| 78:S2:895:G:H2'    | 78:S2:896:U:H4'    | 1.93                     | 0.51              |
| 78:S2:1084:A:OP1   | 78:S2:1858:G:O2'   | 2.27                     | 0.51              |
| 79:L5:278:G:H5'    | 79:L5:329:A:N6     | 2.26                     | 0.51              |
| 2:SA:8:LEU:HD11    | 28:SV:39:VAL:HG21  | 1.92                     | 0.51              |
| 2:SA:76:VAL:HG12   | 2:SA:123:VAL:HB    | 1.93                     | 0.51              |
| 3:LB:14:LEU:HD11   | 3:LB:265:SER:HB3   | 1.93                     | 0.51              |
| 14:SI:5:ARG:NE     | 78:S2:379:C:O2     | 2.43                     | 0.51              |
| 37:LC:95:MET:H     | 37:LC:95:MET:HE2   | 1.76                     | 0.51              |
| 41:LG:165:GLU:HB3  | 47:LN:7:ILE:HG23   | 1.93                     | 0.51              |
| 43:LL:80:GLU:OE1   | 43:LL:102:ARG:NH2  | 2.43                     | 0.51              |
| 60:Lh:72:PHE:O     | 60:Lh:76:LYS:NZ    | 2.44                     | 0.51              |
| 77:mR:35:G:H4'     | 77:mR:36:A:H5'     | 1.91                     | 0.51              |
| 79:L5:926:G:H2'    | 79:L5:927:G:H8     | 1.76                     | 0.51              |
| 79:L5:1582:PSU:O4  | 79:L5:2396:A:N6    | 2.44                     | 0.51              |
| 79:L5:1764:G:O6    | 79:L5:1769:G:N1    | 2.44                     | 0.51              |
| 79:L5:2574:G:N7    | 79:L5:2760:G:N2    | 2.58                     | 0.51              |
| 2:SA:74:VAL:HG13   | 2:SA:121:LEU:HB3   | 1.93                     | 0.51              |
| 12:SH:43:LEU:HD22  | 12:SH:68:GLN:HG3   | 1.92                     | 0.51              |
| 78:S2:455:A:H2'    | 78:S2:456:C:H6     | 1.76                     | 0.51              |
| 78:S2:1382:A:H2'   | 78:S2:1383:A2M:H8  | 1.93                     | 0.51              |
| 79:L5:83:C:O2      | 79:L5:100:C:N4     | 2.34                     | 0.51              |
| 79:L5:1097:C:H2'   | 79:L5:1098:G:H8    | 1.76                     | 0.51              |
| 1:LA:118:GLU:OE1   | 79:L5:3662:A:O2'   | 2.26                     | 0.51              |
| 14:SI:34:ALA:HB2   | 14:SI:56:ARG:HD2   | 1.92                     | 0.51              |
| 29:SY:15:ASN:ND2   | 29:SY:22:GLN:OE1   | 2.43                     | 0.51              |
| 60:Lh:76:LYS:O     | 79:L5:136:C:N4     | 2.44                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 78:S2:65:C:N4      | 78:S2:169:U:O2'    | 2.44                     | 0.51              |
| 78:S2:1354:G:N2    | 78:S2:1357:A:OP2   | 2.36                     | 0.51              |
| 78:S2:1528:G:O2'   | 78:S2:1666:C:OP1   | 2.27                     | 0.51              |
| 79:L5:93:G:H2'     | 79:L5:94:A:C8      | 2.46                     | 0.51              |
| 79:L5:3900:G:O6    | 79:L5:4523:A2M:N6  | 2.41                     | 0.51              |
| 1:LA:65:ASP:OD2    | 1:LA:72:ARG:NE     | 2.41                     | 0.50              |
| 3:LB:161:ARG:HG2   | 3:LB:184:GLN:HA    | 1.93                     | 0.50              |
| 9:SE:160:ILE:HD12  | 9:SE:169:ILE:HG12  | 1.92                     | 0.50              |
| 21:SS:75:ARG:NH1   | 21:SS:81:ASP:OD1   | 2.44                     | 0.50              |
| 72:Lm:109:ASN:ND2  | 72:Lm:117:HIS:O    | 2.43                     | 0.50              |
| 78:S2:604:A:N3     | 78:S2:639:C:O2'    | 2.36                     | 0.50              |
| 79:L5:1933:G:H2'   | 79:L5:1934:A:C8    | 2.45                     | 0.50              |
| 11:SF:122:ARG:HD2  | 33:Sc:57:THR:HG21  | 1.92                     | 0.50              |
| 21:SS:117:ILE:HD11 | 26:SP:110:GLU:HG2  | 1.94                     | 0.50              |
| 41:LG:132:ARG:NH2  | 79:L5:119:G:OP1    | 2.39                     | 0.50              |
| 46:La:36:GLY:HA3   | 46:La:40:HIS:CE1   | 2.46                     | 0.50              |
| 49:LD:109:LEU:HD23 | 49:LD:171:LEU:HD21 | 1.92                     | 0.50              |
| 53:LT:102:ARG:NH1  | 53:LT:105:PHE:HD2  | 2.09                     | 0.50              |
| 78:S2:1259:A:H1'   | 78:S2:1264:C:N4    | 2.26                     | 0.50              |
| 78:S2:1743:G:H21   | 78:S2:1791:A:H62   | 1.60                     | 0.50              |
| 79:L5:717:U:H2'    | 79:L5:718:C:C6     | 2.45                     | 0.50              |
| 79:L5:3910:C:H2'   | 79:L5:3911:C:H6    | 1.76                     | 0.50              |
| 79:L5:5006:U:H4'   | 79:L5:5007:A:H5'   | 1.92                     | 0.50              |
| 6:L7:7:G:OP1       | 49:LD:33:ARG:NH1   | 2.42                     | 0.50              |
| 19:SX:24:ASP:HB3   | 19:SX:27:TYR:HB3   | 1.92                     | 0.50              |
| 25:SR:47:ARG:NH1   | 25:SR:48:ASN:OD1   | 2.44                     | 0.50              |
| 52:LS:17:LEU:HD11  | 53:LT:136:ARG:HH11 | 1.75                     | 0.50              |
| 78:S2:1190:A:N3    | 78:S2:1714:U:O2'   | 2.42                     | 0.50              |
| 79:L5:2494:U:H2'   | 79:L5:2495:U:O4'   | 2.11                     | 0.50              |
| 5:L8:67:U:H2'      | 5:L8:68:G:C8       | 2.47                     | 0.50              |
| 8:SJ:47:LYS:HG3    | 8:SJ:102:ILE:HD12  | 1.92                     | 0.50              |
| 10:SC:123:ARG:NH2  | 78:S2:1358:U:OP2   | 2.45                     | 0.50              |
| 51:LR:62:ARG:NH2   | 79:L5:4646:U:OP2   | 2.31                     | 0.50              |
| 77:mR:33:G:H2'     | 78:S2:961:G:C2     | 2.46                     | 0.50              |
| 78:S2:145:G:H2'    | 78:S2:146:G:C8     | 2.47                     | 0.50              |
| 29:SY:37:LYS:NZ    | 78:S2:572:PSU:OP2  | 2.43                     | 0.50              |
| 40:LE:209:PRO:HB2  | 40:LE:212:LEU:HD23 | 1.93                     | 0.50              |
| 47:LN:68:ARG:HD2   | 47:LN:128:LYS:HG3  | 1.94                     | 0.50              |
| 78:S2:1144:A:H5'   | 78:S2:1355:C:H41   | 1.75                     | 0.50              |
| 3:LB:56:ILE:HD13   | 3:LB:365:LEU:HD22  | 1.92                     | 0.50              |
| 3:LB:92:TYR:HB3    | 3:LB:99:LEU:HD22   | 1.94                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:SE:112:HIS:NE2   | 9:SE:237:SER:O      | 2.45                     | 0.50              |
| 50:LQ:50:ARG:NH1   | 92:LQ:314:HOH:O     | 2.45                     | 0.50              |
| 15:SQ:13:PHE:HB3   | 15:SQ:22:VAL:HG22   | 1.94                     | 0.50              |
| 23:SN:30:SER:HB2   | 23:SN:67:THR:HA     | 1.93                     | 0.50              |
| 37:LC:60:HIS:HA    | 37:LC:92:PHE:HE1    | 1.75                     | 0.50              |
| 47:LN:135:ILE:HG21 | 47:LN:151:ILE:HG21  | 1.92                     | 0.50              |
| 62:LF:89:LEU:HD11  | 62:LF:122:PHE:HB3   | 1.93                     | 0.50              |
| 70:Lk:35:LYS:NZ    | 79:L5:2693:G:OP1    | 2.33                     | 0.50              |
| 78:S2:73:C:O2'     | 78:S2:74:G:N3       | 2.37                     | 0.50              |
| 78:S2:1226:G:N1    | 78:S2:1639:G7M:OP2  | 2.37                     | 0.50              |
| 1:LA:54:ARG:NH2    | 79:L5:3680:U:OP1    | 2.32                     | 0.50              |
| 9:SE:107:GLY:HA2   | 9:SE:189:LEU:HG     | 1.93                     | 0.50              |
| 9:SE:141:THR:OG1   | 9:SE:143:ASP:OD1    | 2.27                     | 0.50              |
| 60:Lh:107:GLN:NE2  | 60:Lh:111:GLU:OE1   | 2.44                     | 0.50              |
| 65:Le:21:ILE:HD13  | 65:Le:33[B]:ARG:HD3 | 1.93                     | 0.50              |
| 79:L5:1669:A:H4'   | 79:L5:1685:G:N2     | 2.26                     | 0.50              |
| 10:SC:242:ASP:O    | 10:SC:246:LYS:HG2   | 2.12                     | 0.50              |
| 17:SK:65:ARG:HH12  | 22:Sd:20:SER:HB2    | 1.76                     | 0.50              |
| 25:SR:66:VAL:HG23  | 25:SR:67:ARG:H      | 1.76                     | 0.50              |
| 46:La:51:GLY:N     | 50:LQ:178:ARG:O     | 2.45                     | 0.50              |
| 62:LF:96:ARG:NH1   | 79:L5:1895:G:OP1    | 2.44                     | 0.50              |
| 69:Lj:13:ASN:ND2   | 79:L5:1618:G:OP1    | 2.36                     | 0.50              |
| 78:S2:656:G:N2     | 78:S2:663:C:H5''    | 2.26                     | 0.50              |
| 78:S2:1139:C:N4    | 78:S2:1149:A:H62    | 2.10                     | 0.50              |
| 79:L5:4594:U:H2'   | 79:L5:4595:G:C8     | 2.44                     | 0.50              |
| 79:L5:4967:A:H2'   | 79:L5:4968:A:C8     | 2.46                     | 0.50              |
| 3:LB:175:GLN:NE2   | 3:LB:177:LYS:O      | 2.35                     | 0.49              |
| 6:L7:24:C:O2       | 6:L7:117:G:N2       | 2.33                     | 0.49              |
| 23:SN:13:GLN:HG3   | 32:Sb:21:LYS:HE3    | 1.93                     | 0.49              |
| 25:SR:56:HIS:NE2   | 78:S2:1465:A:OP1    | 2.35                     | 0.49              |
| 48:LI:47:PRO:HB3   | 48:LI:171:TRP:CZ2   | 2.47                     | 0.49              |
| 66:Lf:78:HIS:HB2   | 66:Lf:85:ARG:HG2    | 1.94                     | 0.49              |
| 78:S2:1101:U:H2'   | 78:S2:1102:G:C8     | 2.47                     | 0.49              |
| 78:S2:1221:G:O2'   | 78:S2:1676:U:O2     | 2.25                     | 0.49              |
| 79:L5:1328:G:O2'   | 79:L5:2349:A:OP1    | 2.29                     | 0.49              |
| 79:L5:1577:G:O2'   | 79:L5:1612:G:H4'    | 2.11                     | 0.49              |
| 79:L5:1700:G:N2    | 79:L5:2097:U:O4'    | 2.41                     | 0.49              |
| 79:L5:4260:U:H2'   | 79:L5:4261:C:C6     | 2.47                     | 0.49              |
| 1:LA:117:GLU:O     | 1:LA:162:ASN:ND2    | 2.45                     | 0.49              |
| 11:SF:29:GLN:H     | 11:SF:110:GLN:NE2   | 2.09                     | 0.49              |
| 11:SF:107:ASN:HB3  | 11:SF:110:GLN:HB2   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:SH:32:MET:SD    | 12:SH:32:MET:N     | 2.85                     | 0.49              |
| 29:SY:105:LYS:NZ   | 78:S2:52:G:O2'     | 2.37                     | 0.49              |
| 49:LD:62:CYS:HB3   | 49:LD:105:LEU:HD22 | 1.94                     | 0.49              |
| 78:S2:1351:G:O2'   | 78:S2:1378:A:N1    | 2.43                     | 0.49              |
| 79:L5:445:U:O4     | 79:L5:1301:C:N4    | 2.42                     | 0.49              |
| 3:LB:49:TYR:OH     | 3:LB:168:MET:SD    | 2.66                     | 0.49              |
| 12:SH:106:ARG:NH1  | 78:S2:801:PSU:O2   | 2.39                     | 0.49              |
| 13:SW:112:ASP:OD1  | 13:SW:112:ASP:N    | 2.38                     | 0.49              |
| 28:SV:17:CYS:HB2   | 28:SV:56:CYS:HB3   | 1.93                     | 0.49              |
| 43:LL:103:ARG:NH1  | 92:LL:426:HOH:O    | 2.44                     | 0.49              |
| 62:LF:236:ARG:NH1  | 92:LF:441:HOH:O    | 2.46                     | 0.49              |
| 5:L8:52:A:H5'      | 71:L1:21:ARG:HD3   | 1.93                     | 0.49              |
| 53:LT:100:LYS:HB2  | 79:L5:1730:U:H4'   | 1.94                     | 0.49              |
| 78:S2:116:OMU:O5'  | 78:S2:116:OMU:H6   | 2.13                     | 0.49              |
| 79:L5:2090:U:H4'   | 79:L5:2091:C:H3'   | 1.94                     | 0.49              |
| 31:Sa:32:LYS:NZ    | 78:S2:989:C:O2     | 2.45                     | 0.49              |
| 47:LN:179:LYS:O    | 79:L5:297:U:O2'    | 2.31                     | 0.49              |
| 49:LD:3:PHE:HB3    | 79:L5:1755:C:N3    | 2.28                     | 0.49              |
| 65:Le:128:ARG:NH1  | 79:L5:2306:G:OP1   | 2.43                     | 0.49              |
| 78:S2:940:U:H3     | 78:S2:1002:U:H3    | 1.61                     | 0.49              |
| 79:L5:699:C:H2'    | 79:L5:700:G:H8     | 1.76                     | 0.49              |
| 79:L5:4638:U:OP1   | 79:L5:5044:A:O2'   | 2.29                     | 0.49              |
| 3:LB:28:LYS:NZ     | 79:L5:4582:C:OP2   | 2.35                     | 0.49              |
| 12:SH:7:LYS:HZ1    | 12:SH:40:LEU:HD22  | 1.78                     | 0.49              |
| 14:SI:22:HIS:HB3   | 78:S2:433:A:H5''   | 1.95                     | 0.49              |
| 27:ST:77:LYS:HD3   | 78:S2:1587:G:H5''  | 1.95                     | 0.49              |
| 51:LR:117:ARG:NH1  | 79:L5:2660:A:OP1   | 2.45                     | 0.49              |
| 57:LY:82:ILE:HB    | 57:LY:85:VAL:HB    | 1.95                     | 0.49              |
| 61:Lb:12:GLN:OE1   | 61:Lb:15:LYS:NZ    | 2.32                     | 0.49              |
| 78:S2:528:A:H2'    | 78:S2:529:A:H8     | 1.78                     | 0.49              |
| 79:L5:162:A:H2'    | 79:L5:163:A:C8     | 2.47                     | 0.49              |
| 79:L5:1245:C:H2'   | 79:L5:1246:G:C8    | 2.45                     | 0.49              |
| 79:L5:2459:G:N2    | 79:L5:2462:C:OP2   | 2.44                     | 0.49              |
| 79:L5:3669:G:H21   | 79:L5:3672:G:H21   | 1.60                     | 0.49              |
| 79:L5:3910:C:H2'   | 79:L5:3911:C:C6    | 2.47                     | 0.49              |
| 3:LB:140:GLU:H     | 3:LB:140:GLU:CD    | 2.20                     | 0.49              |
| 18:SO:116:LEU:HD13 | 31:Sa:45:VAL:HG12  | 1.93                     | 0.49              |
| 26:SP:64:LYS:HE2   | 26:SP:92:SER:HB3   | 1.94                     | 0.49              |
| 51:LR:20:LYS:NZ    | 79:L5:2822:G:N7    | 2.58                     | 0.49              |
| 51:LR:38:ARG:NH2   | 79:L5:2527:A:OP1   | 2.39                     | 0.49              |
| 51:LR:107:ARG:O    | 51:LR:111:GLU:HG2  | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:LZ:41:ALA:HB2   | 58:LZ:77:TYR:HE1   | 1.78                     | 0.49              |
| 78:S2:28:U:H2'     | 78:S2:29:G:H8      | 1.77                     | 0.49              |
| 79:L5:1442:C:H2'   | 79:L5:1443:A:C8    | 2.47                     | 0.49              |
| 79:L5:1872:G:O2'   | 79:L5:4219:A:N3    | 2.44                     | 0.49              |
| 79:L5:3717:A:H2'   | 79:L5:3718:A2M:C8  | 2.42                     | 0.49              |
| 3:LB:176:LYS:HG3   | 79:L5:4986:G:H5''  | 1.94                     | 0.49              |
| 3:LB:261:ARG:HB2   | 42:LO:64:THR:HG21  | 1.95                     | 0.49              |
| 23:SN:3:ARG:HB2    | 23:SN:6:ALA:HB3    | 1.94                     | 0.49              |
| 65:Le:3:ALA:HB1    | 65:Le:121:ARG:HH21 | 1.76                     | 0.49              |
| 79:L5:1740:C:O2    | 79:L5:1786:A:N6    | 2.45                     | 0.49              |
| 79:L5:2588:C:OP1   | 79:L5:2768:C:O2'   | 2.27                     | 0.49              |
| 2:SA:77:ILE:HD11   | 2:SA:99:ILE:HD12   | 1.95                     | 0.49              |
| 10:SC:166:ARG:HB3  | 10:SC:247:THR:HB   | 1.94                     | 0.49              |
| 38:LJ:40:LEU:O     | 38:LJ:44:THR:OG1   | 2.27                     | 0.49              |
| 39:LH:75:SER:OG    | 79:L5:4691:A:OP1   | 2.30                     | 0.49              |
| 42:LO:53:LYS:NZ    | 92:LO:414:HOH:O    | 2.46                     | 0.49              |
| 53:LT:4:THR:O      | 53:LT:9:ARG:NE     | 2.46                     | 0.49              |
| 59:Lr:39:ARG:O     | 59:Lr:103:ARG:NH2  | 2.44                     | 0.49              |
| 60:Lh:14:LYS:HZ1   | 60:Lh:61:ILE:HG23  | 1.78                     | 0.49              |
| 62:LF:32:ARG:NH1   | 79:L5:962:C:O2     | 2.46                     | 0.49              |
| 78:S2:15:U:H2'     | 78:S2:16:G:O4'     | 2.13                     | 0.49              |
| 78:S2:453:C:O2'    | 82:SG:92:ARG:O     | 2.23                     | 0.49              |
| 78:S2:528:A:H2'    | 78:S2:529:A:C8     | 2.48                     | 0.49              |
| 78:S2:1348:G:N1    | 78:S2:1362:U:O4    | 2.40                     | 0.49              |
| 79:L5:478:G:H2'    | 79:L5:479:G:H8     | 1.78                     | 0.49              |
| 79:L5:1279:A:O2'   | 79:L5:1281:G:N7    | 2.41                     | 0.49              |
| 79:L5:4228:OMG:N2  | 79:L5:4375:C:O2    | 2.36                     | 0.49              |
| 3:LB:218:ASP:OD2   | 3:LB:348:ARG:NH2   | 2.33                     | 0.49              |
| 4:SB:34:LYS:NZ     | 4:SB:43:ASN:OD1    | 2.46                     | 0.49              |
| 18:SO:104:ARG:NH2  | 78:S2:959:G:OP1    | 2.46                     | 0.49              |
| 36:Sg:37:ASP:OD1   | 36:Sg:39:THR:OG1   | 2.29                     | 0.49              |
| 40:LE:261:ILE:HG23 | 40:LE:267:LEU:HD12 | 1.93                     | 0.49              |
| 69:Lj:6:SER:OG     | 79:L5:2799:G:O2'   | 2.29                     | 0.49              |
| 78:S2:982:G:H2'    | 78:S2:983:A:H8     | 1.77                     | 0.49              |
| 5:L8:19:C:H2'      | 5:L8:20:A:C8       | 2.47                     | 0.48              |
| 10:SC:88:ILE:HD13  | 10:SC:94:ILE:HD11  | 1.95                     | 0.48              |
| 18:SO:147:ARG:HB3  | 18:SO:150:ARG:HH11 | 1.78                     | 0.48              |
| 24:SL:111:VAL:HG12 | 24:SL:140:PHE:HB2  | 1.94                     | 0.48              |
| 40:LE:247:LYS:HD3  | 79:L5:4938:A:H61   | 1.78                     | 0.48              |
| 47:LN:146:PRO:HB2  | 60:Lh:104:THR:HG23 | 1.95                     | 0.48              |
| 62:LF:156:LYS:NZ   | 62:LF:248:ASN:O    | 2.42                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 79:L5:1333:A:H2'    | 79:L5:1334:A:C8    | 2.48                     | 0.48              |
| 10:SC:205:VAL:O     | 10:SC:224:THR:OG1  | 2.31                     | 0.48              |
| 42:LO:89:PRO:HD3    | 79:L5:1914:C:H4'   | 1.95                     | 0.48              |
| 62:LF:129:SER:HA    | 62:LF:132:MET:HE3  | 1.94                     | 0.48              |
| 78:S2:527:C:H2'     | 78:S2:528:A:H8     | 1.78                     | 0.48              |
| 78:S2:838:G:H1'     | 78:S2:839:C:H5     | 1.78                     | 0.48              |
| 78:S2:942:G:H2'     | 78:S2:943:U:C6     | 2.48                     | 0.48              |
| 78:S2:1130:G:OP2    | 78:S2:1130:G:N2    | 2.43                     | 0.48              |
| 78:S2:1232:PSU:H2'  | 78:S2:1233:G:C8    | 2.48                     | 0.48              |
| 78:S2:1579:A:O2'    | 78:S2:1581:C:OP2   | 2.25                     | 0.48              |
| 78:S2:1588:A:H2'    | 78:S2:1589:A:C8    | 2.48                     | 0.48              |
| 79:L5:4208:U:OP1    | 79:L5:4334:U:O2'   | 2.30                     | 0.48              |
| 2:SA:119:PRO:HG2    | 2:SA:142:LEU:HD21  | 1.94                     | 0.48              |
| 30:SZ:92:LEU:HD12   | 30:SZ:109:TYR:HE1  | 1.78                     | 0.48              |
| 41:LG:230:TYR:OH    | 68:Li:46:GLU:OE2   | 2.23                     | 0.48              |
| 75:Lp:47:MET:HE2    | 75:Lp:57:CYS:HB2   | 1.94                     | 0.48              |
| 78:S2:1534:C:N4     | 78:S2:1600:G:O6    | 2.45                     | 0.48              |
| 78:S2:1834:A:N7     | 78:S2:1837:G:N2    | 2.61                     | 0.48              |
| 79:L5:126:C:H2'     | 79:L5:127:G:H8     | 1.78                     | 0.48              |
| 79:L5:1485:C:O4'    | 79:L5:4349:C:N4    | 2.47                     | 0.48              |
| 11:SF:30:ILE:HG23   | 11:SF:117:ILE:HD11 | 1.95                     | 0.48              |
| 23:SN:40:LEU:HD12   | 23:SN:50:ILE:HG23  | 1.94                     | 0.48              |
| 24:SL:13:GLN:HE22   | 24:SL:63:THR:HB    | 1.78                     | 0.48              |
| 37:LC:95:MET:HE1    | 79:L5:1521:C:H5'   | 1.96                     | 0.48              |
| 41:LG:77:PRO:HG2    | 41:LG:80:ILE:HD12  | 1.95                     | 0.48              |
| 41:LG:133:PRO:HD2   | 79:L5:119:G:H1     | 1.78                     | 0.48              |
| 79:L5:1443:A:N6     | 79:L5:2103:G:O6    | 2.47                     | 0.48              |
| 79:L5:2415:OMU:HM23 | 79:L5:2415:OMU:H1' | 1.65                     | 0.48              |
| 3:LB:77:THR:HG21    | 3:LB:337:VAL:HG22  | 1.95                     | 0.48              |
| 3:LB:252:ALA:HB1    | 79:L5:4524:G:N3    | 2.28                     | 0.48              |
| 7:SD:15:GLY:HA3     | 22:Sd:50:ILE:HG23  | 1.95                     | 0.48              |
| 9:SE:126:VAL:HG22   | 9:SE:139:LEU:HD21  | 1.96                     | 0.48              |
| 62:LF:182:TYR:HB3   | 62:LF:200:ARG:HG3  | 1.95                     | 0.48              |
| 78:S2:158:A:H2'     | 78:S2:159:A2M:O4'  | 2.14                     | 0.48              |
| 78:S2:890:U:H3      | 78:S2:897:U:H5     | 1.62                     | 0.48              |
| 79:L5:4736:C:H2'    | 79:L5:4737:G:H8    | 1.77                     | 0.48              |
| 92:L8:400:HOH:O     | 69:Lj:65:ARG:NH1   | 2.34                     | 0.48              |
| 6:L7:117:G:H5'      | 49:LD:256:LYS:HD2  | 1.96                     | 0.48              |
| 19:SX:93:PHE:HB3    | 19:SX:133:LEU:HD23 | 1.95                     | 0.48              |
| 21:SS:110:ASP:OD1   | 21:SS:113:ARG:NH2  | 2.47                     | 0.48              |
| 25:SR:37:GLU:OE1    | 36:Sg:150:TRP:NE1  | 2.41                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:SZ:73:VAL:HG12   | 30:SZ:79:ILE:HD11  | 1.95                     | 0.48              |
| 37:LC:199:ARG:NH2   | 79:L5:350:C:OP2    | 2.45                     | 0.48              |
| 50:LQ:35:LEU:O      | 50:LQ:39:THR:OG1   | 2.21                     | 0.48              |
| 50:LQ:78:LYS:HD2    | 50:LQ:137:VAL:HG23 | 1.95                     | 0.48              |
| 78:S2:476:A:N3      | 78:S2:488:U:O2'    | 2.34                     | 0.48              |
| 78:S2:955:A:N7      | 78:S2:971:G:N2     | 2.61                     | 0.48              |
| 78:S2:1243:PSU:O2   | 78:S2:1257:G:N2    | 2.42                     | 0.48              |
| 79:L5:956:A:H1'     | 79:L5:2076:G:H5''  | 1.94                     | 0.48              |
| 79:L5:1890:G:OP2    | 79:L5:1890:G:N2    | 2.38                     | 0.48              |
| 79:L5:1916:G:N2     | 79:L5:2067:C:O2    | 2.47                     | 0.48              |
| 79:L5:2411:C:H2'    | 79:L5:2412:A:H8    | 1.78                     | 0.48              |
| 79:L5:3736:A:H2'    | 79:L5:3737:A:C8    | 2.48                     | 0.48              |
| 82:SG:211:LYS:HD3   | 82:SG:211:LYS:HA   | 1.67                     | 0.48              |
| 1:LA:173:GLY:O      | 75:Lp:69:TRP:NE1   | 2.43                     | 0.48              |
| 3:LB:13:SER:HB2     | 79:L5:4622:A:H4'   | 1.94                     | 0.48              |
| 15:SQ:102:GLU:HG2   | 36:Sg:55:PRO:HB2   | 1.95                     | 0.48              |
| 23:SN:76:LYS:HE2    | 23:SN:76:LYS:HB2   | 1.62                     | 0.48              |
| 26:SP:95:GLY:HA2    | 26:SP:104:GLN:HA   | 1.95                     | 0.48              |
| 46:La:53:PHE:O      | 50:LQ:178:ARG:HB2  | 2.13                     | 0.48              |
| 49:LD:83:LEU:HB3    | 49:LD:88:VAL:HB    | 1.94                     | 0.48              |
| 62:LF:36:LYS:NZ     | 79:L5:1702:C:N3    | 2.62                     | 0.48              |
| 67:Lg:62:LYS:HD3    | 79:L5:2517:A:H5'   | 1.96                     | 0.48              |
| 78:S2:12:U:O2       | 78:S2:1356:G:N2    | 2.47                     | 0.48              |
| 78:S2:1562:C:H2'    | 78:S2:1563:G:H8    | 1.79                     | 0.48              |
| 79:L5:2845:A:H62    | 79:L5:3843:C:H42   | 1.61                     | 0.48              |
| 79:L5:4258:C:H2'    | 79:L5:4259:C:H6    | 1.78                     | 0.48              |
| 79:L5:4456:OMC:O2   | 79:L5:4524:G:N2    | 2.39                     | 0.48              |
| 79:L5:4750:G:H2'    | 79:L5:4751:G:C8    | 2.48                     | 0.48              |
| 2:SA:198:MET:HG2    | 2:SA:200:ASP:H     | 1.79                     | 0.48              |
| 6:L7:79:U:O2'       | 79:L5:1795:A:N3    | 2.46                     | 0.48              |
| 14:SI:56:ARG:HA     | 14:SI:180:GLY:HA2  | 1.95                     | 0.48              |
| 19:SX:124:LYS:HA    | 19:SX:129:SER:HA   | 1.96                     | 0.48              |
| 42:LO:54:TYR:OH     | 42:LO:73:PHE:O     | 2.31                     | 0.48              |
| 46:La:85:GLN:HA     | 46:La:88:VAL:HG22  | 1.96                     | 0.48              |
| 53:LT:36[A]:LYS:HE2 | 53:LT:67:VAL:HG23  | 1.96                     | 0.48              |
| 61:Lb:91:ARG:HB2    | 61:Lb:94:ASP:HB2   | 1.95                     | 0.48              |
| 78:S2:520:A:O2'     | 78:S2:825:A:N3     | 2.37                     | 0.48              |
| 78:S2:1036:A:H4'    | 78:S2:1855:G:N2    | 2.28                     | 0.48              |
| 79:L5:3715:PSU:OP1  | 80:Et:4:C:O2'      | 2.28                     | 0.48              |
| 5:L8:13:G:O2'       | 54:LP:121:LYS:O    | 2.28                     | 0.48              |
| 8:SJ:174:LYS:HB2    | 78:S2:560:A:H5'    | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:SE:124:CYS:HB3   | 9:SE:141:THR:HB    | 1.95                     | 0.48              |
| 10:SC:207:ALA:HB2  | 78:S2:4:C:H4'      | 1.95                     | 0.48              |
| 21:SS:98:VAL:HG11  | 21:SS:106:LYS:HG2  | 1.95                     | 0.48              |
| 47:LN:65:ARG:HG3   | 47:LN:127:TYR:HB3  | 1.95                     | 0.48              |
| 48:LI:35:ASP:HB3   | 48:LI:39:LYS:HG2   | 1.95                     | 0.48              |
| 57:LY:31:SER:HA    | 57:LY:48:PRO:HA    | 1.95                     | 0.48              |
| 67:Lg:62:LYS:NZ    | 79:L5:2516:G:O2'   | 2.46                     | 0.48              |
| 79:L5:1558:A:H2'   | 79:L5:1559:G:C8    | 2.48                     | 0.48              |
| 79:L5:1604:G:H2'   | 79:L5:1605:G:C8    | 2.48                     | 0.48              |
| 79:L5:2411:C:H2'   | 79:L5:2412:A:C8    | 2.49                     | 0.48              |
| 79:L5:4734:A:H2'   | 79:L5:4735:G:H8    | 1.78                     | 0.48              |
| 14:SI:142:SER:OG   | 14:SI:143:LYS:N    | 2.45                     | 0.48              |
| 36:Sg:207:CYS:HB2  | 36:Sg:221:LEU:HD21 | 1.96                     | 0.48              |
| 48:LI:129:VAL:HG23 | 48:LI:133:GLN:HG2  | 1.96                     | 0.48              |
| 70:Lk:35:LYS:NZ    | 79:L5:2695:A:OP1   | 2.38                     | 0.48              |
| 78:S2:1203:G:H2'   | 78:S2:1204:A:C8    | 2.49                     | 0.48              |
| 79:L5:3759:A:N6    | 79:L5:3764:PSU:O4  | 2.42                     | 0.48              |
| 5:L8:148:A:H2'     | 5:L8:149:G:C8      | 2.49                     | 0.47              |
| 46:La:2:PRO:HD2    | 79:L5:1509:C:H5''  | 1.96                     | 0.47              |
| 59:Lr:108:MET:HG3  | 79:L5:2263:A:H5''  | 1.95                     | 0.47              |
| 63:Lc:28:VAL:HB    | 63:Lc:33:GLN:HB3   | 1.95                     | 0.47              |
| 66:Lf:20:ASN:ND2   | 79:L5:1885:G:OP1   | 2.40                     | 0.47              |
| 78:S2:1850:MA6:H8  | 78:S2:1850:MA6:O5' | 2.13                     | 0.47              |
| 79:L5:1077:C:OP1   | 79:L5:1215:C:O2'   | 2.32                     | 0.47              |
| 79:L5:1630:A:H5''  | 79:L5:1631:A:N7    | 2.30                     | 0.47              |
| 79:L5:4733:C:H4'   | 79:L5:4734:A:H5'   | 1.96                     | 0.47              |
| 79:L5:4743:G:H2'   | 79:L5:4744:A:C8    | 2.49                     | 0.47              |
| 5:L8:87:G:N1       | 57:LY:114:ASP:OD2  | 2.36                     | 0.47              |
| 6:L7:13:A:O2'      | 49:LD:24:ARG:NH2   | 2.46                     | 0.47              |
| 32:Sb:20:LYS:NZ    | 78:S2:1015:U:OP2   | 2.47                     | 0.47              |
| 36:Sg:248:LEU:HD23 | 36:Sg:259:TRP:HE3  | 1.80                     | 0.47              |
| 37:LC:263:LEU:HG   | 37:LC:273:LEU:HD12 | 1.96                     | 0.47              |
| 41:LG:165:GLU:HG2  | 47:LN:11:TRP:HE1   | 1.79                     | 0.47              |
| 50:LQ:162:HIS:ND1  | 79:L5:1497:A:OP2   | 2.38                     | 0.47              |
| 58:LZ:50:PRO:HD3   | 58:LZ:68:ILE:HG12  | 1.94                     | 0.47              |
| 78:S2:191:A:H62    | 78:S2:208:G:N2     | 2.07                     | 0.47              |
| 78:S2:1036:A:N3    | 78:S2:1844:U:O2'   | 2.45                     | 0.47              |
| 78:S2:1845:A:H2'   | 78:S2:1846:G:C8    | 2.48                     | 0.47              |
| 79:L5:433:A:C2     | 79:L5:3867:A2M:H4' | 2.48                     | 0.47              |
| 79:L5:3878:C:OP1   | 79:L5:4400:G:O2'   | 2.32                     | 0.47              |
| 79:L5:4448:G:H5''  | 79:L5:4449:A:H5''  | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:L5:4459:U:H2'   | 79:L5:4460:U:C6    | 2.49                     | 0.47              |
| 82:SG:176:ILE:HG22 | 82:SG:179:LEU:HB2  | 1.96                     | 0.47              |
| 23:SN:4:MET:HE3    | 78:S2:924:G:H5'    | 1.95                     | 0.47              |
| 30:SZ:85:ARG:NH2   | 78:S2:1597:C:OP2   | 2.46                     | 0.47              |
| 43:LL:79:GLU:HG2   | 43:LL:110:LEU:HD11 | 1.96                     | 0.47              |
| 51:LR:82:LYS:HE3   | 79:L5:2863:G:H1'   | 1.95                     | 0.47              |
| 79:L5:162:A:H2'    | 79:L5:163:A:H8     | 1.79                     | 0.47              |
| 79:L5:1893:C:H1'   | 79:L5:1937:C:O2    | 2.14                     | 0.47              |
| 79:L5:2486:G:H2'   | 79:L5:2487:G:C8    | 2.50                     | 0.47              |
| 79:L5:3656:A:H2'   | 79:L5:3657:U:H6    | 1.80                     | 0.47              |
| 79:L5:3656:A:HO2'  | 79:L5:3747:A:HO2'  | 1.60                     | 0.47              |
| 5:L8:144:U:H2'     | 5:L8:145:C:C6      | 2.50                     | 0.47              |
| 36:Sg:107:ASP:HB2  | 36:Sg:125:ARG:HG3  | 1.97                     | 0.47              |
| 37:LC:242:PRO:HB2  | 79:L5:2297:G:H4'   | 1.96                     | 0.47              |
| 39:LH:117:PHE:O    | 39:LH:120:GLU:HG3  | 2.13                     | 0.47              |
| 40:LE:60:SER:HB2   | 79:L5:1239:C:H5    | 1.79                     | 0.47              |
| 47:LN:125:SER:HB2  | 79:L5:3937:C:H1'   | 1.95                     | 0.47              |
| 53:LT:144:ASN:HB2  | 53:LT:146:LYS:HZ2  | 1.79                     | 0.47              |
| 65:Le:124:ASN:OD1  | 65:Le:124:ASN:N    | 2.47                     | 0.47              |
| 68:Li:28:ARG:NH2   | 79:L5:326:C:OP2    | 2.41                     | 0.47              |
| 79:L5:478:G:H2'    | 79:L5:479:G:C8     | 2.50                     | 0.47              |
| 79:L5:658:C:H2'    | 79:L5:659:G:C8     | 2.49                     | 0.47              |
| 79:L5:4237:C:OP1   | 79:L5:4327:C:O2'   | 2.32                     | 0.47              |
| 21:SS:89:ASP:OD2   | 21:SS:106:LYS:NZ   | 2.48                     | 0.47              |
| 39:LH:153:LEU:O    | 39:LH:157:SER:OG   | 2.29                     | 0.47              |
| 48:LI:158:LYS:NZ   | 79:L5:4413:C:O2    | 2.44                     | 0.47              |
| 56:LX:77:ILE:HD13  | 56:LX:100:VAL:HG12 | 1.96                     | 0.47              |
| 62:LF:93:ILE:HD12  | 62:LF:243:LEU:HD23 | 1.95                     | 0.47              |
| 78:S2:952:G:H2'    | 78:S2:953:C:C6     | 2.49                     | 0.47              |
| 79:L5:2486:G:H2'   | 79:L5:2487:G:H8    | 1.78                     | 0.47              |
| 5:L8:58:G:N7       | 69:Lj:63:ARG:NH2   | 2.53                     | 0.47              |
| 12:SH:83:LEU:HB3   | 12:SH:92:VAL:HG21  | 1.96                     | 0.47              |
| 39:LH:43:VAL:HG21  | 39:LH:73:ILE:HD12  | 1.96                     | 0.47              |
| 59:Lr:98:ARG:NH2   | 79:L5:2262:G:OP2   | 2.33                     | 0.47              |
| 71:Li:37:TYR:O     | 79:L5:362:A:N6     | 2.47                     | 0.47              |
| 78:S2:1423:C:H3'   | 78:S2:1424:G:H8    | 1.79                     | 0.47              |
| 3:LB:76:VAL:HB     | 3:LB:332:MET:HG2   | 1.97                     | 0.47              |
| 3:LB:80:GLU:OE1    | 3:LB:323:TYR:OH    | 2.33                     | 0.47              |
| 5:L8:106:G:H4'     | 5:L8:137:A:H5'     | 1.97                     | 0.47              |
| 24:SL:82:MET:HE1   | 78:S2:372:U:O2'    | 2.14                     | 0.47              |
| 30:SZ:73:VAL:HG13  | 30:SZ:77:LEU:HD21  | 1.97                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:Sa:98:PRO:O     | 78:S2:1868:U:N3     | 2.38                     | 0.47              |
| 36:Sg:79:LEU:HD11  | 36:Sg:87:LEU:HD23   | 1.96                     | 0.47              |
| 39:LH:64:ARG:NH1   | 79:L5:1949:U:OP1    | 2.48                     | 0.47              |
| 40:LE:151:ILE:HB   | 40:LE:195:ILE:HB    | 1.95                     | 0.47              |
| 43:LL:36:ARG:HH21  | 79:L5:1363:C:H3'    | 1.80                     | 0.47              |
| 44:LV:24:ALA:HB3   | 44:LV:39:ILE:HD12   | 1.96                     | 0.47              |
| 46:La:132:ARG:NH1  | 79:L5:1396:G:H5''   | 2.30                     | 0.47              |
| 52:LS:96:GLU:HB3   | 52:LS:142:VAL:HG21  | 1.97                     | 0.47              |
| 57:LY:10:ASP:HB3   | 57:LY:13:LYS:HB2    | 1.97                     | 0.47              |
| 61:Lb:18:ARG:NH1   | 79:L5:1686:C:O2'    | 2.48                     | 0.47              |
| 62:LF:91:PHE:HB2   | 62:LF:145:PRO:HG3   | 1.97                     | 0.47              |
| 78:S2:1113:A:H2'   | 78:S2:1114:U:C6     | 2.50                     | 0.47              |
| 78:S2:1531:A:H4'   | 78:S2:1605:G:H4'    | 1.95                     | 0.47              |
| 79:L5:1538:U:H2'   | 79:L5:1539:G:H8     | 1.80                     | 0.47              |
| 79:L5:3669:G:H21   | 79:L5:3672:G:N2     | 2.13                     | 0.47              |
| 79:L5:4138:C:H2'   | 79:L5:4139:G:C8     | 2.50                     | 0.47              |
| 1:LA:245[B]:ARG:HE | 1:LA:245[B]:ARG:HB2 | 1.54                     | 0.47              |
| 8:SJ:149:VAL:HG11  | 8:SJ:157:ILE:HD11   | 1.97                     | 0.47              |
| 21:SS:105:ASN:OD1  | 21:SS:108:ARG:NH2   | 2.47                     | 0.47              |
| 49:LD:65:ALA:HB2   | 49:LD:74:ILE:HD13   | 1.97                     | 0.47              |
| 52:LS:62:VAL:HA    | 62:LF:83:VAL:HG22   | 1.97                     | 0.47              |
| 57:LY:58:VAL:HG23  | 57:LY:59:ARG:HG2    | 1.97                     | 0.47              |
| 68:Li:67:LYS:NZ    | 79:L5:3725:G:N7     | 2.41                     | 0.47              |
| 78:S2:1288:OMU:HN3 | 78:S2:1311:C:H42    | 1.61                     | 0.47              |
| 79:L5:256:G:H2'    | 79:L5:257:C:C6      | 2.50                     | 0.47              |
| 79:L5:1188:C:H2'   | 79:L5:1189:G:H8     | 1.80                     | 0.47              |
| 79:L5:2318:G:N2    | 79:L5:2321:G:OP2    | 2.41                     | 0.47              |
| 79:L5:4924:C:H1'   | 79:L5:4926:C:N4     | 2.30                     | 0.47              |
| 2:SA:110:ASN:HB3   | 2:SA:113:GLN:HB3    | 1.97                     | 0.47              |
| 37:LC:321:ASN:OD1  | 79:L5:1280:C:O2'    | 2.22                     | 0.47              |
| 42:LO:44:SER:OG    | 79:L5:2054:U:OP2    | 2.25                     | 0.47              |
| 50:LQ:130:SER:O    | 50:LQ:130:SER:OG    | 2.25                     | 0.47              |
| 65:Le:7:LEU:HB2    | 65:Le:93:LYS:HB3    | 1.96                     | 0.47              |
| 78:S2:150:A:N6     | 78:S2:168:C:N3      | 2.62                     | 0.47              |
| 78:S2:531:A:H2'    | 78:S2:532:C:C6      | 2.49                     | 0.47              |
| 78:S2:891:G:O2'    | 78:S2:893:U:OP1     | 2.29                     | 0.47              |
| 79:L5:2481:G:H2'   | 79:L5:2482:C:C6     | 2.49                     | 0.47              |
| 80:Et:36:U:N3      | 80:Et:38:A:N7       | 2.62                     | 0.47              |
| 2:SA:137:ALA:HB1   | 2:SA:142:LEU:HB3    | 1.97                     | 0.47              |
| 54:LP:111:SER:HB2  | 54:LP:154:GLU:HB2   | 1.96                     | 0.47              |
| 57:LY:32:SER:OG    | 57:LY:101:PRO:O     | 2.22                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 58:LZ:48:ARG:H      | 58:LZ:69:LYS:HB3   | 1.80                     | 0.47              |
| 62:LF:90:ALA:HB2    | 62:LF:125:LEU:HD11 | 1.97                     | 0.47              |
| 62:LF:148:LYS:HD3   | 62:LF:245:ARG:HH21 | 1.79                     | 0.47              |
| 79:L5:2845:A:N6     | 79:L5:3843:C:H42   | 2.13                     | 0.47              |
| 79:L5:3732:A:H2'    | 79:L5:3733:A:H8    | 1.80                     | 0.47              |
| 5:L8:8:U:H2'        | 5:L8:9:A:C8        | 2.50                     | 0.46              |
| 8:SJ:89:GLU:H       | 8:SJ:89:GLU:CD     | 2.22                     | 0.46              |
| 14:SI:170:LYS:HB2   | 14:SI:170:LYS:HE3  | 1.61                     | 0.46              |
| 22:Sd:53:ILE:HD12   | 22:Sd:55:LEU:HD21  | 1.96                     | 0.46              |
| 43:LL:90:VAL:O      | 43:LL:93:THR:OG1   | 2.31                     | 0.46              |
| 49:LD:119:TYR:OH    | 49:LD:139:PRO:O    | 2.25                     | 0.46              |
| 55:LU:105:ASN:OD1   | 55:LU:106:SER:N    | 2.48                     | 0.46              |
| 78:S2:126:G:H5''    | 82:SG:195:LYS:HG2  | 1.97                     | 0.46              |
| 78:S2:1010:G:H2'    | 78:S2:1011:A:H8    | 1.80                     | 0.46              |
| 79:L5:3911:C:H2'    | 79:L5:3912:U:H6    | 1.80                     | 0.46              |
| 18:SO:103:ASN:OD1   | 18:SO:103:ASN:N    | 2.44                     | 0.46              |
| 29:SY:117:VAL:O     | 29:SY:122:LYS:NZ   | 2.48                     | 0.46              |
| 31:Sa:33:ASP:OD1    | 31:Sa:34:LYS:N     | 2.49                     | 0.46              |
| 37:LC:44:LEU:HD13   | 79:L5:1373:A:H5''  | 1.96                     | 0.46              |
| 43:LL:165:LYS:HD3   | 43:LL:165:LYS:N    | 2.31                     | 0.46              |
| 49:LD:208:MET:HE2   | 49:LD:233:PRO:HD3  | 1.98                     | 0.46              |
| 58:LZ:36:ARG:HG2    | 58:LZ:38:TYR:CZ    | 2.51                     | 0.46              |
| 78:S2:65:C:N3       | 82:SG:133:LEU:HB3  | 2.30                     | 0.46              |
| 79:L5:3893:C:H2'    | 79:L5:3894:A:C8    | 2.50                     | 0.46              |
| 3:LB:252:ALA:HB3    | 79:L5:4457:PSU:H1' | 1.96                     | 0.46              |
| 21:SS:35:GLY:O      | 21:SS:97:GLN:NE2   | 2.49                     | 0.46              |
| 23:SN:55:ARG:HD3    | 78:S2:1017:U:H5'   | 1.97                     | 0.46              |
| 36:Sg:139:LYS:HD3   | 36:Sg:139:LYS:HA   | 1.72                     | 0.46              |
| 38:LJ:29:SER:OG     | 38:LJ:66:GLU:OE2   | 2.29                     | 0.46              |
| 52:LS:2:LYS:HG3     | 79:L5:2062:C:OP1   | 2.15                     | 0.46              |
| 62:LF:63:GLN:NE2    | 79:L5:1212:G:H5''  | 2.31                     | 0.46              |
| 63:Lc:9:LYS:HD2     | 63:Lc:13:SER:HB3   | 1.96                     | 0.46              |
| 67:Lg:25:THR:HG22   | 79:L5:2521:G:H5''  | 1.96                     | 0.46              |
| 67:Lg:97:ILE:HD13   | 79:L5:4120:U:C4    | 2.50                     | 0.46              |
| 78:S2:532:C:H2'     | 78:S2:533:A:H8     | 1.80                     | 0.46              |
| 79:L5:2520:C:H2'    | 79:L5:2521:G:C8    | 2.50                     | 0.46              |
| 79:L5:3785:A2M:HM'1 | 79:L5:4537:C:H1'   | 1.96                     | 0.46              |
| 79:L5:4699:U:H1'    | 79:L5:4700:A:H5''  | 1.97                     | 0.46              |
| 9:SE:128:LYS:HB3    | 9:SE:140:VAL:HB    | 1.97                     | 0.46              |
| 39:LH:103:VAL:HG11  | 39:LH:144:LEU:HD11 | 1.97                     | 0.46              |
| 78:S2:1037:G:H4'    | 78:S2:1845:A:H4'   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:L5:1662:C:H2'  | 79:L5:1663:C:C6    | 2.51                     | 0.46              |
| 79:L5:1765:A:O2'  | 79:L5:1766:A:OP1   | 2.30                     | 0.46              |
| 79:L5:4260:U:H2'  | 79:L5:4261:C:H6    | 1.79                     | 0.46              |
| 82:SG:56:ASN:HB2  | 82:SG:108:VAL:HG12 | 1.96                     | 0.46              |
| 3:LB:210:VAL:O    | 3:LB:349:LYS:NZ    | 2.48                     | 0.46              |
| 15:SQ:140:ARG:HB2 | 78:S2:1644:C:H4'   | 1.97                     | 0.46              |
| 27:ST:41:LYS:HE3  | 27:ST:93:SER:HB2   | 1.98                     | 0.46              |
| 78:S2:121:OMU:N3  | 78:S2:343:A:N1     | 2.53                     | 0.46              |
| 78:S2:484:A2M:H8  | 78:S2:484:A2M:O5'  | 2.15                     | 0.46              |
| 78:S2:600:G:H2'   | 78:S2:601:OMG:H8   | 1.81                     | 0.46              |
| 79:L5:257:C:H3'   | 79:L5:258:G:H8     | 1.79                     | 0.46              |
| 79:L5:1173:G:H2'  | 79:L5:1174:G:C8    | 2.50                     | 0.46              |
| 79:L5:1541:C:O2   | 79:L5:2448:G:N2    | 2.49                     | 0.46              |
| 79:L5:3664:G:H2'  | 79:L5:3665:G:H8    | 1.80                     | 0.46              |
| 79:L5:4188:U:H2'  | 79:L5:4189:U:C6    | 2.50                     | 0.46              |
| 79:L5:4770:U:H2'  | 79:L5:4771:C:C6    | 2.50                     | 0.46              |
| 3:LB:7:SER:OG     | 79:L5:4492:U:OP2   | 2.32                     | 0.46              |
| 3:LB:139:ASP:OD2  | 3:LB:140:GLU:N     | 2.49                     | 0.46              |
| 4:SB:83:LYS:HB2   | 4:SB:83:LYS:HE3    | 1.74                     | 0.46              |
| 32:Sb:30:SER:OG   | 78:S2:1016:U:OP1   | 2.22                     | 0.46              |
| 54:LP:10:ASN:N    | 54:LP:10:ASN:OD1   | 2.47                     | 0.46              |
| 79:L5:9:C:O2      | 79:L5:2472:A:N6    | 2.48                     | 0.46              |
| 79:L5:1617:G:H1'  | 79:L5:2513:A:N6    | 2.31                     | 0.46              |
| 79:L5:4954:G:H2'  | 79:L5:4955:A:C8    | 2.51                     | 0.46              |
| 80:Et:28:U:H2'    | 80:Et:29:G:C8      | 2.51                     | 0.46              |
| 1:LA:188:LYS:NZ   | 79:L5:2739:C:O2    | 2.41                     | 0.46              |
| 2:SA:196:GLU:OE2  | 2:SA:196:GLU:N     | 2.30                     | 0.46              |
| 47:LN:49:ARG:NH2  | 79:L5:152:U:OP2    | 2.30                     | 0.46              |
| 58:LZ:79:HIS:ND1  | 79:L5:2580:U:O2'   | 2.47                     | 0.46              |
| 68:Li:79:THR:HG22 | 68:Li:82:ARG:H     | 1.81                     | 0.46              |
| 79:L5:1333:A:H2'  | 79:L5:1334:A:H8    | 1.80                     | 0.46              |
| 79:L5:1598:C:H2'  | 79:L5:1599:A:H8    | 1.80                     | 0.46              |
| 79:L5:2103:G:H2'  | 79:L5:2104:G:H8    | 1.81                     | 0.46              |
| 2:SA:134:LEU:HD23 | 2:SA:134:LEU:HA    | 1.76                     | 0.46              |
| 5:L8:7:U:O2'      | 79:L5:1305:C:OP1   | 2.34                     | 0.46              |
| 9:SE:148:ARG:NH2  | 82:SG:202:ASN:OD1  | 2.49                     | 0.46              |
| 38:LJ:56:THR:OG1  | 38:LJ:64:ARG:N     | 2.45                     | 0.46              |
| 44:LV:19:GLY:O    | 79:L5:2846:G:O2'   | 2.27                     | 0.46              |
| 78:S2:367:U:H4'   | 78:S2:371:A:C8     | 2.51                     | 0.46              |
| 78:S2:569:A:H2'   | 78:S2:570:C:O4'    | 2.15                     | 0.46              |
| 78:S2:900:C:H2'   | 78:S2:901:G:H8     | 1.81                     | 0.46              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 78:S2:1232:PSU:H2'   | 78:S2:1233:G:H8    | 1.81                     | 0.46              |
| 79:L5:381:U:H4'      | 79:L5:415:G:H5'    | 1.98                     | 0.46              |
| 79:L5:2079:G:H2'     | 79:L5:2080:U:C6    | 2.50                     | 0.46              |
| 79:L5:4195:G:O2'     | 79:L5:4442:PSU:OP1 | 2.29                     | 0.46              |
| 79:L5:4739:C:H2'     | 79:L5:4740:G:H5'   | 1.97                     | 0.46              |
| 29:SY:29:HIS:ND1     | 29:SY:29:HIS:O     | 2.49                     | 0.46              |
| 36:Sg:70:VAL:HG21    | 36:Sg:113:PHE:HB2  | 1.97                     | 0.46              |
| 36:Sg:153:CYS:HB2    | 36:Sg:168:CYS:N    | 2.28                     | 0.46              |
| 42:LO:197:LYS:HG2    | 42:LO:202:LEU:HB2  | 1.97                     | 0.46              |
| 78:S2:1798:C:H2'     | 78:S2:1799:G:O4'   | 2.16                     | 0.46              |
| 79:L5:3711:A:H4'     | 79:L5:3712:A:C8    | 2.51                     | 0.46              |
| 80:Et:58:A:O2'       | 80:Et:60:A:OP2     | 2.22                     | 0.46              |
| 1:LA:245[B]:ARG:HH12 | 79:L5:3698:G:P     | 2.39                     | 0.46              |
| 5:L8:9:A:H2'         | 5:L8:10:G:H8       | 1.80                     | 0.46              |
| 5:L8:141:C:H2'       | 5:L8:142:U:C6      | 2.50                     | 0.46              |
| 12:SH:10:LYS:HG2     | 12:SH:11:PRO:HD2   | 1.98                     | 0.46              |
| 24:SL:126:VAL:HG12   | 24:SL:145:VAL:HG22 | 1.97                     | 0.46              |
| 27:ST:11:GLN:OE1     | 27:ST:62:ARG:NH1   | 2.39                     | 0.46              |
| 39:LH:76:HIS:O       | 39:LH:80:MET:HG3   | 2.16                     | 0.46              |
| 49:LD:164:LYS:NZ     | 49:LD:168:ASP:OD1  | 2.47                     | 0.46              |
| 51:LR:136:ARG:O      | 51:LR:140:GLU:HG2  | 2.16                     | 0.46              |
| 54:LP:135:ARG:NH2    | 79:L5:1596:U:O2'   | 2.39                     | 0.46              |
| 66:Lf:68:ARG:NH1     | 79:L5:442:G:OP1    | 2.42                     | 0.46              |
| 74:Lo:44:LYS:HE3     | 74:Lo:52:THR:HB    | 1.98                     | 0.46              |
| 78:S2:116:OMU:N3     | 78:S2:347:G:O6     | 2.43                     | 0.46              |
| 78:S2:649:PSU:H2'    | 78:S2:650:A:H8     | 1.81                     | 0.46              |
| 79:L5:2434:G:O2'     | 79:L5:2527:A:N1    | 2.47                     | 0.46              |
| 79:L5:4899:G:H2'     | 79:L5:4901:G:C8    | 2.51                     | 0.46              |
| 14:SI:56:ARG:NH1     | 14:SI:180:GLY:O    | 2.46                     | 0.45              |
| 19:SX:63:ASN:ND2     | 19:SX:114:ASP:OD2  | 2.39                     | 0.45              |
| 23:SN:22:VAL:HG13    | 23:SN:66:VAL:HG22  | 1.99                     | 0.45              |
| 38:LJ:78:LYS:HE3     | 38:LJ:82:ILE:HD11  | 1.98                     | 0.45              |
| 39:LH:107:GLU:OE1    | 39:LH:127:ARG:NH1  | 2.36                     | 0.45              |
| 42:LO:165:LYS:HD2    | 42:LO:165:LYS:HA   | 1.77                     | 0.45              |
| 78:S2:530:U:H2'      | 78:S2:531:A:C8     | 2.51                     | 0.45              |
| 79:L5:24:G:N2        | 79:L5:55:G:O6      | 2.50                     | 0.45              |
| 79:L5:4088:C:H2'     | 79:L5:4089:G:C8    | 2.50                     | 0.45              |
| 79:L5:4239:A:H2'     | 79:L5:4240:G:C8    | 2.51                     | 0.45              |
| 79:L5:4620:OMU:HM23  | 79:L5:4620:OMU:H1' | 1.68                     | 0.45              |
| 79:L5:4637:OMG:HM23  | 79:L5:4637:OMG:H1' | 1.69                     | 0.45              |
| 6:L7:103:A:O2'       | 79:L5:1741:G:O6    | 2.22                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:SW:31:SER:HB3  | 78:S2:685:A:H5''   | 1.97                     | 0.45              |
| 30:SZ:69:THR:HG22 | 30:SZ:108:ILE:HA   | 1.98                     | 0.45              |
| 42:LO:82:ARG:HH22 | 79:L5:3886:G:H5''  | 1.80                     | 0.45              |
| 53:LT:115:LYS:HA  | 53:LT:115:LYS:HD2  | 1.64                     | 0.45              |
| 54:LP:94:MET:HG2  | 54:LP:148:MET:HE3  | 1.97                     | 0.45              |
| 79:L5:325:U:H2'   | 79:L5:326:C:C6     | 2.51                     | 0.45              |
| 79:L5:703:G:H2'   | 79:L5:704:C:H5''   | 1.98                     | 0.45              |
| 79:L5:1669:A:H4'  | 79:L5:1685:G:H22   | 1.81                     | 0.45              |
| 79:L5:4991:U:H2'  | 79:L5:4992:G:H8    | 1.82                     | 0.45              |
| 82:SG:38:ALA:HB2  | 82:SG:50:VAL:HG22  | 1.99                     | 0.45              |
| 6:L7:30:C:O2'     | 49:LD:221:LYS:NZ   | 2.43                     | 0.45              |
| 14:SI:139:LYS:HD2 | 14:SI:141:ARG:HE   | 1.81                     | 0.45              |
| 21:SS:15:VAL:HG13 | 21:SS:68:ILE:HD11  | 1.98                     | 0.45              |
| 27:ST:42:HIS:CD2  | 27:ST:43:LYS:HD3   | 2.51                     | 0.45              |
| 31:Sa:66:LYS:HE2  | 31:Sa:66:LYS:HB3   | 1.85                     | 0.45              |
| 41:LG:131:LYS:HA  | 41:LG:131:LYS:HD3  | 1.72                     | 0.45              |
| 54:LP:33:ALA:HB1  | 54:LP:117:ILE:HG12 | 1.99                     | 0.45              |
| 55:LU:22:THR:HB   | 55:LU:109:SER:HB2  | 1.98                     | 0.45              |
| 57:LY:46:SER:OG   | 79:L5:239:C:OP1    | 2.34                     | 0.45              |
| 75:Lp:48:LYS:HB2  | 75:Lp:48:LYS:HE2   | 1.75                     | 0.45              |
| 78:S2:184:G:H2'   | 78:S2:185:G:C8     | 2.52                     | 0.45              |
| 78:S2:1010:G:H2'  | 78:S2:1011:A:C8    | 2.51                     | 0.45              |
| 78:S2:1013:U:OP1  | 78:S2:1129:G:O2'   | 2.31                     | 0.45              |
| 79:L5:197:A:N3    | 79:L5:222:C:O2'    | 2.44                     | 0.45              |
| 79:L5:1271:G:OP2  | 79:L5:1271:G:N2    | 2.36                     | 0.45              |
| 79:L5:1437:C:N4   | 79:L5:2098:G:N3    | 2.65                     | 0.45              |
| 79:L5:2444:U:O4   | 79:L5:2516:G:N2    | 2.49                     | 0.45              |
| 79:L5:5004:C:H2'  | 79:L5:5005:G:O4'   | 2.17                     | 0.45              |
| 82:SG:51:ARG:NH1  | 82:SG:53:SER:OG    | 2.49                     | 0.45              |
| 4:SB:145:LYS:HG3  | 4:SB:149:GLN:NE2   | 2.32                     | 0.45              |
| 11:SF:79:HIS:O    | 11:SF:81:ARG:N     | 2.50                     | 0.45              |
| 14:SI:79:ILE:HG13 | 14:SI:170:LYS:HG2  | 1.98                     | 0.45              |
| 29:SY:10:ARG:HG3  | 29:SY:11:LYS:HG3   | 1.97                     | 0.45              |
| 29:SY:37:LYS:HD2  | 29:SY:57:VAL:HG23  | 1.97                     | 0.45              |
| 49:LD:215:ASP:OD1 | 49:LD:218:ALA:N    | 2.38                     | 0.45              |
| 57:LY:130:LYS:HE2 | 57:LY:130:LYS:HB2  | 1.62                     | 0.45              |
| 59:Lr:20:ARG:NH2  | 65:Le:84:GLU:OE1   | 2.37                     | 0.45              |
| 71:Ll:3:SER:O     | 79:L5:2781:G:O2'   | 2.34                     | 0.45              |
| 74:Lo:23:VAL:HG22 | 74:Lo:70:LEU:HD23  | 1.98                     | 0.45              |
| 78:S2:455:A:H2'   | 78:S2:456:C:C6     | 2.52                     | 0.45              |
| 79:L5:462:G:H2'   | 79:L5:463:A:C8     | 2.51                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:L5:3720:G:H22   | 79:L5:3733:A:H2    | 1.65                     | 0.45              |
| 79:L5:4088:C:H2'   | 79:L5:4089:G:H8    | 1.82                     | 0.45              |
| 82:SG:154:ARG:HH11 | 82:SG:154:ARG:HB2  | 1.82                     | 0.45              |
| 2:SA:125:THR:HG23  | 2:SA:175:TRP:HE1   | 1.81                     | 0.45              |
| 9:SE:95:THR:HG22   | 29:SY:16:ARG:HB2   | 1.98                     | 0.45              |
| 15:SQ:18:THR:HG21  | 78:S2:1546:G:H5'   | 1.99                     | 0.45              |
| 18:SO:26:ASN:OD1   | 18:SO:26:ASN:N     | 2.48                     | 0.45              |
| 46:La:27:LYS:HE3   | 79:L5:1518:A:H5'   | 1.98                     | 0.45              |
| 46:La:42:ARG:NH2   | 79:L5:4377:G:N7    | 2.64                     | 0.45              |
| 47:LN:14:LYS:HE2   | 79:L5:280:G:H5''   | 1.98                     | 0.45              |
| 69:Lj:63:ARG:HE    | 69:Lj:65:ARG:HG3   | 1.82                     | 0.45              |
| 78:S2:1035:A:O2'   | 78:S2:1856:C:O2    | 2.30                     | 0.45              |
| 79:L5:1274:A:H2'   | 79:L5:1275:G:C8    | 2.52                     | 0.45              |
| 79:L5:1683:PSU:H2' | 79:L5:1684:A:C8    | 2.51                     | 0.45              |
| 79:L5:1733:G:N3    | 79:L5:4214:A:H2'   | 2.31                     | 0.45              |
| 79:L5:2521:G:H5'   | 79:L5:2640:G:H1'   | 1.98                     | 0.45              |
| 79:L5:2539:C:H2'   | 79:L5:2540:C:C6    | 2.51                     | 0.45              |
| 79:L5:4163:U:H5'   | 79:L5:4164:C:H5''  | 1.99                     | 0.45              |
| 5:L8:21:C:OP1      | 37:LC:195:LYS:NZ   | 2.49                     | 0.45              |
| 6:L7:55:A:H4'      | 38:LJ:155:HIS:HB2  | 1.98                     | 0.45              |
| 10:SC:173:LYS:HB3  | 28:SV:3:ASN:HA     | 1.98                     | 0.45              |
| 42:LO:81:TRP:HB2   | 42:LO:104:VAL:HG21 | 1.99                     | 0.45              |
| 50:LQ:22:ASP:O     | 50:LQ:26:ARG:HG2   | 2.17                     | 0.45              |
| 65:Le:11:LYS:HE2   | 65:Le:11:LYS:HB2   | 1.78                     | 0.45              |
| 76:Pt:24:C:H2'     | 76:Pt:25:U:C6      | 2.52                     | 0.45              |
| 79:L5:2517:A:N3    | 79:L5:2539:C:O2'   | 2.49                     | 0.45              |
| 79:L5:3870:C:H2'   | 79:L5:3871:A:H8    | 1.82                     | 0.45              |
| 79:L5:3938:G:N2    | 79:L5:4171:C:OP2   | 2.49                     | 0.45              |
| 79:L5:4591:U:H2'   | 79:L5:4592:C:C6    | 2.52                     | 0.45              |
| 24:SL:49:GLU:H     | 24:SL:49:GLU:CD    | 2.23                     | 0.45              |
| 48:LI:36:LEU:HG    | 48:LI:87:ILE:HB    | 1.99                     | 0.45              |
| 79:L5:156:G:N2     | 79:L5:157:U:O4     | 2.49                     | 0.45              |
| 79:L5:1802:A:H5''  | 79:L5:1803:G:H5'   | 1.98                     | 0.45              |
| 79:L5:2023:C:H2'   | 79:L5:2024:G:O4'   | 2.17                     | 0.45              |
| 3:LB:168:MET:HG3   | 3:LB:178:ALA:HA    | 1.99                     | 0.45              |
| 3:LB:228:TYR:O     | 79:L5:2835:A:O2'   | 2.25                     | 0.45              |
| 9:SE:44:LEU:HD11   | 9:SE:70:ILE:HG21   | 1.98                     | 0.45              |
| 14:SI:38:ILE:HD11  | 14:SI:81:VAL:HG23  | 1.98                     | 0.45              |
| 39:LH:48:LEU:HD11  | 39:LH:56:ARG:HB2   | 1.98                     | 0.45              |
| 45:LM:113:MET:HG3  | 79:L5:4881:U:N3    | 2.31                     | 0.45              |
| 78:S2:1409:A:H2'   | 78:S2:1410:C:C6    | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:L5:258:G:H2'    | 79:L5:259:C:C6     | 2.52                     | 0.45              |
| 79:L5:732:A:H2'    | 79:L5:733:A:O4'    | 2.17                     | 0.45              |
| 79:L5:1097:C:H2'   | 79:L5:1098:G:C8    | 2.52                     | 0.45              |
| 79:L5:1249:C:H2'   | 79:L5:1250:C:C6    | 2.52                     | 0.45              |
| 79:L5:1274:A:H2'   | 79:L5:1275:G:H8    | 1.80                     | 0.45              |
| 79:L5:3707:U:H2'   | 79:L5:3708:C:C6    | 2.51                     | 0.45              |
| 79:L5:3839:G:N2    | 79:L5:3843:C:O2'   | 2.50                     | 0.45              |
| 79:L5:4619:U:H2'   | 79:L5:4620:OMU:H6  | 1.98                     | 0.45              |
| 2:SA:30:LEU:HB2    | 2:SA:47:TYR:CE2    | 2.52                     | 0.45              |
| 5:L8:60:G:OP1      | 56:LX:70:LYS:NZ    | 2.50                     | 0.45              |
| 6:L7:69:U:H2'      | 6:L7:70:G:C8       | 2.52                     | 0.45              |
| 14:SI:5:ARG:HB3    | 78:S2:386:C:H1'    | 1.99                     | 0.45              |
| 24:SL:107:LYS:NZ   | 78:S2:354:OMU:OP2  | 2.50                     | 0.45              |
| 36:Sg:65:PHE:O     | 36:Sg:83:TRP:N     | 2.44                     | 0.45              |
| 36:Sg:298:LEU:HB3  | 36:Sg:310:TRP:HB2  | 1.99                     | 0.45              |
| 38:LJ:167:GLN:HE21 | 38:LJ:174:ILE:HG12 | 1.80                     | 0.45              |
| 54:LP:6:LEU:HD23   | 54:LP:6:LEU:HA     | 1.86                     | 0.45              |
| 62:LF:36:LYS:HD2   | 62:LF:36:LYS:HA    | 1.70                     | 0.45              |
| 78:S2:57:U:OP1     | 78:S2:504:G:O2'    | 2.35                     | 0.45              |
| 78:S2:1801:A:H2'   | 78:S2:1802:C:C6    | 2.52                     | 0.45              |
| 79:L5:153:G:H2'    | 79:L5:154:G:H8     | 1.82                     | 0.45              |
| 79:L5:1346:C:H2'   | 79:L5:1347:G:H8    | 1.81                     | 0.45              |
| 79:L5:1773:U:H2'   | 79:L5:1774:C:C6    | 2.52                     | 0.45              |
| 4:SB:82:ARG:NH1    | 4:SB:189:ILE:O     | 2.50                     | 0.45              |
| 78:S2:982:G:H2'    | 78:S2:983:A:C8     | 2.52                     | 0.45              |
| 79:L5:394:G:N2     | 79:L5:397:G:OP2    | 2.37                     | 0.45              |
| 79:L5:2505:C:H42   | 79:L5:4084:G:H4'   | 1.82                     | 0.45              |
| 79:L5:3707:U:H2'   | 79:L5:3708:C:H6    | 1.81                     | 0.45              |
| 79:L5:3848:U:H2'   | 79:L5:3849:A:H8    | 1.82                     | 0.45              |
| 79:L5:4584:A:H2'   | 79:L5:4585:U:O4'   | 2.17                     | 0.45              |
| 8:SJ:145:PRO:HD2   | 78:S2:522:A:H5''   | 1.99                     | 0.44              |
| 10:SC:73:MET:HE3   | 10:SC:73:MET:HB3   | 1.80                     | 0.44              |
| 23:SN:94:LYS:O     | 23:SN:98:VAL:HG23  | 2.17                     | 0.44              |
| 24:SL:111:VAL:HG11 | 24:SL:128:VAL:HG11 | 1.99                     | 0.44              |
| 40:LE:149:ILE:O    | 40:LE:197:THR:OG1  | 2.27                     | 0.44              |
| 53:LT:80:VAL:HG21  | 79:L5:4305:G:C6    | 2.52                     | 0.44              |
| 62:LF:32:ARG:HH12  | 79:L5:962:C:H1'    | 1.81                     | 0.44              |
| 65:Le:16:ARG:NH2   | 65:Le:19:LYS:O     | 2.46                     | 0.44              |
| 71:Ll:48:LYS:HE3   | 79:L5:2406:G:H4'   | 1.98                     | 0.44              |
| 77:mR:35:G:H1'     | 78:S2:1207:G:C2    | 2.51                     | 0.44              |
| 78:S2:5:U:H2'      | 78:S2:6:G:H8       | 1.83                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 78:S2:189:U:H2'    | 78:S2:190:G:O4'    | 2.17                     | 0.44              |
| 78:S2:1410:C:H2'   | 78:S2:1411:G:H8    | 1.82                     | 0.44              |
| 79:L5:223:G:H4'    | 79:L5:225:G:N7     | 2.32                     | 0.44              |
| 80:Et:17:C:O2'     | 80:Et:61:C:OP1     | 2.34                     | 0.44              |
| 4:SB:139:CYS:HA    | 4:SB:213:ARG:H     | 1.81                     | 0.44              |
| 21:SS:148:VAL:HG22 | 26:SP:131:PRO:HB2  | 1.98                     | 0.44              |
| 36:Sg:248:LEU:HD23 | 36:Sg:259:TRP:CE3  | 2.53                     | 0.44              |
| 43:LL:56:ARG:NH1   | 43:LL:74:ARG:O     | 2.44                     | 0.44              |
| 47:LN:4:TYR:OH     | 79:L5:151:G:OP2    | 2.21                     | 0.44              |
| 49:LD:116:ASP:OD1  | 49:LD:116:ASP:N    | 2.43                     | 0.44              |
| 51:LR:99:MET:HE1   | 51:LR:127:VAL:O    | 2.17                     | 0.44              |
| 52:LS:17:LEU:HD23  | 52:LS:17:LEU:HA    | 1.87                     | 0.44              |
| 54:LP:8:PRO:HD3    | 54:LP:149:ILE:HD13 | 1.98                     | 0.44              |
| 59:Lr:63:VAL:HG22  | 59:Lr:79:ARG:HD2   | 1.99                     | 0.44              |
| 68:Li:53:TYR:OH    | 68:Li:86:LYS:NZ    | 2.51                     | 0.44              |
| 74:Lo:63:THR:OG1   | 79:L5:4229:U:OP1   | 2.28                     | 0.44              |
| 78:S2:354:OMU:HM23 | 78:S2:354:OMU:H1'  | 1.63                     | 0.44              |
| 78:S2:1215:C:O2'   | 78:S2:1645:C:OP2   | 2.33                     | 0.44              |
| 79:L5:207:G:N3     | 79:L5:232:G:N2     | 2.58                     | 0.44              |
| 79:L5:4389:C:H2'   | 79:L5:4390:A:C8    | 2.52                     | 0.44              |
| 4:SB:116:LYS:HG3   | 78:S2:988:C:H5''   | 1.98                     | 0.44              |
| 18:SO:151:LEU:HD23 | 18:SO:151:LEU:HA   | 1.81                     | 0.44              |
| 36:Sg:134:THR:O    | 36:Sg:134:THR:OG1  | 2.34                     | 0.44              |
| 37:LC:350:ARG:HD3  | 79:L5:724:C:OP1    | 2.18                     | 0.44              |
| 39:LH:71:ARG:NH1   | 79:L5:4691:A:H5'   | 2.32                     | 0.44              |
| 40:LE:133:PHE:O    | 40:LE:138:ARG:NH2  | 2.47                     | 0.44              |
| 79:L5:257:C:H2'    | 79:L5:258:G:O4'    | 2.17                     | 0.44              |
| 79:L5:1754:U:O2'   | 79:L5:1755:C:O5'   | 2.34                     | 0.44              |
| 79:L5:1867:A:H2'   | 79:L5:1868:A:C8    | 2.52                     | 0.44              |
| 79:L5:2900:U:H2'   | 79:L5:2901:G:C8    | 2.52                     | 0.44              |
| 79:L5:4570:G:H2'   | 79:L5:4571:A2M:H8  | 1.99                     | 0.44              |
| 79:L5:4694:G:OP1   | 79:L5:4694:G:N2    | 2.50                     | 0.44              |
| 7:SD:219:PRO:HB2   | 36:Sg:190:GLY:HA2  | 2.00                     | 0.44              |
| 11:SF:159:ARG:NH1  | 78:S2:1535:U:O4    | 2.50                     | 0.44              |
| 12:SH:24:SER:HA    | 12:SH:27:LEU:HD12  | 1.98                     | 0.44              |
| 27:ST:39:LEU:HA    | 27:ST:39:LEU:HD23  | 1.72                     | 0.44              |
| 43:LL:126:LEU:HD12 | 43:LL:126:LEU:HA   | 1.85                     | 0.44              |
| 46:La:132:ARG:HH12 | 79:L5:1396:G:H5''  | 1.82                     | 0.44              |
| 57:LY:100:HIS:CD2  | 79:L5:231:U:H4'    | 2.52                     | 0.44              |
| 68:Li:85:ARG:NH1   | 68:Li:85:ARG:HB2   | 2.33                     | 0.44              |
| 79:L5:215:C:H5''   | 79:L5:216:C:H5'    | 1.99                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:L5:456:C:H2'    | 79:L5:457:G:C8    | 2.53                     | 0.44              |
| 79:L5:3861:A:H2'   | 79:L5:3862:A:C8   | 2.51                     | 0.44              |
| 4:SB:36:PRO:HD2    | 4:SB:86:LEU:HD13  | 2.00                     | 0.44              |
| 8:SJ:136:ARG:HH11  | 8:SJ:139:LYS:HA   | 1.82                     | 0.44              |
| 12:SH:11:PRO:HD3   | 12:SH:46:THR:HG23 | 1.99                     | 0.44              |
| 29:SY:8:ARG:HG2    | 29:SY:8:ARG:HH11  | 1.82                     | 0.44              |
| 36:Sg:17:TRP:H     | 36:Sg:36:ARG:HB2  | 1.81                     | 0.44              |
| 36:Sg:256:ILE:HB   | 36:Sg:270:LEU:HB2 | 1.99                     | 0.44              |
| 48:LI:180:GLU:HG3  | 48:LI:184:MET:HE2 | 1.99                     | 0.44              |
| 76:Pt:23:G:O6      | 76:Pt:47:G7M:N2   | 2.51                     | 0.44              |
| 76:Pt:33:OMC:HM22  | 76:Pt:34:U:H5'    | 2.00                     | 0.44              |
| 78:S2:1201:U:H2'   | 78:S2:1202:U:C6   | 2.52                     | 0.44              |
| 79:L5:1194:G:OP2   | 79:L5:1194:G:N2   | 2.43                     | 0.44              |
| 79:L5:1250:C:H2'   | 79:L5:1251:C:C6   | 2.52                     | 0.44              |
| 79:L5:1846:G:H2'   | 79:L5:1847:C:C6   | 2.52                     | 0.44              |
| 79:L5:3654:G:O2'   | 79:L5:3693:U:OP1  | 2.35                     | 0.44              |
| 3:LB:224:LYS:HG2   | 3:LB:340:THR:HG23 | 1.99                     | 0.44              |
| 6:L7:57:C:H2'      | 6:L7:58:A:H8      | 1.83                     | 0.44              |
| 8:SJ:6:SER:OG      | 78:S2:828:G:OP1   | 2.35                     | 0.44              |
| 27:ST:5:THR:HG21   | 78:S2:1425:G:H21  | 1.82                     | 0.44              |
| 41:LG:242:LEU:HD23 | 41:LG:242:LEU:HA  | 1.89                     | 0.44              |
| 67:Lg:60:ARG:HD2   | 67:Lg:60:ARG:HA   | 1.70                     | 0.44              |
| 78:S2:609:PSU:H2'  | 78:S2:610:G:H8    | 1.83                     | 0.44              |
| 78:S2:980:A:H2'    | 78:S2:981:A:C8    | 2.53                     | 0.44              |
| 78:S2:1816:G:O2'   | 79:L5:3807:A:O2'  | 2.31                     | 0.44              |
| 79:L5:177:G:H2'    | 79:L5:178:C:H5''  | 1.99                     | 0.44              |
| 79:L5:1773:U:H2'   | 79:L5:1774:C:H6   | 1.82                     | 0.44              |
| 79:L5:1967:A:H2'   | 79:L5:1968:G:C8   | 2.53                     | 0.44              |
| 79:L5:2103:G:H2'   | 79:L5:2104:G:C8   | 2.53                     | 0.44              |
| 79:L5:3721:U:H2'   | 79:L5:3722:G:H8   | 1.82                     | 0.44              |
| 79:L5:4478:G:O2'   | 79:L5:4602:A:N1   | 2.45                     | 0.44              |
| 13:SW:14:ILE:HG23  | 13:SW:65:LEU:HD21 | 1.99                     | 0.44              |
| 24:SL:132:ARG:HD2  | 78:S2:383:G:H4'   | 2.00                     | 0.44              |
| 25:SR:66:VAL:HG23  | 25:SR:67:ARG:N    | 2.33                     | 0.44              |
| 43:LL:117:LEU:HD23 | 43:LL:117:LEU:HA  | 1.85                     | 0.44              |
| 49:LD:238:GLU:OE1  | 49:LD:238:GLU:N   | 2.51                     | 0.44              |
| 62:LF:182:TYR:CZ   | 62:LF:203:GLU:HG2 | 2.53                     | 0.44              |
| 79:L5:653:U:H2'    | 79:L5:654:C:C6    | 2.52                     | 0.44              |
| 79:L5:1696:C:H2'   | 79:L5:1697:G:O4'  | 2.18                     | 0.44              |
| 1:LA:243:THR:N     | 79:L5:3745:U:O2'  | 2.47                     | 0.44              |
| 3:LB:287:ILE:HD13  | 3:LB:331:VAL:HG22 | 2.00                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:SB:146:ARG:HB2    | 4:SB:149:GLN:HB2   | 2.00                     | 0.44              |
| 6:L7:4:U:H2'        | 6:L7:5:A:H8        | 1.83                     | 0.44              |
| 6:L7:110:G:H2'      | 6:L7:111:C:C6      | 2.53                     | 0.44              |
| 9:SE:18:TRP:O       | 9:SE:51:ARG:NH2    | 2.51                     | 0.44              |
| 18:SO:95:ILE:HD12   | 18:SO:126:ILE:HG23 | 2.00                     | 0.44              |
| 39:LH:65:LYS:HD3    | 39:LH:65:LYS:HA    | 1.75                     | 0.44              |
| 42:LO:67:SER:HA     | 79:L5:4586:G:H4'   | 2.00                     | 0.44              |
| 51:LR:14:VAL:HG11   | 51:LR:42:ARG:HG2   | 2.00                     | 0.44              |
| 60:Lh:74:LYS:HE2    | 60:Lh:74:LYS:HB2   | 1.80                     | 0.44              |
| 61:Lb:25:ARG:HA     | 61:Lb:25:ARG:HD2   | 1.69                     | 0.44              |
| 62:LF:220:MET:HE1   | 62:LF:223:LYS:HB3  | 1.99                     | 0.44              |
| 78:S2:1432:U:OP1    | 78:S2:1434:C:N4    | 2.50                     | 0.44              |
| 79:L5:1316:OMG:HM23 | 79:L5:1316:OMG:H1' | 1.79                     | 0.44              |
| 79:L5:1327:C:H2'    | 79:L5:1328:G:C8    | 2.52                     | 0.44              |
| 79:L5:2049:G:O2'    | 79:L5:3884:PSU:O2' | 2.28                     | 0.44              |
| 79:L5:2391:G:OP1    | 79:L5:4653:C:O2'   | 2.36                     | 0.44              |
| 79:L5:2694:G:H5'    | 79:L5:2695:A:C2    | 2.52                     | 0.44              |
| 1:LA:201:GLY:HA2    | 1:LA:204:MET:HG3   | 2.00                     | 0.44              |
| 4:SB:120:MET:HB2    | 4:SB:142:PHE:CE2   | 2.53                     | 0.44              |
| 5:L8:23:C:O2        | 57:LY:20:ASN:ND2   | 2.40                     | 0.44              |
| 36:Sg:89:LEU:O      | 36:Sg:98:THR:N     | 2.51                     | 0.44              |
| 37:LC:328:LEU:HD22  | 62:LF:187:MET:HG3  | 2.00                     | 0.44              |
| 44:LV:45:ILE:HG21   | 44:LV:53:PRO:HB3   | 2.00                     | 0.44              |
| 52:LS:2:LYS:HD3     | 62:LF:230:GLY:HA3  | 2.00                     | 0.44              |
| 61:Lb:10:HIS:O      | 61:Lb:12:GLN:NE2   | 2.48                     | 0.44              |
| 65:Le:106:LYS:HB3   | 65:Le:106:LYS:HE2  | 1.84                     | 0.44              |
| 66:Lf:15:LYS:HB3    | 66:Lf:25:THR:HB    | 1.99                     | 0.44              |
| 78:S2:1308:U:H2'    | 78:S2:1309:C:H6    | 1.83                     | 0.44              |
| 79:L5:496:G:H2'     | 79:L5:497:G:H8     | 1.83                     | 0.44              |
| 79:L5:1204:C:H2'    | 79:L5:1205:G:H8    | 1.82                     | 0.44              |
| 79:L5:1734:G:N2     | 79:L5:1735:U:O4    | 2.40                     | 0.44              |
| 79:L5:1787:A:N3     | 79:L5:4210:U:O2'   | 2.49                     | 0.44              |
| 79:L5:3736:A:H2'    | 79:L5:3737:A:H8    | 1.83                     | 0.44              |
| 79:L5:4991:U:H2'    | 79:L5:4992:G:C8    | 2.53                     | 0.44              |
| 82:SG:58:LYS:H      | 82:SG:58:LYS:HG2   | 1.57                     | 0.44              |
| 9:SE:174:LYS:HB3    | 9:SE:174:LYS:HE3   | 1.70                     | 0.43              |
| 15:SQ:73:LYS:HE3    | 15:SQ:73:LYS:HB3   | 1.72                     | 0.43              |
| 19:SX:98:ASP:OD2    | 19:SX:140:ARG:NH2  | 2.51                     | 0.43              |
| 25:SR:132:ARG:NH2   | 78:S2:1100:A:OP1   | 2.51                     | 0.43              |
| 31:Sa:12:LYS:HB2    | 31:Sa:33:ASP:OD2   | 2.18                     | 0.43              |
| 41:LG:110:LYS:HG3   | 41:LG:114:LEU:HD23 | 2.00                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 57:LY:30:MET:HB3   | 57:LY:101:PRO:HG3   | 2.00                     | 0.43              |
| 58:LZ:48:ARG:NH2   | 79:L5:2575:U:OP1    | 2.46                     | 0.43              |
| 78:S2:1408:U:H2'   | 78:S2:1409:A:C8     | 2.53                     | 0.43              |
| 79:L5:1253:G:N2    | 79:L5:1256:G:OP2    | 2.51                     | 0.43              |
| 79:L5:1382:G:H2'   | 79:L5:1383:G:H8     | 1.83                     | 0.43              |
| 79:L5:3848:U:H2'   | 79:L5:3849:A:C8     | 2.52                     | 0.43              |
| 5:L8:87:G:P        | 60:Lh:7:ARG:HH22    | 2.41                     | 0.43              |
| 6:L7:12:U:OP2      | 6:L7:67:C:O2'       | 2.36                     | 0.43              |
| 9:SE:49:ARG:NH1    | 78:S2:496:C:OP2     | 2.50                     | 0.43              |
| 36:Sg:152:SER:OG   | 36:Sg:168:CYS:SG    | 2.73                     | 0.43              |
| 59:Lr:47:LYS:O     | 59:Lr:103:ARG:NH1   | 2.47                     | 0.43              |
| 73:Ln:10:MET:HE1   | 73:Ln:14:LYS:HG3    | 2.00                     | 0.43              |
| 78:S2:644:OMG:HM23 | 78:S2:644:OMG:H1'   | 1.81                     | 0.43              |
| 79:L5:2052:G:O2'   | 79:L5:2057:A:N1     | 2.44                     | 0.43              |
| 79:L5:5001:PSU:H2' | 79:L5:5002:U:O4'    | 2.18                     | 0.43              |
| 82:SG:154:ARG:HB2  | 82:SG:154:ARG:NH1   | 2.33                     | 0.43              |
| 6:L7:3:C:H2'       | 6:L7:4:U:H6         | 1.83                     | 0.43              |
| 10:SC:74:LYS:HD3   | 10:SC:74:LYS:HA     | 1.64                     | 0.43              |
| 30:SZ:92:LEU:HD12  | 30:SZ:109:TYR:CE1   | 2.53                     | 0.43              |
| 44:LV:16:ILE:HD11  | 44:LV:56:GLY:HA3    | 2.00                     | 0.43              |
| 47:LN:15:GLN:O     | 47:LN:20:ARG:NH1    | 2.51                     | 0.43              |
| 52:LS:9:GLU:HG3    | 52:LS:33:PHE:CE2    | 2.52                     | 0.43              |
| 59:Lr:49:VAL:HG11  | 59:Lr:97:ILE:HD11   | 2.00                     | 0.43              |
| 65:Le:90:MET:HE3   | 65:Le:90:MET:HB3    | 1.83                     | 0.43              |
| 73:Ln:1:MET:HE3    | 78:S2:1851:MA6:H5'  | 1.99                     | 0.43              |
| 78:S2:1589:A:N3    | 78:S2:1653:U:O2'    | 2.46                     | 0.43              |
| 79:L5:1072:C:H2'   | 79:L5:1073:G:C8     | 2.53                     | 0.43              |
| 79:L5:1278:C:H2'   | 79:L5:1279:A:O4'    | 2.18                     | 0.43              |
| 79:L5:1741:G:N3    | 79:L5:1781:PSU:H5'' | 2.34                     | 0.43              |
| 79:L5:5003:U:H2'   | 79:L5:5004:C:C6     | 2.53                     | 0.43              |
| 80:Et:16:G:N2      | 80:Et:48:C:H42      | 2.15                     | 0.43              |
| 5:L8:130:C:H2'     | 5:L8:131:G:H8       | 1.83                     | 0.43              |
| 14:SI:190:LEU:HD22 | 14:SI:194:GLU:HG2   | 2.00                     | 0.43              |
| 27:ST:71:GLY:HA3   | 78:S2:1562:C:H5''   | 2.00                     | 0.43              |
| 39:LH:129:ARG:HH21 | 39:LH:160:LEU:HD21  | 1.82                     | 0.43              |
| 40:LE:183:ARG:HA   | 40:LE:183:ARG:HD2   | 1.72                     | 0.43              |
| 43:LL:42:LYS:HE3   | 43:LL:46:ILE:HD13   | 2.00                     | 0.43              |
| 46:La:83:SER:OG    | 46:La:86:THR:OG1    | 2.33                     | 0.43              |
| 62:LF:148:LYS:O    | 62:LF:152:GLU:HG2   | 2.19                     | 0.43              |
| 75:Lp:4:ARG:NH1    | 79:L5:1555:G:O6     | 2.50                     | 0.43              |
| 76:Pt:63:C:H2'     | 76:Pt:64:G:C8       | 2.53                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 78:S2:223:C:H2'     | 78:S2:224:A:C8      | 2.53                     | 0.43              |
| 78:S2:1408:U:H2'    | 78:S2:1409:A:H8     | 1.82                     | 0.43              |
| 78:S2:1447:OMG:HM23 | 78:S2:1447:OMG:H1'  | 1.81                     | 0.43              |
| 79:L5:711:A:H2'     | 79:L5:712:C:C6      | 2.53                     | 0.43              |
| 79:L5:1762:C:H42    | 79:L5:1770:A:H61    | 1.65                     | 0.43              |
| 79:L5:2376:A:H2'    | 79:L5:2377:C:C6     | 2.54                     | 0.43              |
| 79:L5:4578:G:H2'    | 79:L5:4579:PSU:C6   | 2.54                     | 0.43              |
| 79:L5:5058:A:H2'    | 79:L5:5059:C:C6     | 2.52                     | 0.43              |
| 7:SD:50:ILE:HD11    | 7:SD:86:LEU:HD23    | 2.01                     | 0.43              |
| 15:SQ:53:GLU:HG3    | 15:SQ:85:ARG:HH21   | 1.83                     | 0.43              |
| 40:LE:95:PRO:HG2    | 79:L5:687:U:C4      | 2.53                     | 0.43              |
| 40:LE:140:LEU:HB2   | 40:LE:167:GLN:HE22  | 1.83                     | 0.43              |
| 47:LN:171:SER:O     | 47:LN:171:SER:OG    | 2.36                     | 0.43              |
| 49:LD:59:ASP:OD1    | 49:LD:60:ILE:N      | 2.51                     | 0.43              |
| 51:LR:76:MET:HE2    | 51:LR:76:MET:HB3    | 1.86                     | 0.43              |
| 54:LP:115:GLU:OE1   | 54:LP:151:THR:OG1   | 2.34                     | 0.43              |
| 69:Lj:67:LEU:HD12   | 69:Lj:67:LEU:HA     | 1.88                     | 0.43              |
| 71:Ll:24:PRO:HD2    | 71:Ll:27:ILE:HG13   | 2.01                     | 0.43              |
| 78:S2:12:U:H2'      | 78:S2:13:C:C6       | 2.53                     | 0.43              |
| 78:S2:844:U:H2'     | 78:S2:845:G:H8      | 1.82                     | 0.43              |
| 78:S2:1139:C:H42    | 78:S2:1149:A:N6     | 2.13                     | 0.43              |
| 78:S2:1390:U:H2'    | 78:S2:1391:OMC:C6   | 2.53                     | 0.43              |
| 79:L5:492:U:H2'     | 79:L5:493:G:C8      | 2.54                     | 0.43              |
| 79:L5:1177:U:H2'    | 79:L5:1178:G:C8     | 2.52                     | 0.43              |
| 79:L5:1248:C:H2'    | 79:L5:1249:C:C6     | 2.53                     | 0.43              |
| 79:L5:1662:C:H2'    | 79:L5:1663:C:H6     | 1.83                     | 0.43              |
| 79:L5:2019:C:H2'    | 79:L5:2020:U:C6     | 2.54                     | 0.43              |
| 79:L5:3656:A:H2'    | 79:L5:3657:U:C6     | 2.53                     | 0.43              |
| 79:L5:4093:G:H2'    | 79:L5:4094:G:H8     | 1.83                     | 0.43              |
| 79:L5:4460:U:H2'    | 79:L5:4461:C:H6     | 1.84                     | 0.43              |
| 81:LW:50:ASN:OD1    | 81:LW:50:ASN:N      | 2.50                     | 0.43              |
| 3:LB:241:PRO:HD3    | 79:L5:4456:OMC:HM21 | 2.00                     | 0.43              |
| 17:SK:53:LYS:HB3    | 17:SK:53:LYS:HE2    | 1.59                     | 0.43              |
| 18:SO:19:PRO:HG2    | 18:SO:27:VAL:HG21   | 2.00                     | 0.43              |
| 32:Sb:68:GLY:O      | 78:S2:928:G:N2      | 2.47                     | 0.43              |
| 39:LH:95:VAL:HG22   | 72:Lm:82:LEU:HD23   | 1.99                     | 0.43              |
| 49:LD:271:MET:HG2   | 49:LD:275:GLN:HB2   | 1.99                     | 0.43              |
| 62:LF:34:ARG:HD2    | 79:L5:1272:C:H5'    | 2.00                     | 0.43              |
| 78:S2:495:U:H2'     | 78:S2:496:C:O4'     | 2.19                     | 0.43              |
| 78:S2:1134:G:H2'    | 78:S2:1135:C:C6     | 2.54                     | 0.43              |
| 79:L5:318:A:H2'     | 79:L5:319:A:H8      | 1.84                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 79:L5:1271:G:H21    | 79:L5:1271:G:P     | 2.39                     | 0.43              |
| 79:L5:2323:C:H2'    | 79:L5:2324:C:H6    | 1.84                     | 0.43              |
| 79:L5:2864:A:H2'    | 79:L5:2865:U:C6    | 2.54                     | 0.43              |
| 79:L5:4992:G:H2'    | 79:L5:4993:G:C8    | 2.53                     | 0.43              |
| 79:L5:5066:U:H2'    | 79:L5:5067:U:C6    | 2.54                     | 0.43              |
| 80:Et:21:A:O4'      | 80:Et:48:C:N4      | 2.52                     | 0.43              |
| 82:SG:72:ARG:HD3    | 82:SG:96:SER:HB3   | 2.01                     | 0.43              |
| 1:LA:37:ARG:NH2     | 79:L5:4088:C:OP1   | 2.45                     | 0.43              |
| 5:L8:90:C:H2'       | 5:L8:91:A:C8       | 2.54                     | 0.43              |
| 14:SI:60:LEU:HD13   | 14:SI:185:ALA:HB2  | 2.00                     | 0.43              |
| 21:SS:46:ARG:HG2    | 27:ST:35:ASP:HB2   | 2.00                     | 0.43              |
| 25:SR:60:ARG:HB3    | 25:SR:66:VAL:HG11  | 2.01                     | 0.43              |
| 42:LO:181:ALA:O     | 42:LO:185:VAL:HG22 | 2.18                     | 0.43              |
| 47:LN:177:GLY:HA2   | 79:L5:67:C:O3'     | 2.18                     | 0.43              |
| 48:LI:38:ARG:HG2    | 48:LI:41:ALA:HB2   | 2.00                     | 0.43              |
| 48:LI:48:LEU:HD11   | 48:LI:167:ILE:HD12 | 2.00                     | 0.43              |
| 53:LT:158:PHE:HD1   | 53:LT:159:MET:N    | 2.17                     | 0.43              |
| 63:Lc:18:LEU:HD23   | 63:Lc:18:LEU:HA    | 1.86                     | 0.43              |
| 78:S2:98:C:H2'      | 78:S2:426:A:H4'    | 2.00                     | 0.43              |
| 78:S2:568:C:H42     | 78:S2:582:U:H3     | 1.67                     | 0.43              |
| 78:S2:1007:C:H2'    | 78:S2:1008:A:C8    | 2.54                     | 0.43              |
| 78:S2:1328:OMG:HM23 | 78:S2:1328:OMG:HI' | 1.74                     | 0.43              |
| 79:L5:1404:G:H2'    | 79:L5:1405:C:C6    | 2.53                     | 0.43              |
| 79:L5:2568:C:H2'    | 79:L5:2569:G:C8    | 2.52                     | 0.43              |
| 79:L5:2900:U:H2'    | 79:L5:2901:G:H8    | 1.83                     | 0.43              |
| 1:LA:243:THR:HB     | 79:L5:3748:A:H5''  | 2.01                     | 0.43              |
| 3:LB:47:LEU:HB2     | 3:LB:84:MET:SD     | 2.59                     | 0.43              |
| 9:SE:127:ARG:HG3    | 9:SE:142:HIS:HA    | 2.01                     | 0.43              |
| 21:SS:136:THR:OG1   | 78:S2:1521:C:OP2   | 2.32                     | 0.43              |
| 23:SN:33:VAL:HG21   | 23:SN:66:VAL:HG11  | 2.00                     | 0.43              |
| 33:Sc:36:ASP:OD2    | 33:Sc:37:ASP:N     | 2.52                     | 0.43              |
| 37:LC:237:ILE:HD12  | 37:LC:237:ILE:HA   | 1.87                     | 0.43              |
| 44:LV:123:LYS:HE3   | 44:LV:123:LYS:HB3  | 1.87                     | 0.43              |
| 48:LI:162:ARG:HH21  | 48:LI:164:LYS:HE3  | 1.83                     | 0.43              |
| 52:LS:37:HIS:NE2    | 62:LF:238:ASP:OD2  | 2.40                     | 0.43              |
| 54:LP:83:TRP:O      | 79:L5:3856:A:H5''  | 2.18                     | 0.43              |
| 61:Lb:95:ARG:HG3    | 79:L5:1266:G:C8    | 2.54                     | 0.43              |
| 78:S2:51:U:H2'      | 78:S2:52:G:C8      | 2.54                     | 0.43              |
| 78:S2:106:C:H2'     | 78:S2:107:A:C8     | 2.53                     | 0.43              |
| 78:S2:1083:A:N7     | 78:S2:1841:C:O2'   | 2.44                     | 0.43              |
| 79:L5:257:C:H3'     | 79:L5:258:G:C8     | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:L5:268:G:H2'    | 79:L5:269:G:H8     | 1.83                     | 0.43              |
| 79:L5:2894:A:H2'   | 79:L5:2895:A:C8    | 2.54                     | 0.43              |
| 79:L5:4071:U:H2'   | 79:L5:4072:C:H6    | 1.84                     | 0.43              |
| 79:L5:4538:G:H2'   | 79:L5:4539:U:C6    | 2.54                     | 0.43              |
| 79:L5:4593:C:H2'   | 79:L5:4594:U:H6    | 1.84                     | 0.43              |
| 1:LA:30:ARG:NH1    | 1:LA:36:GLU:OE1    | 2.52                     | 0.43              |
| 3:LB:58:ARG:HA     | 3:LB:366:LYS:HG3   | 2.00                     | 0.43              |
| 17:SK:45:VAL:O     | 17:SK:49:MET:HG2   | 2.18                     | 0.43              |
| 25:SR:81:ARG:HD3   | 25:SR:81:ARG:HA    | 1.78                     | 0.43              |
| 27:ST:39:LEU:HD21  | 27:ST:52:TRP:CZ3   | 2.54                     | 0.43              |
| 28:SV:59:ILE:HD13  | 28:SV:62:MET:HE3   | 2.01                     | 0.43              |
| 36:Sg:304:ASP:O    | 36:Sg:306:LEU:N    | 2.52                     | 0.43              |
| 37:LC:60:HIS:NE2   | 37:LC:100:ARG:HD3  | 2.34                     | 0.43              |
| 37:LC:230:LEU:HD23 | 37:LC:230:LEU:HA   | 1.88                     | 0.43              |
| 40:LE:41:LYS:HB2   | 40:LE:41:LYS:HE2   | 1.82                     | 0.43              |
| 49:LD:108:ARG:NE   | 49:LD:253:TYR:HB2  | 2.33                     | 0.43              |
| 54:LP:108:ASP:N    | 54:LP:152:GLU:OE2  | 2.39                     | 0.43              |
| 62:LF:53:LYS:NZ    | 62:LF:189:ASP:OD2  | 2.43                     | 0.43              |
| 78:S2:118:C:H1'    | 78:S2:445:A:C5     | 2.54                     | 0.43              |
| 78:S2:494:C:N4     | 78:S2:509:OMG:HN22 | 2.15                     | 0.43              |
| 78:S2:1142:G:N2    | 78:S2:1145:A:OP2   | 2.42                     | 0.43              |
| 78:S2:1410:C:H2'   | 78:S2:1411:G:C8    | 2.53                     | 0.43              |
| 78:S2:1452:A:O2'   | 78:S2:1475:G:N2    | 2.52                     | 0.43              |
| 78:S2:1545:A:N3    | 78:S2:1671:G:O2'   | 2.42                     | 0.43              |
| 79:L5:223:G:H4'    | 79:L5:225:G:C8     | 2.54                     | 0.43              |
| 79:L5:1676:C:H41   | 79:L5:4378:A:H5''  | 1.83                     | 0.43              |
| 79:L5:2607:C:H2'   | 79:L5:2608:G:H8    | 1.84                     | 0.43              |
| 79:L5:4578:G:H2'   | 79:L5:4579:PSU:H6  | 1.83                     | 0.43              |
| 80:Et:53:G:H2'     | 80:Et:54:A:C8      | 2.51                     | 0.43              |
| 3:LB:29:VAL:HG23   | 3:LB:346:THR:HG21  | 2.01                     | 0.43              |
| 3:LB:72:VAL:HA     | 44:LV:92:ASP:HA    | 2.01                     | 0.43              |
| 11:SF:154:LEU:HD22 | 11:SF:177:LEU:HD23 | 2.00                     | 0.43              |
| 41:LG:165:GLU:OE2  | 47:LN:22:LEU:HD13  | 2.19                     | 0.43              |
| 41:LG:213:GLY:O    | 41:LG:217:LYS:HG2  | 2.19                     | 0.43              |
| 43:LL:142:GLU:HG3  | 43:LL:146:LEU:HD13 | 2.00                     | 0.43              |
| 44:LV:33:GLY:HA3   | 44:LV:69:LYS:HD2   | 2.01                     | 0.43              |
| 44:LV:51:ARG:NH1   | 79:L5:4620:OMU:OP1 | 2.48                     | 0.43              |
| 48:LI:53:VAL:HG12  | 48:LI:134:VAL:HG22 | 2.00                     | 0.43              |
| 51:LR:74:ARG:H     | 51:LR:74:ARG:HG2   | 1.66                     | 0.43              |
| 57:LY:57:VAL:HA    | 57:LY:104:VAL:HG12 | 2.00                     | 0.43              |
| 73:Ln:16:LYS:HD2   | 73:Ln:16:LYS:N     | 2.34                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 78:S2:186:C:H2'     | 78:S2:187:G:H8     | 1.84                     | 0.43              |
| 78:S2:1112:U:O2     | 78:S2:1121:G:O6    | 2.37                     | 0.43              |
| 78:S2:1653:U:H2'    | 78:S2:1654:G:C8    | 2.54                     | 0.43              |
| 79:L5:456:C:H2'     | 79:L5:457:G:H8     | 1.83                     | 0.43              |
| 79:L5:3923:A:H2'    | 79:L5:3924:C:C6    | 2.54                     | 0.43              |
| 79:L5:4069:U:H2'    | 79:L5:4070:U:H6    | 1.84                     | 0.43              |
| 1:LA:244:GLY:HA3    | 79:L5:3746:A:H5''  | 2.00                     | 0.42              |
| 2:SA:145:ILE:HG12   | 2:SA:159:ILE:HB    | 2.01                     | 0.42              |
| 27:ST:22:LEU:HD13   | 27:ST:28:LEU:HD13  | 2.00                     | 0.42              |
| 37:LC:52:TYR:O      | 92:LC:616:HOH:O    | 2.21                     | 0.42              |
| 39:LH:43:VAL:O      | 79:L5:4764:A:O2'   | 2.34                     | 0.42              |
| 40:LE:188:ARG:NH2   | 79:L5:4941:G:OP2   | 2.48                     | 0.42              |
| 41:LG:176:LYS:HD3   | 68:Li:43:MET:HE1   | 2.00                     | 0.42              |
| 48:LI:93:PRO:HB2    | 48:LI:125:THR:HB   | 2.01                     | 0.42              |
| 51:LR:106:LEU:HB3   | 51:LR:120:TYR:CE1  | 2.55                     | 0.42              |
| 57:LY:69:LYS:H      | 57:LY:83:GLU:HB2   | 1.84                     | 0.42              |
| 61:Lb:102:PRO:HA    | 61:Lb:109:ARG:HH12 | 1.84                     | 0.42              |
| 62:LF:232:ASP:OD2   | 62:LF:236:ARG:NH2  | 2.52                     | 0.42              |
| 67:Lg:33:LEU:HD23   | 67:Lg:33:LEU:HA    | 1.94                     | 0.42              |
| 92:Lj:205:HOH:O     | 79:L5:2794:C:OP1   | 2.21                     | 0.42              |
| 78:S2:1643:PSU:H2'  | 78:S2:1644:C:C6    | 2.54                     | 0.42              |
| 78:S2:1733:U:H2'    | 78:S2:1734:G:O4'   | 2.19                     | 0.42              |
| 79:L5:132:G:O2'     | 79:L5:133:C:O4'    | 2.20                     | 0.42              |
| 79:L5:3880:G:H2'    | 79:L5:3881:G:C8    | 2.54                     | 0.42              |
| 79:L5:4504:C:H2'    | 79:L5:4505:C:C6    | 2.53                     | 0.42              |
| 79:L5:4536:OMC:HM22 | 79:L5:4537:C:O4'   | 2.19                     | 0.42              |
| 2:SA:63:ARG:HG3     | 2:SA:185:MET:HE1   | 2.01                     | 0.42              |
| 6:L7:16:A:H2'       | 6:L7:17:C:C6       | 2.54                     | 0.42              |
| 14:SI:3:ILE:H       | 14:SI:3:ILE:HG13   | 1.66                     | 0.42              |
| 15:SQ:138:ARG:HD3   | 15:SQ:138:ARG:HA   | 1.76                     | 0.42              |
| 27:ST:34:VAL:O      | 27:ST:52:TRP:NE1   | 2.40                     | 0.42              |
| 37:LC:12:SER:HA     | 37:LC:155:GLU:HG2  | 2.02                     | 0.42              |
| 40:LE:89:LEU:HD12   | 40:LE:89:LEU:HA    | 1.84                     | 0.42              |
| 41:LG:120:LYS:HA    | 41:LG:120:LYS:HD3  | 1.74                     | 0.42              |
| 42:LO:192:TYR:CZ    | 45:LM:118:MET:HG2  | 2.53                     | 0.42              |
| 44:LV:21:PRO:HA     | 44:LV:54:ALA:HA    | 2.01                     | 0.42              |
| 47:LN:82:GLY:O      | 47:LN:87:HIS:HE1   | 2.02                     | 0.42              |
| 54:LP:122:ALA:HB3   | 54:LP:143:PRO:HG2  | 2.01                     | 0.42              |
| 57:LY:11:ARG:HG3    | 79:L5:229:G:H5''   | 2.00                     | 0.42              |
| 57:LY:103:LYS:NZ    | 79:L5:200:U:O4     | 2.31                     | 0.42              |
| 78:S2:534:G:H2'     | 78:S2:535:G:C8     | 2.54                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 78:S2:655:A:H4'     | 78:S2:656:G:H3'     | 2.01                     | 0.42              |
| 78:S2:659:G:O2'     | 78:S2:662:G:O2'     | 2.33                     | 0.42              |
| 79:L5:459:C:H2'     | 79:L5:460:C:H6      | 1.83                     | 0.42              |
| 79:L5:1086:C:H2'    | 79:L5:1087:A:H8     | 1.85                     | 0.42              |
| 79:L5:2488:C:H2'    | 79:L5:2489:C:O4'    | 2.17                     | 0.42              |
| 79:L5:2876:OMG:HM22 | 79:L5:2876:OMG:H1'  | 1.74                     | 0.42              |
| 79:L5:4452:U:O4'    | 90:L5:5101:ANM:H10  | 2.19                     | 0.42              |
| 18:SO:36:SER:OG     | 18:SO:37:PHE:N      | 2.51                     | 0.42              |
| 31:Sa:2:THR:OG1     | 78:S2:1199:A:OP1    | 2.32                     | 0.42              |
| 36:Sg:255:SER:HB3   | 36:Sg:271:LYS:HD2   | 2.00                     | 0.42              |
| 37:LC:143:ARG:NH2   | 37:LC:145:GLU:OE2   | 2.52                     | 0.42              |
| 37:LC:204:ARG:NH1   | 37:LC:205:ARG:O     | 2.52                     | 0.42              |
| 45:LM:63:LYS:HB2    | 45:LM:63:LYS:HE2    | 1.72                     | 0.42              |
| 47:LN:12:ARG:HD3    | 79:L5:279:A:C5      | 2.54                     | 0.42              |
| 48:LI:51:HIS:ND1    | 48:LI:137:SER:HB3   | 2.34                     | 0.42              |
| 49:LD:164:LYS:HD2   | 49:LD:164:LYS:HA    | 1.76                     | 0.42              |
| 57:LY:33:PRO:HG2    | 57:LY:105:VAL:HG23  | 2.01                     | 0.42              |
| 76:Pt:31:G:OP1      | 78:S2:1524:G:O2'    | 2.37                     | 0.42              |
| 79:L5:25:A:N3       | 79:L5:339:C:O2'     | 2.44                     | 0.42              |
| 79:L5:1260:G:H2'    | 79:L5:1261:G:C8     | 2.54                     | 0.42              |
| 79:L5:3911:C:H4'    | 79:L5:4196:OMG:HM23 | 2.01                     | 0.42              |
| 79:L5:4978:G:H2'    | 79:L5:4979:A:H5''   | 2.01                     | 0.42              |
| 80:Et:27:C:H2'      | 80:Et:28:U:C6       | 2.54                     | 0.42              |
| 6:L7:6:C:O2'        | 49:LD:50:ARG:NH2    | 2.52                     | 0.42              |
| 10:SC:171:GLY:HA3   | 13:SW:97:ARG:HH21   | 1.82                     | 0.42              |
| 15:SQ:16:LYS:HD2    | 15:SQ:17:LYS:H      | 1.83                     | 0.42              |
| 15:SQ:34:VAL:HB     | 15:SQ:42:ILE:HD11   | 2.01                     | 0.42              |
| 24:SL:78:THR:HG21   | 24:SL:89:ARG:HB2    | 2.01                     | 0.42              |
| 27:ST:84:ARG:NH2    | 78:S2:1531:A:OP1    | 2.45                     | 0.42              |
| 36:Sg:107:ASP:C     | 36:Sg:124:SER:HG    | 2.26                     | 0.42              |
| 36:Sg:254:PRO:HB3   | 36:Sg:283:PRO:HB2   | 2.00                     | 0.42              |
| 40:LE:112:MET:CE    | 79:L5:2261:G:H5''   | 2.50                     | 0.42              |
| 43:LL:37:LYS:HD3    | 79:L5:1366:G:N7     | 2.34                     | 0.42              |
| 45:LM:113:MET:HG3   | 79:L5:4881:U:C4     | 2.54                     | 0.42              |
| 47:LN:93:LYS:HD3    | 79:L5:300:A:H2      | 1.85                     | 0.42              |
| 74:Lo:30:LYS:HE2    | 74:Lo:30:LYS:HB2    | 1.92                     | 0.42              |
| 78:S2:1511:U:H2'    | 78:S2:1512:C:C6     | 2.55                     | 0.42              |
| 78:S2:1841:C:H2'    | 78:S2:1842:4AC:H6   | 2.00                     | 0.42              |
| 79:L5:3627:OMG:HM23 | 79:L5:3627:OMG:H1'  | 1.88                     | 0.42              |
| 79:L5:5002:U:H2'    | 79:L5:5003:U:C6     | 2.55                     | 0.42              |
| 80:Et:54:A:N6       | 80:Et:58:A:N7       | 2.57                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:123:ARG:NH1   | 79:L5:4083:U:OP1   | 2.52                     | 0.42              |
| 13:SW:32:LYS:HE2   | 13:SW:32:LYS:HB2   | 1.78                     | 0.42              |
| 30:SZ:50:PHE:HB2   | 30:SZ:54:THR:HB    | 2.02                     | 0.42              |
| 44:LV:82:ILE:HG22  | 44:LV:125:CYS:SG   | 2.60                     | 0.42              |
| 49:LD:30:TYR:HA    | 49:LD:33:ARG:HB3   | 2.02                     | 0.42              |
| 50:LQ:49:LYS:HE3   | 50:LQ:49:LYS:HB3   | 1.71                     | 0.42              |
| 71:Ll:41:ARG:HD2   | 71:Ll:41:ARG:HA    | 1.75                     | 0.42              |
| 78:S2:29:G:H2'     | 78:S2:30:C:C6      | 2.55                     | 0.42              |
| 78:S2:96:C:H2'     | 78:S2:97:U:C6      | 2.54                     | 0.42              |
| 78:S2:116:OMU:HM23 | 78:S2:116:OMU:H1'  | 1.76                     | 0.42              |
| 78:S2:553:U:H2'    | 78:S2:555:A:C8     | 2.55                     | 0.42              |
| 78:S2:1144:A:H2'   | 78:S2:1145:A:C8    | 2.55                     | 0.42              |
| 78:S2:1458:G:H2'   | 78:S2:1459:G:C8    | 2.55                     | 0.42              |
| 79:L5:90:G:OP2     | 79:L5:92:C:N4      | 2.46                     | 0.42              |
| 79:L5:679:C:H2'    | 79:L5:680:G:H8     | 1.85                     | 0.42              |
| 79:L5:1094:G:H2'   | 79:L5:1095:A:C8    | 2.55                     | 0.42              |
| 79:L5:1341:U:H2'   | 79:L5:1342:A:C8    | 2.54                     | 0.42              |
| 79:L5:1494:U:H2'   | 79:L5:1495:G:C8    | 2.54                     | 0.42              |
| 3:LB:223:THR:O     | 3:LB:343:ARG:NH2   | 2.52                     | 0.42              |
| 5:L8:60:G:O6       | 5:L8:96:C:O2'      | 2.32                     | 0.42              |
| 6:L7:23:A:N3       | 6:L7:118:C:O2'     | 2.38                     | 0.42              |
| 9:SE:213:ALA:HB3   | 9:SE:244:ILE:HD11  | 2.01                     | 0.42              |
| 11:SF:192:LYS:HA   | 11:SF:192:LYS:HD2  | 1.82                     | 0.42              |
| 33:Sc:34:PHE:CZ    | 33:Sc:61:SER:HB2   | 2.54                     | 0.42              |
| 39:LH:50:LYS:O     | 39:LH:51:LYS:HG3   | 2.20                     | 0.42              |
| 46:La:79:TRP:HB3   | 46:La:87:ARG:HH11  | 1.84                     | 0.42              |
| 49:LD:82:GLU:OE1   | 49:LD:108:ARG:NH2  | 2.50                     | 0.42              |
| 49:LD:164:LYS:HG2  | 49:LD:195:HIS:CE1  | 2.55                     | 0.42              |
| 55:LU:24:ASP:OD2   | 55:LU:26:THR:OG1   | 2.37                     | 0.42              |
| 69:Lj:43:ARG:HG2   | 79:L5:21:G:H5'     | 2.02                     | 0.42              |
| 76:Pt:5:G:H2'      | 76:Pt:6:G:C8       | 2.55                     | 0.42              |
| 78:S2:674:C:H2'    | 78:S2:675:U:C6     | 2.54                     | 0.42              |
| 79:L5:1204:C:H2'   | 79:L5:1205:G:C8    | 2.55                     | 0.42              |
| 79:L5:4884:G:H2'   | 79:L5:4885:U:C6    | 2.55                     | 0.42              |
| 2:SA:81:ASN:OD1    | 2:SA:81:ASN:N      | 2.53                     | 0.42              |
| 4:SB:92:GLN:HG3    | 4:SB:97:LEU:HD11   | 2.02                     | 0.42              |
| 9:SE:197:ASN:HB2   | 9:SE:209:HIS:HB2   | 2.02                     | 0.42              |
| 19:SX:87:ASN:N     | 78:S2:618:C:OP1    | 2.51                     | 0.42              |
| 42:LO:76:PRO:HB3   | 42:LO:138:LEU:HG   | 2.02                     | 0.42              |
| 46:La:4:ARG:H      | 46:La:4:ARG:HG2    | 1.61                     | 0.42              |
| 73:Ln:2:ARG:NE     | 78:S2:1842:4AC:OP2 | 2.45                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 78:S2:677:G:N1     | 78:S2:1027:A:OP2    | 2.32                     | 0.42              |
| 78:S2:1293:A:N6    | 78:S2:1294:G:O6     | 2.52                     | 0.42              |
| 78:S2:1678:A2M:H1' | 78:S2:1678:A2M:HM'3 | 1.77                     | 0.42              |
| 79:L5:106:A:H2'    | 79:L5:107:G:O4'     | 2.20                     | 0.42              |
| 79:L5:381:U:O2     | 79:L5:385:A:N6      | 2.52                     | 0.42              |
| 79:L5:490:C:H2'    | 79:L5:491:G:C8      | 2.55                     | 0.42              |
| 79:L5:1475:G:H2'   | 79:L5:1476:C:C6     | 2.55                     | 0.42              |
| 79:L5:1699:A:N1    | 79:L5:1705:G:H4'    | 2.35                     | 0.42              |
| 79:L5:1763:C:H2'   | 79:L5:1764:G:C8     | 2.53                     | 0.42              |
| 79:L5:2693:G:H2'   | 79:L5:2694:G:N2     | 2.34                     | 0.42              |
| 79:L5:5030:U:H2'   | 79:L5:5031:G:H8     | 1.85                     | 0.42              |
| 3:LB:19:ARG:HB2    | 3:LB:234:ARG:NH2    | 2.35                     | 0.42              |
| 4:SB:146:ARG:HD3   | 4:SB:146:ARG:HA     | 1.87                     | 0.42              |
| 17:SK:52:LEU:HB3   | 17:SK:58:VAL:HG22   | 2.02                     | 0.42              |
| 18:SO:32:HIS:N     | 18:SO:43:HIS:O      | 2.50                     | 0.42              |
| 23:SN:55:ARG:HH22  | 32:Sb:51:GLN:NE2    | 2.18                     | 0.42              |
| 25:SR:82:ASP:OD2   | 25:SR:83:ASN:N      | 2.53                     | 0.42              |
| 47:LN:46:ASP:OD2   | 92:LN:421:HOH:O     | 2.21                     | 0.42              |
| 61:Lb:111:ARG:NH2  | 79:L5:1268:G:N7     | 2.67                     | 0.42              |
| 78:S2:85:A:H2'     | 78:S2:86:C:H6       | 1.84                     | 0.42              |
| 79:L5:173:C:H2'    | 79:L5:174:C:C6      | 2.55                     | 0.42              |
| 79:L5:1878:G:H2'   | 79:L5:1879:C:C6     | 2.54                     | 0.42              |
| 82:SG:147:LEU:HD23 | 82:SG:153:VAL:HG12  | 2.01                     | 0.42              |
| 3:LB:120:LYS:HZ2   | 79:L5:4578:G:H5''   | 1.85                     | 0.42              |
| 3:LB:200:ARG:HG2   | 3:LB:200:ARG:HH11   | 1.85                     | 0.42              |
| 5:L8:28:C:O2'      | 79:L5:1371:A:N1     | 2.47                     | 0.42              |
| 6:L7:27:G:N7       | 49:LD:58:ARG:NH1    | 2.61                     | 0.42              |
| 9:SE:51:ARG:HD3    | 9:SE:51:ARG:HA      | 1.88                     | 0.42              |
| 13:SW:50:PHE:HB3   | 13:SW:63:VAL:HG13   | 2.01                     | 0.42              |
| 21:SS:14:ARG:HA    | 21:SS:14:ARG:HD2    | 1.87                     | 0.42              |
| 37:LC:156:ASP:OD2  | 37:LC:255:SER:OG    | 2.31                     | 0.42              |
| 46:La:13:GLY:HA2   | 79:L5:1660:U:H3'    | 2.01                     | 0.42              |
| 92:La:345:HOH:O    | 79:L5:2282:A:OP2    | 2.22                     | 0.42              |
| 54:LP:96:LYS:HE2   | 54:LP:96:LYS:HB3    | 1.72                     | 0.42              |
| 61:Lb:64:ALA:HB1   | 61:Lb:68:ARG:CZ     | 2.50                     | 0.42              |
| 62:LF:213:LEU:O    | 79:L5:2072:C:O2'    | 2.35                     | 0.42              |
| 70:Lk:12:LEU:HB3   | 70:Lk:16:ARG:HH12   | 1.85                     | 0.42              |
| 78:S2:77:A:H2      | 82:SG:175:LYS:HG3   | 1.85                     | 0.42              |
| 78:S2:656:G:H5'    | 78:S2:662:G:N2      | 2.35                     | 0.42              |
| 79:L5:2424:OMG:H1' | 79:L5:2424:OMG:HM23 | 1.82                     | 0.42              |
| 3:LB:96:PRO:HD3    | 42:LO:156:LEU:HD12  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:L7:3:C:H2'      | 6:L7:4:U:C6        | 2.55                     | 0.42              |
| 6:L7:69:U:H2'     | 6:L7:70:G:H8       | 1.85                     | 0.42              |
| 15:SQ:126:ARG:HD3 | 15:SQ:126:ARG:HA   | 1.81                     | 0.42              |
| 17:SK:42:ASN:O    | 17:SK:46:MET:HG3   | 2.20                     | 0.42              |
| 52:LS:115:ALA:HB2 | 79:L5:2060:G:N2    | 2.35                     | 0.42              |
| 54:LP:30:ARG:HD2  | 54:LP:63:TYR:HE1   | 1.85                     | 0.42              |
| 55:LU:31:ASP:OD2  | 55:LU:114:TYR:OH   | 2.29                     | 0.42              |
| 71:L1:48:LYS:HD2  | 71:L1:48:LYS:HA    | 1.74                     | 0.42              |
| 78:S2:388:U:H2'   | 78:S2:389:A:C8     | 2.53                     | 0.42              |
| 78:S2:440:G:OP1   | 78:S2:1798:C:O2'   | 2.34                     | 0.42              |
| 78:S2:568:C:H2'   | 78:S2:569:A:H8     | 1.84                     | 0.42              |
| 78:S2:903:A:H2'   | 78:S2:904:A:C8     | 2.54                     | 0.42              |
| 78:S2:1217:A:H2'  | 78:S2:1218:C:C6    | 2.55                     | 0.42              |
| 78:S2:1457:U:H2'  | 78:S2:1458:G:H8    | 1.84                     | 0.42              |
| 78:S2:1458:G:H2'  | 78:S2:1459:G:H8    | 1.85                     | 0.42              |
| 78:S2:1746:U:H5'' | 82:SG:33:ALA:HB3   | 2.02                     | 0.42              |
| 79:L5:926:G:H2'   | 79:L5:927:G:C8     | 2.53                     | 0.42              |
| 79:L5:2264:C:H2'  | 79:L5:2265:G:O4'   | 2.20                     | 0.42              |
| 79:L5:4069:U:H2'  | 79:L5:4070:U:C6    | 2.55                     | 0.42              |
| 79:L5:4460:U:H2'  | 79:L5:4461:C:C6    | 2.55                     | 0.42              |
| 1:LA:20:VAL:HG12  | 1:LA:23:ARG:HD2    | 2.01                     | 0.41              |
| 1:LA:126:LEU:HD13 | 1:LA:150:LEU:HD21  | 2.02                     | 0.41              |
| 7:SD:70:THR:HA    | 7:SD:86:LEU:HD13   | 2.01                     | 0.41              |
| 7:SD:74:GLN:NE2   | 7:SD:79:PHE:O      | 2.52                     | 0.41              |
| 10:SC:94:ILE:HG21 | 10:SC:162:ILE:HD12 | 2.01                     | 0.41              |
| 11:SF:40:ALA:HB1  | 11:SF:45:TYR:CG    | 2.55                     | 0.41              |
| 12:SH:115:LYS:HE2 | 78:S2:868:G:C2     | 2.54                     | 0.41              |
| 36:Sg:217:MET:HE2 | 36:Sg:219:TRP:CZ2  | 2.55                     | 0.41              |
| 50:LQ:64:SER:OG   | 50:LQ:89:ASP:OD2   | 2.36                     | 0.41              |
| 51:LR:128:LYS:NZ  | 92:LR:322:HOH:O    | 2.52                     | 0.41              |
| 70:Lk:12:LEU:HB3  | 70:Lk:16:ARG:NH1   | 2.35                     | 0.41              |
| 75:Lp:9:GLY:O     | 79:L5:1553:A:O2'   | 2.33                     | 0.41              |
| 76:Pt:39:A:O2'    | 78:S2:1058:A:OP1   | 2.33                     | 0.41              |
| 78:S2:300:U:H2'   | 78:S2:301:A:C8     | 2.55                     | 0.41              |
| 78:S2:959:G:H1'   | 78:S2:964:A:N6     | 2.34                     | 0.41              |
| 78:S2:1183:A:H2'  | 78:S2:1184:G:H8    | 1.85                     | 0.41              |
| 78:S2:1856:C:H2'  | 78:S2:1857:G:C8    | 2.55                     | 0.41              |
| 79:L5:186:G:H2'   | 79:L5:187:U:H4'    | 2.01                     | 0.41              |
| 79:L5:446:C:H2'   | 79:L5:447:C:C6     | 2.54                     | 0.41              |
| 79:L5:3910:C:O2'  | 79:L5:4196:OMG:N2  | 2.53                     | 0.41              |
| 79:L5:3948:C:O2   | 79:L5:4065:G:N1    | 2.43                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:LB:238:LYS:HE2    | 3:LB:238:LYS:HB2    | 1.75                     | 0.41              |
| 8:SJ:5:ARG:HG3      | 78:S2:38:A:OP1      | 2.20                     | 0.41              |
| 14:SI:36:THR:HG21   | 14:SI:60:LEU:HD12   | 2.02                     | 0.41              |
| 23:SN:125:LEU:HD12  | 23:SN:125:LEU:HA    | 1.88                     | 0.41              |
| 26:SP:130:ARG:HG3   | 26:SP:130:ARG:HH11  | 1.85                     | 0.41              |
| 37:LC:152:LEU:HD21  | 37:LC:174:LEU:HB3   | 2.02                     | 0.41              |
| 39:LH:180:TYR:OH    | 72:Lm:90:ASN:ND2    | 2.50                     | 0.41              |
| 40:LE:57:TYR:HB2    | 40:LE:62:MET:HG2    | 2.01                     | 0.41              |
| 45:LM:114:LYS:HD3   | 79:L5:4929:C:H5''   | 2.02                     | 0.41              |
| 68:Li:45:ARG:NH1    | 68:Li:49:GLY:O      | 2.41                     | 0.41              |
| 78:S2:1786:U:H2'    | 78:S2:1787:G:H8     | 1.84                     | 0.41              |
| 78:S2:1797:U:H2'    | 78:S2:1798:C:C6     | 2.55                     | 0.41              |
| 78:S2:1810:U:H2'    | 78:S2:1811:C:C6     | 2.55                     | 0.41              |
| 79:L5:1399:G:H2'    | 79:L5:1400:G:C8     | 2.55                     | 0.41              |
| 79:L5:1751:A:H2'    | 79:L5:1752:G:H8     | 1.84                     | 0.41              |
| 79:L5:1895:G:H2'    | 79:L5:1896:A:O4'    | 2.20                     | 0.41              |
| 79:L5:2744:A:H2'    | 79:L5:2745:A:C8     | 2.55                     | 0.41              |
| 79:L5:3925:OMU:H1'  | 79:L5:3925:OMU:HM23 | 1.62                     | 0.41              |
| 7:SD:58:VAL:HG12    | 7:SD:66:ILE:HD13    | 2.03                     | 0.41              |
| 38:LJ:174:ILE:HD13  | 38:LJ:174:ILE:HA    | 1.87                     | 0.41              |
| 41:LG:53:ARG:HE     | 41:LG:53:ARG:HB3    | 1.43                     | 0.41              |
| 59:Lr:65:LYS:NZ     | 92:Lr:322:HOH:O     | 2.51                     | 0.41              |
| 76:Pt:10:G:N2       | 76:Pt:27:G:H1'      | 2.36                     | 0.41              |
| 78:S2:1360:U:O2'    | 78:S2:1379:A:OP2    | 2.31                     | 0.41              |
| 78:S2:1562:C:H2'    | 78:S2:1563:G:C8     | 2.54                     | 0.41              |
| 78:S2:1804:OMU:HM23 | 78:S2:1804:OMU:H1'  | 1.73                     | 0.41              |
| 79:L5:498:C:H2'     | 79:L5:499:G:C8      | 2.55                     | 0.41              |
| 79:L5:2020:U:H2'    | 79:L5:2021:G:C8     | 2.50                     | 0.41              |
| 79:L5:2413:U:H2'    | 79:L5:2414:G:H8     | 1.85                     | 0.41              |
| 79:L5:3868:G:H22    | 79:L5:3900:G:H1'    | 1.84                     | 0.41              |
| 79:L5:3911:C:H2'    | 79:L5:3912:U:C6     | 2.55                     | 0.41              |
| 79:L5:4195:G:C8     | 79:L5:4442:PSU:H5'  | 2.55                     | 0.41              |
| 8:SJ:38:ARG:HA      | 34:Se:105:ARG:HB2   | 2.03                     | 0.41              |
| 21:SS:84:LEU:HD12   | 21:SS:95:TYR:HB3    | 2.02                     | 0.41              |
| 36:Sg:207:CYS:O     | 36:Sg:219:TRP:HD1   | 2.03                     | 0.41              |
| 37:LC:41:HIS:CE1    | 37:LC:45:ARG:HD3    | 2.55                     | 0.41              |
| 52:LS:2:LYS:HE3     | 79:L5:2062:C:H5'    | 2.01                     | 0.41              |
| 56:LX:74:TYR:OH     | 60:Lh:22:ASP:OD1    | 2.35                     | 0.41              |
| 62:LF:60:GLU:O      | 62:LF:64:MET:HG3    | 2.21                     | 0.41              |
| 78:S2:1706:G:H2'    | 78:S2:1707:U:H6     | 1.86                     | 0.41              |
| 79:L5:699:C:H2'     | 79:L5:700:G:C8      | 2.53                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 79:L5:2029:A:H2'   | 79:L5:2030:A:C8     | 2.56                     | 0.41              |
| 79:L5:2362:U:H2'   | 79:L5:2363:A2M:H8   | 2.02                     | 0.41              |
| 79:L5:4071:U:H2'   | 79:L5:4072:C:C6     | 2.55                     | 0.41              |
| 79:L5:4313:A:H2'   | 79:L5:4314:C:O4'    | 2.20                     | 0.41              |
| 1:LA:17:ARG:HE     | 1:LA:17:ARG:HB2     | 1.61                     | 0.41              |
| 13:SW:12:LYS:HD3   | 13:SW:12:LYS:HA     | 1.78                     | 0.41              |
| 29:SY:120:THR:OG1  | 78:S2:151:C:OP1     | 2.31                     | 0.41              |
| 37:LC:163:LYS:HE3  | 37:LC:163:LYS:HB3   | 1.94                     | 0.41              |
| 65:Le:104:SER:OG   | 65:Le:107:ASN:ND2   | 2.54                     | 0.41              |
| 78:S2:1446:A:O2'   | 78:S2:1447:OMG:H5'' | 2.21                     | 0.41              |
| 78:S2:1648:G:O2'   | 78:S2:1674:G:O6     | 2.35                     | 0.41              |
| 78:S2:1809:A:H2'   | 78:S2:1810:U:C6     | 2.55                     | 0.41              |
| 78:S2:1823:A:H2'   | 78:S2:1824:A:C8     | 2.55                     | 0.41              |
| 79:L5:434:A:H2'    | 79:L5:435:A:O4'     | 2.20                     | 0.41              |
| 79:L5:734:G:C2     | 79:L5:735:G:C8      | 3.08                     | 0.41              |
| 79:L5:1086:C:H2'   | 79:L5:1087:A:C8     | 2.55                     | 0.41              |
| 79:L5:2503:G:H21   | 79:L5:4084:G:H5'    | 1.85                     | 0.41              |
| 79:L5:3893:C:H2'   | 79:L5:3894:A:H8     | 1.84                     | 0.41              |
| 79:L5:4499:OMG:C2  | 79:L5:4529:G:H1'    | 2.56                     | 0.41              |
| 82:SG:2:LYS:HD3    | 82:SG:15:LEU:HD21   | 2.02                     | 0.41              |
| 2:SA:77:ILE:HD12   | 2:SA:122:LEU:HD11   | 2.03                     | 0.41              |
| 3:LB:163:ILE:HG22  | 3:LB:180:LEU:HD22   | 2.02                     | 0.41              |
| 6:L7:119:U:H2'     | 49:LD:261:VAL:HG21  | 2.01                     | 0.41              |
| 9:SE:62:LYS:HB3    | 9:SE:62:LYS:HE2     | 1.84                     | 0.41              |
| 15:SQ:113:ILE:HD13 | 15:SQ:113:ILE:HA    | 1.94                     | 0.41              |
| 15:SQ:116:ASP:C    | 15:SQ:118:THR:H     | 2.29                     | 0.41              |
| 41:LG:53:ARG:HD3   | 79:L5:4161:G:C6     | 2.56                     | 0.41              |
| 42:LO:8:VAL:HG12   | 42:LO:117:ARG:HG3   | 2.02                     | 0.41              |
| 48:LI:171:TRP:O    | 48:LI:174:THR:OG1   | 2.30                     | 0.41              |
| 51:LR:7:GLN:HG2    | 51:LR:32:ILE:HG22   | 2.03                     | 0.41              |
| 58:LZ:5:MET:O      | 58:LZ:28:ASN:ND2    | 2.53                     | 0.41              |
| 58:LZ:47:ASP:N     | 58:LZ:69:LYS:O      | 2.50                     | 0.41              |
| 60:Lh:82:ASP:OD1   | 60:Lh:82:ASP:N      | 2.40                     | 0.41              |
| 78:S2:964:A:H2'    | 78:S2:965:U:H6      | 1.86                     | 0.41              |
| 78:S2:1374:C:H2'   | 78:S2:1375:G:O4'    | 2.20                     | 0.41              |
| 79:L5:272:U:H2'    | 79:L5:273:U:C6      | 2.56                     | 0.41              |
| 79:L5:1661:C:H2'   | 79:L5:1662:C:H6     | 1.85                     | 0.41              |
| 79:L5:1754:U:H1'   | 79:L5:1755:C:H5     | 1.85                     | 0.41              |
| 79:L5:1762:C:H2'   | 79:L5:1763:C:C6     | 2.56                     | 0.41              |
| 79:L5:1916:G:N3    | 79:L5:2067:C:O2'    | 2.51                     | 0.41              |
| 1:LA:233:ARG:HB2   | 79:L5:4184:G:H5'    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:LB:115:LYS:NZ    | 3:LB:129:ALA:O     | 2.46                     | 0.41              |
| 4:SB:38:MET:H      | 4:SB:38:MET:HG3    | 1.65                     | 0.41              |
| 5:L8:144:U:H2'     | 5:L8:145:C:H6      | 1.85                     | 0.41              |
| 6:L7:58:A:H2'      | 6:L7:59:G:C8       | 2.56                     | 0.41              |
| 6:L7:83:A:H4'      | 62:LF:224:THR:HB   | 2.02                     | 0.41              |
| 7:SD:160:SER:OG    | 78:S2:1386:A:OP2   | 2.32                     | 0.41              |
| 15:SQ:112:LEU:HD22 | 15:SQ:119:LEU:HD13 | 2.03                     | 0.41              |
| 37:LC:83:GLY:O     | 79:L5:367:C:O2'    | 2.27                     | 0.41              |
| 38:LJ:63:ARG:HE    | 38:LJ:63:ARG:HB2   | 1.73                     | 0.41              |
| 41:LG:197:LYS:HG2  | 79:L5:6:C:H5''     | 2.02                     | 0.41              |
| 49:LD:200:MET:HB3  | 49:LD:237:GLU:HG3  | 2.02                     | 0.41              |
| 53:LT:71:ALA:HB3   | 79:L5:4313:A:H4'   | 2.02                     | 0.41              |
| 58:LZ:35:ASP:OD2   | 58:LZ:35:ASP:N     | 2.54                     | 0.41              |
| 58:LZ:60:LYS:HE2   | 58:LZ:60:LYS:HB3   | 1.82                     | 0.41              |
| 61:Lb:120:ARG:HA   | 61:Lb:121:PRO:HD3  | 1.92                     | 0.41              |
| 67:Lg:44:SER:OG    | 67:Lg:46:CYS:SG    | 2.75                     | 0.41              |
| 78:S2:76:U:H5'     | 78:S2:77:A:OP2     | 2.21                     | 0.41              |
| 78:S2:160:U:O2'    | 78:S2:162:C:O5'    | 2.38                     | 0.41              |
| 78:S2:443:U:H2'    | 78:S2:444:G:O4'    | 2.20                     | 0.41              |
| 79:L5:86:U:H2'     | 79:L5:87:A:C8      | 2.54                     | 0.41              |
| 79:L5:323:C:H2'    | 79:L5:324:A:H8     | 1.86                     | 0.41              |
| 79:L5:2079:G:H2'   | 79:L5:2080:U:H6    | 1.85                     | 0.41              |
| 79:L5:2448:G:H2'   | 79:L5:2449:A:C8    | 2.55                     | 0.41              |
| 8:SJ:18:ARG:NH2    | 78:S2:4:C:O2'      | 2.50                     | 0.41              |
| 9:SE:22:LYS:HG3    | 9:SE:23:LEU:HD23   | 2.03                     | 0.41              |
| 26:SP:96:VAL:HG13  | 26:SP:120:SER:HB2  | 2.02                     | 0.41              |
| 44:LV:106:VAL:HG12 | 44:LV:112:MET:HG2  | 2.02                     | 0.41              |
| 49:LD:153:THR:HG21 | 79:L5:4323:A:C6    | 2.56                     | 0.41              |
| 49:LD:193:GLU:OE2  | 49:LD:196:ARG:NH1  | 2.53                     | 0.41              |
| 53:LT:102:ARG:HD2  | 53:LT:102:ARG:HA   | 1.77                     | 0.41              |
| 53:LT:124:THR:OG1  | 53:LT:125:TRP:N    | 2.54                     | 0.41              |
| 68:Li:35:LYS:HB3   | 68:Li:35:LYS:HE3   | 1.68                     | 0.41              |
| 76:Pt:5:G:H2'      | 76:Pt:6:G:H8       | 1.84                     | 0.41              |
| 78:S2:656:G:H21    | 78:S2:663:C:H5''   | 1.86                     | 0.41              |
| 78:S2:1179:G:N2    | 78:S2:1182:A:OP2   | 2.37                     | 0.41              |
| 79:L5:288:G:H2'    | 79:L5:289:C:C6     | 2.55                     | 0.41              |
| 79:L5:1967:A:H2'   | 79:L5:1968:G:H8    | 1.86                     | 0.41              |
| 79:L5:2844:A:O2'   | 79:L5:4631:G:H4'   | 2.20                     | 0.41              |
| 79:L5:2884:G:H2'   | 79:L5:2885:A:C8    | 2.55                     | 0.41              |
| 79:L5:3732:A:H2'   | 79:L5:3733:A:C8    | 2.56                     | 0.41              |
| 79:L5:4239:A:H2'   | 79:L5:4240:G:H8    | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:L5:4458:C:H2'   | 79:L5:4459:U:C6    | 2.55                     | 0.41              |
| 1:LA:175:ILE:H     | 1:LA:175:ILE:HG13  | 1.66                     | 0.41              |
| 3:LB:33:PRO:HA     | 3:LB:351:LEU:HD23  | 2.02                     | 0.41              |
| 5:L8:89:U:H2'      | 5:L8:90:C:C6       | 2.55                     | 0.41              |
| 7:SD:161:GLY:HA3   | 78:S2:1388:A:H61   | 1.85                     | 0.41              |
| 7:SD:218:LEU:HA    | 7:SD:219:PRO:HD3   | 1.96                     | 0.41              |
| 14:SI:80:ASP:OD2   | 14:SI:81:VAL:N     | 2.50                     | 0.41              |
| 14:SI:103:LEU:HD23 | 14:SI:103:LEU:HA   | 1.94                     | 0.41              |
| 19:SX:40:PRO:HA    | 19:SX:79:LYS:HD2   | 2.02                     | 0.41              |
| 21:SS:120:HIS:NE2  | 26:SP:123:TYR:OH   | 2.42                     | 0.41              |
| 26:SP:84:ILE:HG12  | 26:SP:115:TYR:HE1  | 1.85                     | 0.41              |
| 26:SP:134:GLY:O    | 78:S2:1235:G:O2'   | 2.37                     | 0.41              |
| 37:LC:339:THR:OG1  | 37:LC:342:ARG:NH2  | 2.54                     | 0.41              |
| 40:LE:121:VAL:HG21 | 79:L5:702:U:H5'    | 2.02                     | 0.41              |
| 41:LG:147:VAL:HG13 | 41:LG:179:VAL:HG21 | 2.03                     | 0.41              |
| 44:LV:43:LYS:HG3   | 44:LV:60:MET:HG2   | 2.02                     | 0.41              |
| 46:La:3:SER:OG     | 79:L5:2344:U:O4    | 2.37                     | 0.41              |
| 51:LR:145:LEU:HD23 | 51:LR:145:LEU:HA   | 1.91                     | 0.41              |
| 53:LT:14:MET:HE3   | 53:LT:14:MET:HB2   | 1.88                     | 0.41              |
| 57:LY:55:VAL:HG12  | 57:LY:106:ILE:HA   | 2.03                     | 0.41              |
| 57:LY:132:LYS:HE3  | 79:L5:247:G:H5'    | 2.01                     | 0.41              |
| 78:S2:28:U:H2'     | 78:S2:29:G:C8      | 2.56                     | 0.41              |
| 78:S2:454:U:H2'    | 78:S2:455:A:C8     | 2.55                     | 0.41              |
| 78:S2:553:U:H3'    | 78:S2:555:A:H5''   | 2.03                     | 0.41              |
| 78:S2:563:G:O2'    | 78:S2:564:A:H8     | 2.04                     | 0.41              |
| 78:S2:863:PSU:H2'  | 78:S2:864:A:H8     | 1.85                     | 0.41              |
| 78:S2:1292:C:N4    | 78:S2:1302:G:O6    | 2.51                     | 0.41              |
| 78:S2:1628:C:H2'   | 78:S2:1629:C:C6    | 2.56                     | 0.41              |
| 78:S2:1633:A:H2'   | 78:S2:1634:A:C8    | 2.56                     | 0.41              |
| 78:S2:1705:C:H2'   | 78:S2:1706:G:C8    | 2.56                     | 0.41              |
| 79:L5:459:C:H2'    | 79:L5:460:C:C6     | 2.56                     | 0.41              |
| 79:L5:1317:U:H2'   | 79:L5:1318:C:C6    | 2.55                     | 0.41              |
| 79:L5:1661:C:H2'   | 79:L5:1662:C:C6    | 2.56                     | 0.41              |
| 79:L5:4378:A:O2'   | 79:L5:4379:A:H2'   | 2.20                     | 0.41              |
| 79:L5:4887:C:H2'   | 79:L5:4888:U:O4'   | 2.21                     | 0.41              |
| 2:SA:25:LEU:HD23   | 2:SA:25:LEU:HA     | 1.86                     | 0.41              |
| 5:L8:130:C:H2'     | 5:L8:131:G:C8      | 2.55                     | 0.41              |
| 6:L7:15:C:H2'      | 6:L7:16:A:H8       | 1.86                     | 0.41              |
| 14:SI:153:LYS:HB2  | 14:SI:153:LYS:HE2  | 1.81                     | 0.41              |
| 26:SP:108:LYS:HB2  | 26:SP:111:MET:HG3  | 2.02                     | 0.41              |
| 36:Sg:122:SER:HB3  | 36:Sg:132:TRP:HE1  | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LE:258:LEU:HD23 | 40:LE:258:LEU:HA   | 1.89                     | 0.41              |
| 51:LR:44:LEU:HD22  | 51:LR:49:LEU:HD22  | 2.02                     | 0.41              |
| 62:LF:94:ARG:NH1   | 62:LF:114:LEU:O    | 2.54                     | 0.41              |
| 62:LF:136:VAL:O    | 62:LF:140:ILE:HG12 | 2.21                     | 0.41              |
| 78:S2:1253:A:OP2   | 78:S2:1526:G:N2    | 2.40                     | 0.41              |
| 79:L5:1693:U:H2'   | 79:L5:1694:C:O4'   | 2.20                     | 0.41              |
| 79:L5:2884:G:H2'   | 79:L5:2885:A:H8    | 1.85                     | 0.41              |
| 79:L5:3934:G:H2'   | 79:L5:3935:C:C6    | 2.56                     | 0.41              |
| 79:L5:5037:U:H2'   | 79:L5:5038:A:C8    | 2.55                     | 0.41              |
| 3:LB:194:LEU:HA    | 3:LB:194:LEU:HD23  | 1.78                     | 0.40              |
| 4:SB:44:ILE:HG23   | 4:SB:69:VAL:HG11   | 2.02                     | 0.40              |
| 5:L8:39:G:O2'      | 5:L8:104:A:N1      | 2.54                     | 0.40              |
| 7:SD:145:GLN:O     | 78:S2:1332:A:O2'   | 2.36                     | 0.40              |
| 10:SC:110:MET:HA   | 10:SC:111:PRO:HD3  | 1.89                     | 0.40              |
| 32:Sb:15:GLU:HG3   | 32:Sb:23:ARG:HG2   | 2.02                     | 0.40              |
| 36:Sg:35:SER:OG    | 36:Sg:36:ARG:N     | 2.54                     | 0.40              |
| 41:LG:136:LEU:HD12 | 41:LG:136:LEU:HA   | 1.92                     | 0.40              |
| 43:LL:91:ALA:HB1   | 43:LL:96:ILE:HB    | 2.03                     | 0.40              |
| 43:LL:129:ARG:HD3  | 79:L5:173:C:OP1    | 2.21                     | 0.40              |
| 43:LL:150:LEU:HD12 | 43:LL:150:LEU:HA   | 1.92                     | 0.40              |
| 44:LV:90:ARG:NH2   | 44:LV:96:LEU:HD22  | 2.36                     | 0.40              |
| 49:LD:106:ALA:HB2  | 49:LD:166:ALA:HA   | 2.02                     | 0.40              |
| 49:LD:211:LEU:HB3  | 49:LD:219:TYR:HB2  | 2.04                     | 0.40              |
| 56:LX:90:ILE:HG22  | 56:LX:147:LEU:HD22 | 2.03                     | 0.40              |
| 58:LZ:36:ARG:NH1   | 79:L5:2580:U:OP1   | 2.40                     | 0.40              |
| 60:Lh:105:LYS:HE3  | 60:Lh:105:LYS:HB2  | 1.87                     | 0.40              |
| 73:Ln:4:LYS:HB2    | 78:S2:1842:4AC:OP2 | 2.20                     | 0.40              |
| 78:S2:96:C:O2      | 78:S2:473:A:O2'    | 2.35                     | 0.40              |
| 78:S2:102:A:H4'    | 78:S2:104:A:C8     | 2.56                     | 0.40              |
| 78:S2:836:G:H21    | 78:S2:837:A:H3'    | 1.85                     | 0.40              |
| 78:S2:1712:A:H2'   | 78:S2:1713:C:C6    | 2.56                     | 0.40              |
| 79:L5:23:C:H2'     | 79:L5:24:G:O4'     | 2.21                     | 0.40              |
| 79:L5:426:A:H2'    | 79:L5:427:A:C8     | 2.56                     | 0.40              |
| 79:L5:1346:C:H2'   | 79:L5:1347:G:C8    | 2.56                     | 0.40              |
| 79:L5:3619:G:H22   | 79:L5:3624:A:H1'   | 1.85                     | 0.40              |
| 79:L5:4178:A:H2'   | 79:L5:4179:G:C8    | 2.56                     | 0.40              |
| 3:LB:189:THR:OG1   | 3:LB:192:GLU:HG3   | 2.21                     | 0.40              |
| 9:SE:89:VAL:HG13   | 9:SE:114:ILE:HD11  | 2.03                     | 0.40              |
| 12:SH:41:ARG:HE    | 12:SH:41:ARG:HB3   | 1.62                     | 0.40              |
| 14:SI:160:SER:HA   | 14:SI:163:GLU:HB2  | 2.03                     | 0.40              |
| 15:SQ:139:ALA:HB2  | 78:S2:1650:A:H5''  | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:SS:38:ARG:HB3   | 27:ST:45:LEU:HD21  | 2.03                     | 0.40              |
| 36:Sg:29:ASP:N     | 36:Sg:29:ASP:OD2   | 2.54                     | 0.40              |
| 39:LH:52:LYS:HD3   | 39:LH:52:LYS:HA    | 1.86                     | 0.40              |
| 40:LE:242:ILE:H    | 40:LE:242:ILE:HG12 | 1.72                     | 0.40              |
| 44:LV:13:LYS:NZ    | 44:LV:59:ASP:OD2   | 2.54                     | 0.40              |
| 45:LM:104:MET:HE3  | 45:LM:109:ARG:HG2  | 2.02                     | 0.40              |
| 51:LR:98:ARG:NH1   | 51:LR:132:PHE:O    | 2.54                     | 0.40              |
| 52:LS:94:TYR:OH    | 52:LS:96:GLU:OE2   | 2.34                     | 0.40              |
| 54:LP:61:ARG:NH2   | 54:LP:76:TRP:HB3   | 2.36                     | 0.40              |
| 92:LX:205:HOH:O    | 79:L5:2782:U:O4    | 2.21                     | 0.40              |
| 62:LF:57:TYR:HD2   | 62:LF:188:GLU:HB3  | 1.86                     | 0.40              |
| 78:S2:454:U:H2'    | 78:S2:455:A:H8     | 1.86                     | 0.40              |
| 78:S2:929:G:N2     | 78:S2:1104:G:H4'   | 2.36                     | 0.40              |
| 78:S2:962:A:N1     | 78:S2:1055:A:O2'   | 2.53                     | 0.40              |
| 78:S2:1856:C:H2'   | 78:S2:1857:G:H8    | 1.86                     | 0.40              |
| 79:L5:365:U:H2'    | 79:L5:366:A:H8     | 1.85                     | 0.40              |
| 79:L5:1416:G:H2'   | 79:L5:1417:C:C6    | 2.57                     | 0.40              |
| 79:L5:2484:A:H2'   | 79:L5:2485:U:C6    | 2.56                     | 0.40              |
| 79:L5:3663:A:N6    | 79:L5:4168:G:HO2'  | 2.18                     | 0.40              |
| 79:L5:4238:G:H2'   | 79:L5:4239:A:C8    | 2.57                     | 0.40              |
| 79:L5:4454:G:O2'   | 79:L5:4500:PSU:O2' | 2.29                     | 0.40              |
| 3:LB:354:GLN:HB3   | 3:LB:359:ALA:HB1   | 2.02                     | 0.40              |
| 4:SB:9:LEU:H       | 4:SB:9:LEU:HD12    | 1.87                     | 0.40              |
| 4:SB:140:VAL:HG12  | 4:SB:213:ARG:HB2   | 2.03                     | 0.40              |
| 14:SI:104:ILE:HD13 | 14:SI:173:ALA:HB2  | 2.04                     | 0.40              |
| 21:SS:101:ASN:O    | 21:SS:105:ASN:ND2  | 2.54                     | 0.40              |
| 26:SP:133:ILE:HD13 | 26:SP:133:ILE:HA   | 1.87                     | 0.40              |
| 29:SY:8:ARG:HG2    | 29:SY:8:ARG:NH1    | 2.36                     | 0.40              |
| 37:LC:97:ARG:HG3   | 79:L5:354:U:H1'    | 2.03                     | 0.40              |
| 37:LC:201:ARG:HE   | 37:LC:201:ARG:HB3  | 1.69                     | 0.40              |
| 37:LC:275:SER:N    | 79:L5:1376:C:OP1   | 2.42                     | 0.40              |
| 63:Lc:90:ARG:NH1   | 92:Lc:302:HOH:O    | 2.52                     | 0.40              |
| 78:S2:635:G:H2'    | 78:S2:636:C:C6     | 2.57                     | 0.40              |
| 78:S2:1405:A:H2'   | 78:S2:1406:G:O4'   | 2.21                     | 0.40              |
| 78:S2:1845:A:H2'   | 78:S2:1846:G:H8    | 1.85                     | 0.40              |
| 79:L5:318:A:H2'    | 79:L5:319:A:C8     | 2.56                     | 0.40              |
| 79:L5:1405:C:H2'   | 79:L5:1406:G:C8    | 2.56                     | 0.40              |
| 79:L5:1701:A:H5'   | 79:L5:2096:G:N2    | 2.36                     | 0.40              |
| 79:L5:2508:PSU:H2' | 79:L5:2509:C:C6    | 2.56                     | 0.40              |
| 79:L5:3907:G:H1'   | 79:L5:3908[A]:A:N7 | 2.37                     | 0.40              |
| 79:L5:4068:U:H2'   | 79:L5:4069:U:C6    | 2.56                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:L5:4749:C:H2'   | 79:L5:4750:G:O4'   | 2.22                     | 0.40              |
| 1:LA:199:VAL:HG21  | 79:L5:1631:A:N7    | 2.36                     | 0.40              |
| 2:SA:34:MET:HE3    | 2:SA:34:MET:HB3    | 1.84                     | 0.40              |
| 3:LB:245:HIC:HB2   | 79:L5:4525:C:H5''  | 2.04                     | 0.40              |
| 18:SO:59:GLY:HA2   | 18:SO:68:GLU:HG2   | 2.03                     | 0.40              |
| 21:SS:127:TRP:HE3  | 21:SS:129:LEU:HD12 | 1.86                     | 0.40              |
| 23:SN:124:ARG:HD2  | 78:S2:677:G:OP1    | 2.21                     | 0.40              |
| 24:SL:82:MET:HG3   | 24:SL:85:THR:O     | 2.22                     | 0.40              |
| 24:SL:104:LYS:HB3  | 24:SL:104:LYS:HE3  | 1.93                     | 0.40              |
| 36:Sg:227:LEU:HB3  | 36:Sg:228:TYR:CD1  | 2.56                     | 0.40              |
| 39:LH:20:LEU:HD23  | 39:LH:20:LEU:HA    | 1.94                     | 0.40              |
| 40:LE:162:VAL:HG11 | 40:LE:184:VAL:HG11 | 2.04                     | 0.40              |
| 42:LO:78:ARG:HA    | 42:LO:78:ARG:HD2   | 1.95                     | 0.40              |
| 70:Lk:17:ARG:HB3   | 70:Lk:19:ASP:OD2   | 2.22                     | 0.40              |
| 76:Pt:19:G:N1      | 76:Pt:56:PSU:O4    | 2.46                     | 0.40              |
| 78:S2:300:U:H2'    | 78:S2:301:A:H8     | 1.87                     | 0.40              |
| 78:S2:312:G:OP2    | 82:SG:195:LYS:NZ   | 2.54                     | 0.40              |
| 78:S2:509:OMG:HM23 | 78:S2:509:OMG:H1'  | 1.85                     | 0.40              |
| 78:S2:639:C:H2'    | 78:S2:640:A:C8     | 2.57                     | 0.40              |
| 78:S2:1291:A:OP2   | 78:S2:1302:G:O2'   | 2.37                     | 0.40              |
| 79:L5:3870:C:H2'   | 79:L5:3871:A:C8    | 2.57                     | 0.40              |
| 5:L8:75:OMG:HM23   | 5:L8:75:OMG:H1'    | 1.84                     | 0.40              |
| 5:L8:115:G:H2'     | 5:L8:116:C:H6      | 1.85                     | 0.40              |
| 5:L8:115:G:H2'     | 5:L8:116:C:C6      | 2.57                     | 0.40              |
| 8:SJ:134:HIS:ND1   | 8:SJ:163:SER:HB2   | 2.36                     | 0.40              |
| 11:SF:119:SER:OG   | 11:SF:189:ALA:HB1  | 2.21                     | 0.40              |
| 13:SW:76:SER:OG    | 78:S2:1159:G:OP1   | 2.37                     | 0.40              |
| 15:SQ:117:ARG:HD3  | 15:SQ:117:ARG:O    | 2.21                     | 0.40              |
| 41:LG:165:GLU:HG2  | 47:LN:11:TRP:NE1   | 2.35                     | 0.40              |
| 41:LG:193:LEU:HD12 | 41:LG:193:LEU:HA   | 1.89                     | 0.40              |
| 78:S2:531:A:H2'    | 78:S2:532:C:H6     | 1.86                     | 0.40              |
| 78:S2:1220:A:H2'   | 78:S2:1221:G:O4'   | 2.21                     | 0.40              |
| 79:L5:1431:C:H2'   | 79:L5:1432:G:O4'   | 2.21                     | 0.40              |
| 79:L5:2508:PSU:H2' | 79:L5:2509:C:H6    | 1.86                     | 0.40              |
| 79:L5:3711:A:N6    | 79:L5:3736:A:OP1   | 2.54                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | LA    | 248/257 (96%) | 238 (96%) | 10 (4%) | 0        | 100         | 100 |
| 2   | SA    | 215/294 (73%) | 211 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 3   | LB    | 391/403 (97%) | 383 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 4   | SB    | 217/264 (82%) | 212 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 7   | SD    | 222/243 (91%) | 211 (95%) | 11 (5%) | 0        | 100         | 100 |
| 8   | SJ    | 177/194 (91%) | 170 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 9   | SE    | 256/263 (97%) | 253 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 10  | SC    | 219/293 (75%) | 211 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 11  | SF    | 178/204 (87%) | 174 (98%) | 3 (2%)  | 1 (1%)   | 21          | 53  |
| 12  | SH    | 179/194 (92%) | 171 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 13  | SW    | 127/130 (98%) | 123 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 14  | SI    | 204/208 (98%) | 196 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 15  | SQ    | 138/146 (94%) | 134 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 16  | SU    | 99/119 (83%)  | 95 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 17  | SK    | 94/165 (57%)  | 91 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 18  | SO    | 132/151 (87%) | 125 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 19  | SX    | 137/143 (96%) | 131 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 20  | SM    | 38/132 (29%)  | 37 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 21  | SS    | 146/152 (96%) | 141 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 22  | Sd    | 53/56 (95%)   | 52 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 23  | SN    | 149/151 (99%) | 144 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 24  | SL    | 138/158 (87%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 25  | SR    | 130/135 (96%) | 125 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 26  | SP    | 126/145 (87%) | 120 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 27  | ST    | 141/145 (97%) | 135 (96%) | 6 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 28  | SV    | 80/82 (98%)   | 78 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 29  | SY    | 120/133 (90%) | 119 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 30  | SZ    | 73/125 (58%)  | 70 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 31  | Sa    | 97/115 (84%)  | 96 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 32  | Sb    | 81/84 (96%)   | 75 (93%)   | 6 (7%)  | 0        | 100         | 100 |
| 33  | Sc    | 56/69 (81%)   | 54 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 34  | Se    | 44/133 (33%)  | 42 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 35  | Sf    | 33/156 (21%)  | 30 (91%)   | 3 (9%)  | 0        | 100         | 100 |
| 36  | Sg    | 309/317 (98%) | 282 (91%)  | 27 (9%) | 0        | 100         | 100 |
| 37  | LC    | 364/427 (85%) | 357 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 38  | LJ    | 168/178 (94%) | 167 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 39  | LH    | 188/192 (98%) | 184 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 40  | LE    | 217/288 (75%) | 207 (95%)  | 10 (5%) | 0        | 100         | 100 |
| 41  | LG    | 230/266 (86%) | 223 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 42  | LO    | 200/203 (98%) | 199 (100%) | 0       | 1 (0%)   | 24          | 58  |
| 43  | LL    | 205/211 (97%) | 201 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 44  | LV    | 128/140 (91%) | 126 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 45  | LM    | 134/215 (62%) | 128 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 46  | La    | 144/148 (97%) | 136 (94%)  | 8 (6%)  | 0        | 100         | 100 |
| 47  | LN    | 201/204 (98%) | 195 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 48  | LI    | 199/214 (93%) | 196 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 49  | LD    | 292/297 (98%) | 285 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 50  | LQ    | 185/188 (98%) | 181 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 51  | LR    | 185/196 (94%) | 181 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 52  | LS    | 174/176 (99%) | 172 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 53  | LT    | 159/160 (99%) | 155 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 54  | LP    | 152/184 (83%) | 149 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 55  | LU    | 97/128 (76%)  | 93 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 56  | LX    | 116/156 (74%) | 113 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 57  | LY    | 131/145 (90%) | 130 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 58  | LZ    | 134/136 (98%) | 129 (96%)  | 5 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 59  | Lr    | 123/136 (90%)     | 121 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 60  | Lh    | 120/123 (98%)     | 117 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 61  | Lb    | 106/159 (67%)     | 104 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 62  | LF    | 225/248 (91%)     | 218 (97%)   | 6 (3%)   | 1 (0%)   | 30          | 62  |
| 63  | Lc    | 97/115 (84%)      | 95 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 64  | Ld    | 105/125 (84%)     | 105 (100%)  | 0        | 0        | 100         | 100 |
| 65  | Le    | 127/135 (94%)     | 125 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 66  | Lf    | 107/110 (97%)     | 107 (100%)  | 0        | 0        | 100         | 100 |
| 67  | Lg    | 110/117 (94%)     | 109 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 68  | Li    | 100/105 (95%)     | 99 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 69  | Lj    | 85/97 (88%)       | 85 (100%)   | 0        | 0        | 100         | 100 |
| 70  | Lk    | 67/70 (96%)       | 66 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 71  | Ll    | 48/51 (94%)       | 48 (100%)   | 0        | 0        | 100         | 100 |
| 72  | Lm    | 50/128 (39%)      | 49 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 73  | Ln    | 23/25 (92%)       | 23 (100%)   | 0        | 0        | 100         | 100 |
| 74  | Lo    | 103/106 (97%)     | 100 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 75  | Lp    | 90/92 (98%)       | 85 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 81  | LW    | 60/157 (38%)      | 60 (100%)   | 0        | 0        | 100         | 100 |
| 82  | SG    | 216/249 (87%)     | 211 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| All | All   | 11012/12759 (86%) | 10698 (97%) | 311 (3%) | 3 (0%)   | 100         | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | LO    | 186 | GLU  |
| 11  | SF    | 80  | GLY  |
| 62  | LF    | 197 | 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   | LA    | 191/198 (96%)  | 188 (98%)  | 3 (2%)   | 55          | 78  |
| 2   | SA    | 175/242 (72%)  | 171 (98%)  | 4 (2%)   | 44          | 72  |
| 3   | LB    | 309/348 (89%)  | 306 (99%)  | 3 (1%)   | 68          | 83  |
| 4   | SB    | 192/231 (83%)  | 186 (97%)  | 6 (3%)   | 35          | 66  |
| 7   | SD    | 160/202 (79%)  | 157 (98%)  | 3 (2%)   | 50          | 75  |
| 8   | SJ    | 155/168 (92%)  | 154 (99%)  | 1 (1%)   | 78          | 88  |
| 9   | SE    | 220/225 (98%)  | 218 (99%)  | 2 (1%)   | 70          | 85  |
| 10  | SC    | 177/225 (79%)  | 174 (98%)  | 3 (2%)   | 53          | 77  |
| 11  | SF    | 152/170 (89%)  | 151 (99%)  | 1 (1%)   | 76          | 87  |
| 12  | SH    | 147/174 (84%)  | 144 (98%)  | 3 (2%)   | 48          | 75  |
| 13  | SW    | 111/113 (98%)  | 110 (99%)  | 1 (1%)   | 70          | 85  |
| 14  | SI    | 168/180 (93%)  | 168 (100%) | 0        | 100         | 100 |
| 15  | SQ    | 114/121 (94%)  | 112 (98%)  | 2 (2%)   | 51          | 76  |
| 16  | SU    | 7/107 (6%)     | 6 (86%)    | 1 (14%)  | 3           | 14  |
| 17  | SK    | 51/136 (38%)   | 51 (100%)  | 0        | 100         | 100 |
| 18  | SO    | 101/119 (85%)  | 100 (99%)  | 1 (1%)   | 68          | 83  |
| 19  | SX    | 111/114 (97%)  | 109 (98%)  | 2 (2%)   | 51          | 76  |
| 21  | SS    | 120/132 (91%)  | 117 (98%)  | 3 (2%)   | 42          | 71  |
| 22  | Sd    | 48/49 (98%)    | 45 (94%)   | 3 (6%)   | 16          | 46  |
| 23  | SN    | 131/131 (100%) | 127 (97%)  | 4 (3%)   | 35          | 66  |
| 24  | SL    | 124/142 (87%)  | 121 (98%)  | 3 (2%)   | 43          | 72  |
| 25  | SR    | 109/122 (89%)  | 105 (96%)  | 4 (4%)   | 30          | 62  |
| 26  | SP    | 114/130 (88%)  | 112 (98%)  | 2 (2%)   | 51          | 76  |
| 27  | ST    | 84/115 (73%)   | 82 (98%)   | 2 (2%)   | 43          | 72  |
| 28  | SV    | 66/66 (100%)   | 65 (98%)   | 1 (2%)   | 57          | 79  |
| 29  | SY    | 98/115 (85%)   | 97 (99%)   | 1 (1%)   | 68          | 83  |
| 30  | SZ    | 61/103 (59%)   | 59 (97%)   | 2 (3%)   | 33          | 65  |
| 31  | Sa    | 84/98 (86%)    | 82 (98%)   | 2 (2%)   | 43          | 72  |
| 32  | Sb    | 73/76 (96%)    | 71 (97%)   | 2 (3%)   | 39          | 70  |
| 33  | Sc    | 51/62 (82%)    | 47 (92%)   | 4 (8%)   | 11          | 37  |
| 34  | Se    | 36/104 (35%)   | 35 (97%)   | 1 (3%)   | 38          | 69  |
| 35  | Sf    | 8/140 (6%)     | 8 (100%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 36  | Sg    | 260/275 (94%)  | 247 (95%)  | 13 (5%)  | 22          | 54  |
| 37  | LC    | 305/348 (88%)  | 299 (98%)  | 6 (2%)   | 48          | 75  |
| 38  | LJ    | 141/149 (95%)  | 136 (96%)  | 5 (4%)   | 32          | 63  |
| 39  | LH    | 169/171 (99%)  | 165 (98%)  | 4 (2%)   | 43          | 72  |
| 40  | LE    | 196/252 (78%)  | 194 (99%)  | 2 (1%)   | 68          | 83  |
| 41  | LG    | 195/223 (87%)  | 186 (95%)  | 9 (5%)   | 24          | 57  |
| 42  | LO    | 170/174 (98%)  | 168 (99%)  | 2 (1%)   | 63          | 82  |
| 43  | LL    | 170/177 (96%)  | 168 (99%)  | 2 (1%)   | 63          | 82  |
| 44  | LV    | 100/107 (94%)  | 98 (98%)   | 2 (2%)   | 48          | 75  |
| 45  | LM    | 115/161 (71%)  | 110 (96%)  | 5 (4%)   | 26          | 58  |
| 46  | La    | 116/120 (97%)  | 115 (99%)  | 1 (1%)   | 70          | 85  |
| 47  | LN    | 171/172 (99%)  | 167 (98%)  | 4 (2%)   | 44          | 72  |
| 48  | LI    | 173/181 (96%)  | 170 (98%)  | 3 (2%)   | 53          | 77  |
| 49  | LD    | 247/250 (99%)  | 239 (97%)  | 8 (3%)   | 34          | 65  |
| 50  | LQ    | 164/165 (99%)  | 161 (98%)  | 3 (2%)   | 51          | 76  |
| 51  | LR    | 144/175 (82%)  | 142 (99%)  | 2 (1%)   | 59          | 80  |
| 52  | LS    | 157/157 (100%) | 151 (96%)  | 6 (4%)   | 29          | 61  |
| 53  | LT    | 141/140 (101%) | 136 (96%)  | 5 (4%)   | 32          | 63  |
| 54  | LP    | 135/163 (83%)  | 134 (99%)  | 1 (1%)   | 76          | 87  |
| 55  | LU    | 88/115 (76%)   | 84 (96%)   | 4 (4%)   | 24          | 57  |
| 56  | LX    | 106/133 (80%)  | 104 (98%)  | 2 (2%)   | 50          | 75  |
| 57  | LY    | 122/135 (90%)  | 118 (97%)  | 4 (3%)   | 33          | 65  |
| 58  | LZ    | 118/118 (100%) | 115 (98%)  | 3 (2%)   | 42          | 71  |
| 59  | Lr    | 109/120 (91%)  | 107 (98%)  | 2 (2%)   | 51          | 76  |
| 60  | Lh    | 109/110 (99%)  | 108 (99%)  | 1 (1%)   | 70          | 85  |
| 61  | Lb    | 90/125 (72%)   | 89 (99%)   | 1 (1%)   | 65          | 82  |
| 62  | LF    | 196/215 (91%)  | 196 (100%) | 0        | 100         | 100 |
| 63  | Lc    | 84/97 (87%)    | 82 (98%)   | 2 (2%)   | 43          | 72  |
| 64  | Ld    | 20/110 (18%)   | 15 (75%)   | 5 (25%)  | 0           | 3   |
| 65  | Le    | 115/121 (95%)  | 113 (98%)  | 2 (2%)   | 53          | 77  |
| 66  | Lf    | 88/89 (99%)    | 84 (96%)   | 4 (4%)   | 24          | 57  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 67  | Lg    | 92/100 (92%)     | 89 (97%)   | 3 (3%)   | 33          | 65  |
| 68  | Li    | 83/89 (93%)      | 82 (99%)   | 1 (1%)   | 63          | 82  |
| 69  | Lj    | 74/80 (92%)      | 72 (97%)   | 2 (3%)   | 39          | 70  |
| 70  | Lk    | 64/65 (98%)      | 62 (97%)   | 2 (3%)   | 35          | 66  |
| 71  | Ll    | 46/48 (96%)      | 44 (96%)   | 2 (4%)   | 26          | 58  |
| 72  | Lm    | 48/115 (42%)     | 47 (98%)   | 1 (2%)   | 47          | 74  |
| 73  | Ln    | 24/24 (100%)     | 24 (100%)  | 0        | 100         | 100 |
| 74  | Lo    | 93/93 (100%)     | 92 (99%)   | 1 (1%)   | 65          | 82  |
| 75  | Lp    | 75/75 (100%)     | 75 (100%)  | 0        | 100         | 100 |
| 81  | LW    | 54/126 (43%)     | 52 (96%)   | 2 (4%)   | 30          | 62  |
| 82  | SG    | 167/218 (77%)    | 161 (96%)  | 6 (4%)   | 31          | 63  |
| All | All   | 9082/10739 (85%) | 8879 (98%) | 203 (2%) | 45          | 73  |

All (203) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | LA    | 77  | ILE  |
| 1   | LA    | 104 | VAL  |
| 1   | LA    | 243 | THR  |
| 2   | SA    | 28  | THR  |
| 2   | SA    | 87  | VAL  |
| 2   | SA    | 152 | SER  |
| 2   | SA    | 190 | SER  |
| 3   | LB    | 41  | VAL  |
| 3   | LB    | 317 | LEU  |
| 3   | LB    | 381 | THR  |
| 4   | SB    | 22  | VAL  |
| 4   | SB    | 38  | MET  |
| 4   | SB    | 57  | ILE  |
| 4   | SB    | 108 | ASP  |
| 4   | SB    | 154 | SER  |
| 4   | SB    | 172 | MET  |
| 7   | SD    | 94  | ARG  |
| 7   | SD    | 179 | GLN  |
| 7   | SD    | 217 | ILE  |
| 8   | SJ    | 15  | THR  |
| 9   | SE    | 117 | GLU  |
| 9   | SE    | 220 | THR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 10  | SC    | 102    | LEU  |
| 10  | SC    | 221    | ASP  |
| 10  | SC    | 254    | ASP  |
| 11  | SF    | 37     | ASP  |
| 12  | SH    | 8      | ILE  |
| 12  | SH    | 10     | LYS  |
| 12  | SH    | 32     | MET  |
| 13  | SW    | 105    | THR  |
| 15  | SQ    | 29     | ASN  |
| 15  | SQ    | 49     | TYR  |
| 16  | SU    | 111    | GLU  |
| 18  | SO    | 36     | SER  |
| 19  | SX    | 105    | PHE  |
| 19  | SX    | 115    | ILE  |
| 21  | SS    | 83     | PHE  |
| 21  | SS    | 99     | LEU  |
| 21  | SS    | 118    | ARG  |
| 22  | Sd    | 18     | SER  |
| 22  | Sd    | 36     | LEU  |
| 22  | Sd    | 53     | ILE  |
| 23  | SN    | 123[A] | HIS  |
| 23  | SN    | 123[B] | HIS  |
| 23  | SN    | 144    | SER  |
| 23  | SN    | 145    | THR  |
| 24  | SL    | 7      | GLU  |
| 24  | SL    | 19     | ASN  |
| 24  | SL    | 74     | SER  |
| 25  | SR    | 22     | THR  |
| 25  | SR    | 80     | ARG  |
| 25  | SR    | 85     | VAL  |
| 25  | SR    | 105    | MET  |
| 26  | SP    | 21     | ASP  |
| 26  | SP    | 121    | ILE  |
| 27  | ST    | 4      | VAL  |
| 27  | ST    | 87     | VAL  |
| 28  | SV    | 10     | ASP  |
| 29  | SY    | 24     | VAL  |
| 30  | SZ    | 50     | PHE  |
| 30  | SZ    | 51     | ASP  |
| 31  | Sa    | 76     | SER  |
| 31  | Sa    | 88     | SER  |
| 32  | Sb    | 26     | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | Sb    | 34  | ASP  |
| 33  | Sc    | 18  | LEU  |
| 33  | Sc    | 21  | THR  |
| 33  | Sc    | 40  | ARG  |
| 33  | Sc    | 50  | VAL  |
| 34  | Se    | 79  | SER  |
| 36  | Sg    | 66  | VAL  |
| 36  | Sg    | 69  | VAL  |
| 36  | Sg    | 70  | VAL  |
| 36  | Sg    | 105 | THR  |
| 36  | Sg    | 107 | ASP  |
| 36  | Sg    | 113 | PHE  |
| 36  | Sg    | 135 | LEU  |
| 36  | Sg    | 142 | VAL  |
| 36  | Sg    | 173 | LEU  |
| 36  | Sg    | 199 | THR  |
| 36  | Sg    | 213 | ASP  |
| 36  | Sg    | 287 | THR  |
| 36  | Sg    | 309 | VAL  |
| 37  | LC    | 94  | ASN  |
| 37  | LC    | 95  | MET  |
| 37  | LC    | 107 | THR  |
| 37  | LC    | 124 | ILE  |
| 37  | LC    | 198 | ASN  |
| 37  | LC    | 266 | THR  |
| 38  | LJ    | 34  | THR  |
| 38  | LJ    | 39  | VAL  |
| 38  | LJ    | 58  | ARG  |
| 38  | LJ    | 74  | VAL  |
| 38  | LJ    | 174 | ILE  |
| 39  | LH    | 9   | THR  |
| 39  | LH    | 46  | SER  |
| 39  | LH    | 104 | VAL  |
| 39  | LH    | 188 | GLN  |
| 40  | LE    | 107 | VAL  |
| 40  | LE    | 286 | LEU  |
| 41  | LG    | 33  | GLU  |
| 41  | LG    | 53  | ARG  |
| 41  | LG    | 95  | LEU  |
| 41  | LG    | 111 | LYS  |
| 41  | LG    | 198 | THR  |
| 41  | LG    | 201 | THR  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 41  | LG    | 231   | ASP  |
| 41  | LG    | 253   | LEU  |
| 41  | LG    | 257   | LYS  |
| 42  | LO    | 125   | LYS  |
| 42  | LO    | 179   | LYS  |
| 43  | LL    | 59    | VAL  |
| 43  | LL    | 107   | THR  |
| 44  | LV    | 101   | ASN  |
| 44  | LV    | 123   | LYS  |
| 45  | LM    | 28    | VAL  |
| 45  | LM    | 32    | ASP  |
| 45  | LM    | 104   | MET  |
| 45  | LM    | 112   | VAL  |
| 45  | LM    | 125   | ASN  |
| 46  | La    | 15    | VAL  |
| 47  | LN    | 18    | VAL  |
| 47  | LN    | 60    | VAL  |
| 47  | LN    | 66    | VAL  |
| 47  | LN    | 197   | THR  |
| 48  | LI    | 28    | ASP  |
| 48  | LI    | 66    | GLU  |
| 48  | LI    | 123   | GLN  |
| 49  | LD    | 3     | PHE  |
| 49  | LD    | 36    | LEU  |
| 49  | LD    | 75    | VAL  |
| 49  | LD    | 90    | VAL  |
| 49  | LD    | 116   | ASP  |
| 49  | LD    | 129   | GLU  |
| 49  | LD    | 261   | VAL  |
| 49  | LD    | 267   | ASN  |
| 50  | LQ    | 45    | GLN  |
| 50  | LQ    | 76    | GLU  |
| 50  | LQ    | 183   | SER  |
| 51  | LR    | 37    | SER  |
| 51  | LR    | 122   | SER  |
| 52  | LS    | 16    | CYS  |
| 52  | LS    | 48    | VAL  |
| 52  | LS    | 75    | VAL  |
| 52  | LS    | 85    | ASP  |
| 52  | LS    | 129   | VAL  |
| 52  | LS    | 158   | VAL  |
| 53  | LT    | 36[A] | LYS  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 53  | LT    | 36[B]  | LYS  |
| 53  | LT    | 127    | GLN  |
| 53  | LT    | 142[A] | ARG  |
| 53  | LT    | 142[B] | ARG  |
| 54  | LP    | 75     | GLN  |
| 55  | LU    | 62     | THR  |
| 55  | LU    | 63     | ILE  |
| 55  | LU    | 76     | VAL  |
| 55  | LU    | 109    | SER  |
| 56  | LX    | 120    | ASP  |
| 56  | LX    | 147    | LEU  |
| 57  | LY    | 67     | ILE  |
| 57  | LY    | 94     | THR  |
| 57  | LY    | 105    | VAL  |
| 57  | LY    | 112    | ASP  |
| 58  | LZ    | 35     | ASP  |
| 58  | LZ    | 100    | VAL  |
| 58  | LZ    | 109    | LYS  |
| 59  | Lr    | 48     | THR  |
| 59  | Lr    | 124    | VAL  |
| 60  | Lh    | 104    | THR  |
| 61  | Lb    | 9      | THR  |
| 63  | Lc    | 94     | LEU  |
| 63  | Lc    | 103    | ASP  |
| 64  | Ld    | 112    | THR  |
| 64  | Ld    | 118    | GLN  |
| 64  | Ld    | 119    | THR  |
| 64  | Ld    | 120    | VAL  |
| 64  | Ld    | 122    | VAL  |
| 65  | Le    | 53     | ILE  |
| 65  | Le    | 81     | ASN  |
| 66  | Lf    | 7      | SER  |
| 66  | Lf    | 37     | ASP  |
| 66  | Lf    | 46     | ARG  |
| 66  | Lf    | 90     | SER  |
| 67  | Lg    | 28     | ASN  |
| 67  | Lg    | 48     | VAL  |
| 67  | Lg    | 82     | MET  |
| 68  | Li    | 35     | LYS  |
| 69  | Lj    | 66[A]  | HIS  |
| 69  | Lj    | 66[B]  | HIS  |
| 70  | Lk    | 12     | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70  | Lk    | 56  | LEU  |
| 71  | Ll    | 11  | ARG  |
| 71  | Ll    | 23  | ILE  |
| 72  | Lm    | 127 | VAL  |
| 74  | Lo    | 25  | GLN  |
| 81  | LW    | 9   | SER  |
| 81  | LW    | 53  | VAL  |
| 82  | SG    | 15  | LEU  |
| 82  | SG    | 127 | THR  |
| 82  | SG    | 163 | ASN  |
| 82  | SG    | 181 | THR  |
| 82  | SG    | 186 | GLN  |
| 82  | SG    | 217 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | LA    | 22  | HIS  |
| 2   | SA    | 9   | GLN  |
| 2   | SA    | 50  | ASN  |
| 2   | SA    | 164 | ASN  |
| 3   | LB    | 121 | ASN  |
| 3   | LB    | 145 | GLN  |
| 4   | SB    | 149 | GLN  |
| 7   | SD    | 57  | ASN  |
| 7   | SD    | 101 | GLN  |
| 7   | SD    | 159 | HIS  |
| 8   | SJ    | 177 | ASN  |
| 9   | SE    | 50  | ASN  |
| 9   | SE    | 67  | GLN  |
| 9   | SE    | 157 | ASN  |
| 9   | SE    | 224 | ASN  |
| 10  | SC    | 136 | HIS  |
| 10  | SC    | 172 | ASN  |
| 11  | SF    | 79  | HIS  |
| 11  | SF    | 186 | ASN  |
| 12  | SH    | 33  | ASN  |
| 12  | SH    | 44  | ASN  |
| 12  | SH    | 112 | ASN  |
| 15  | SQ    | 11  | GLN  |
| 15  | SQ    | 86  | GLN  |
| 17  | SK    | 42  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | SS    | 19  | ASN  |
| 21  | SS    | 72  | GLN  |
| 22  | Sd    | 26  | ASN  |
| 24  | SL    | 141 | ASN  |
| 25  | SR    | 74  | GLN  |
| 28  | SV    | 33  | GLN  |
| 28  | SV    | 35  | ASN  |
| 29  | SY    | 89  | HIS  |
| 32  | Sb    | 26  | GLN  |
| 33  | Sc    | 29  | GLN  |
| 34  | Se    | 89  | GLN  |
| 36  | Sg    | 237 | ASN  |
| 37  | LC    | 38  | ASN  |
| 37  | LC    | 299 | GLN  |
| 37  | LC    | 317 | ASN  |
| 38  | LJ    | 42  | GLN  |
| 38  | LJ    | 167 | GLN  |
| 39  | LH    | 7   | ASN  |
| 39  | LH    | 102 | ASN  |
| 39  | LH    | 169 | ASN  |
| 40  | LE    | 167 | GLN  |
| 40  | LE    | 284 | HIS  |
| 41  | LG    | 141 | ASN  |
| 42  | LO    | 26  | GLN  |
| 42  | LO    | 46  | ASN  |
| 42  | LO    | 180 | GLN  |
| 43  | LL    | 19  | GLN  |
| 43  | LL    | 149 | GLN  |
| 45  | LM    | 20  | HIS  |
| 45  | LM    | 33  | GLN  |
| 45  | LM    | 34  | ASN  |
| 45  | LM    | 48  | GLN  |
| 47  | LN    | 15  | GLN  |
| 47  | LN    | 87  | HIS  |
| 47  | LN    | 99  | GLN  |
| 47  | LN    | 196 | ASN  |
| 50  | LQ    | 45  | GLN  |
| 51  | LR    | 40  | GLN  |
| 52  | LS    | 125 | GLN  |
| 54  | LP    | 97  | ASN  |
| 56  | LX    | 107 | HIS  |
| 57  | LY    | 96  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | Lr    | 4   | HIS  |
| 59  | Lr    | 30  | ASN  |
| 61  | Lb    | 6   | ASN  |
| 63  | Lc    | 19  | GLN  |
| 64  | Ld    | 118 | GLN  |
| 65  | Le    | 34  | ASN  |
| 65  | Le    | 107 | ASN  |
| 65  | Le    | 126 | ASN  |
| 66  | Lf    | 99  | HIS  |
| 68  | Li    | 15  | HIS  |
| 82  | SG    | 177 | GLN  |
| 82  | SG    | 186 | GLN  |
| 82  | SG    | 197 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 5   | L8    | 155/156 (99%)   | 22 (14%)          | 0               |
| 6   | L7    | 119/120 (99%)   | 7 (5%)            | 0               |
| 76  | Pt    | 76/77 (98%)     | 8 (10%)           | 0               |
| 77  | mR    | 6/27 (22%)      | 3 (50%)           | 0               |
| 78  | S2    | 1627/1869 (87%) | 264 (16%)         | 0               |
| 79  | L5    | 3504/5069 (69%) | 531 (15%)         | 5 (0%)          |
| 80  | Et    | 74/75 (98%)     | 17 (22%)          | 0               |
| All | All   | 5561/7393 (75%) | 852 (15%)         | 5 (0%)          |

All (852) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L8    | 16  | G    |
| 5   | L8    | 23  | C    |
| 5   | L8    | 34  | U    |
| 5   | L8    | 35  | C    |
| 5   | L8    | 51  | U    |
| 5   | L8    | 59  | A    |
| 5   | L8    | 62  | A    |
| 5   | L8    | 63  | U    |
| 5   | L8    | 80  | A    |
| 5   | L8    | 86  | U    |
| 5   | L8    | 87  | G    |
| 5   | L8    | 94  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L8    | 103 | A    |
| 5   | L8    | 105 | C    |
| 5   | L8    | 109 | C    |
| 5   | L8    | 110 | U    |
| 5   | L8    | 114 | G    |
| 5   | L8    | 123 | U    |
| 5   | L8    | 124 | U    |
| 5   | L8    | 125 | C    |
| 5   | L8    | 126 | C    |
| 5   | L8    | 127 | U    |
| 6   | L7    | 33  | U    |
| 6   | L7    | 53  | U    |
| 6   | L7    | 54  | A    |
| 6   | L7    | 64  | G    |
| 6   | L7    | 100 | A    |
| 6   | L7    | 110 | G    |
| 6   | L7    | 120 | U    |
| 76  | Pt    | 2   | G    |
| 76  | Pt    | 8   | 4SU  |
| 76  | Pt    | 9   | G    |
| 76  | Pt    | 16  | C    |
| 76  | Pt    | 19  | G    |
| 76  | Pt    | 21  | H2U  |
| 76  | Pt    | 71  | G    |
| 76  | Pt    | 77  | A    |
| 77  | mR    | 35  | G    |
| 77  | mR    | 36  | A    |
| 77  | mR    | 37  | A    |
| 78  | S2    | 3   | C    |
| 78  | S2    | 17  | C    |
| 78  | S2    | 33  | G    |
| 78  | S2    | 41  | G    |
| 78  | S2    | 42  | A    |
| 78  | S2    | 46  | A    |
| 78  | S2    | 56  | G    |
| 78  | S2    | 59  | U    |
| 78  | S2    | 62  | G    |
| 78  | S2    | 64  | A    |
| 78  | S2    | 65  | C    |
| 78  | S2    | 67  | C    |
| 78  | S2    | 68  | A    |
| 78  | S2    | 74  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | S2    | 75  | G    |
| 78  | S2    | 76  | U    |
| 78  | S2    | 79  | A    |
| 78  | S2    | 80  | G    |
| 78  | S2    | 92  | A    |
| 78  | S2    | 99  | A2M  |
| 78  | S2    | 103 | A    |
| 78  | S2    | 113 | G    |
| 78  | S2    | 114 | G    |
| 78  | S2    | 115 | U    |
| 78  | S2    | 126 | G    |
| 78  | S2    | 127 | C    |
| 78  | S2    | 129 | C    |
| 78  | S2    | 130 | G    |
| 78  | S2    | 140 | C    |
| 78  | S2    | 143 | U    |
| 78  | S2    | 147 | A    |
| 78  | S2    | 155 | G    |
| 78  | S2    | 160 | U    |
| 78  | S2    | 162 | C    |
| 78  | S2    | 168 | C    |
| 78  | S2    | 182 | C    |
| 78  | S2    | 183 | G    |
| 78  | S2    | 184 | G    |
| 78  | S2    | 215 | G    |
| 78  | S2    | 225 | G    |
| 78  | S2    | 302 | A    |
| 78  | S2    | 306 | C    |
| 78  | S2    | 309 | G    |
| 78  | S2    | 312 | G    |
| 78  | S2    | 319 | C    |
| 78  | S2    | 320 | G    |
| 78  | S2    | 323 | C    |
| 78  | S2    | 324 | C    |
| 78  | S2    | 327 | G    |
| 78  | S2    | 328 | U    |
| 78  | S2    | 335 | G    |
| 78  | S2    | 347 | G    |
| 78  | S2    | 361 | U    |
| 78  | S2    | 362 | C    |
| 78  | S2    | 364 | A    |
| 78  | S2    | 370 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | S2    | 385 | G    |
| 78  | S2    | 386 | C    |
| 78  | S2    | 407 | G    |
| 78  | S2    | 409 | C    |
| 78  | S2    | 436 | OMG  |
| 78  | S2    | 441 | C    |
| 78  | S2    | 448 | A    |
| 78  | S2    | 449 | A    |
| 78  | S2    | 450 | C    |
| 78  | S2    | 465 | A    |
| 78  | S2    | 466 | G    |
| 78  | S2    | 467 | G    |
| 78  | S2    | 471 | G    |
| 78  | S2    | 472 | C    |
| 78  | S2    | 474 | G    |
| 78  | S2    | 482 | G    |
| 78  | S2    | 487 | U    |
| 78  | S2    | 492 | C    |
| 78  | S2    | 493 | A    |
| 78  | S2    | 496 | C    |
| 78  | S2    | 508 | A    |
| 78  | S2    | 509 | OMG  |
| 78  | S2    | 512 | A2M  |
| 78  | S2    | 516 | A    |
| 78  | S2    | 525 | A    |
| 78  | S2    | 533 | A    |
| 78  | S2    | 534 | G    |
| 78  | S2    | 554 | A    |
| 78  | S2    | 555 | A    |
| 78  | S2    | 563 | G    |
| 78  | S2    | 564 | A    |
| 78  | S2    | 576 | A2M  |
| 78  | S2    | 587 | A    |
| 78  | S2    | 590 | A2M  |
| 78  | S2    | 591 | U    |
| 78  | S2    | 594 | A    |
| 78  | S2    | 604 | A    |
| 78  | S2    | 606 | G    |
| 78  | S2    | 608 | C    |
| 78  | S2    | 614 | C    |
| 78  | S2    | 617 | G    |
| 78  | S2    | 620 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | S2    | 628 | A    |
| 78  | S2    | 643 | A    |
| 78  | S2    | 644 | OMG  |
| 78  | S2    | 655 | A    |
| 78  | S2    | 660 | C    |
| 78  | S2    | 663 | C    |
| 78  | S2    | 668 | A2M  |
| 78  | S2    | 669 | A    |
| 78  | S2    | 671 | A    |
| 78  | S2    | 672 | A    |
| 78  | S2    | 673 | G    |
| 78  | S2    | 683 | OMG  |
| 78  | S2    | 688 | U    |
| 78  | S2    | 809 | A    |
| 78  | S2    | 821 | G    |
| 78  | S2    | 822 | PSU  |
| 78  | S2    | 827 | A    |
| 78  | S2    | 830 | A    |
| 78  | S2    | 831 | G    |
| 78  | S2    | 835 | C    |
| 78  | S2    | 836 | G    |
| 78  | S2    | 838 | G    |
| 78  | S2    | 847 | A    |
| 78  | S2    | 870 | A    |
| 78  | S2    | 871 | U    |
| 78  | S2    | 872 | A    |
| 78  | S2    | 878 | G    |
| 78  | S2    | 888 | U    |
| 78  | S2    | 889 | U    |
| 78  | S2    | 891 | G    |
| 78  | S2    | 892 | U    |
| 78  | S2    | 895 | G    |
| 78  | S2    | 896 | U    |
| 78  | S2    | 897 | U    |
| 78  | S2    | 903 | A    |
| 78  | S2    | 909 | G    |
| 78  | S2    | 913 | A    |
| 78  | S2    | 920 | A    |
| 78  | S2    | 922 | A    |
| 78  | S2    | 933 | G    |
| 78  | S2    | 943 | U    |
| 78  | S2    | 971 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 78  | S2    | 990  | A    |
| 78  | S2    | 992  | A    |
| 78  | S2    | 1002 | U    |
| 78  | S2    | 1017 | U    |
| 78  | S2    | 1023 | A    |
| 78  | S2    | 1027 | A    |
| 78  | S2    | 1045 | U    |
| 78  | S2    | 1055 | A    |
| 78  | S2    | 1061 | U    |
| 78  | S2    | 1062 | A    |
| 78  | S2    | 1080 | A    |
| 78  | S2    | 1083 | A    |
| 78  | S2    | 1085 | C    |
| 78  | S2    | 1089 | G    |
| 78  | S2    | 1107 | G    |
| 78  | S2    | 1109 | C    |
| 78  | S2    | 1115 | U    |
| 78  | S2    | 1121 | G    |
| 78  | S2    | 1133 | A    |
| 78  | S2    | 1138 | C    |
| 78  | S2    | 1153 | C    |
| 78  | S2    | 1154 | U    |
| 78  | S2    | 1157 | G    |
| 78  | S2    | 1172 | U    |
| 78  | S2    | 1183 | A    |
| 78  | S2    | 1188 | A    |
| 78  | S2    | 1195 | A    |
| 78  | S2    | 1207 | G    |
| 78  | S2    | 1208 | A    |
| 78  | S2    | 1215 | C    |
| 78  | S2    | 1224 | G    |
| 78  | S2    | 1242 | U    |
| 78  | S2    | 1243 | PSU  |
| 78  | S2    | 1251 | A    |
| 78  | S2    | 1253 | A    |
| 78  | S2    | 1256 | G    |
| 78  | S2    | 1257 | G    |
| 78  | S2    | 1259 | A    |
| 78  | S2    | 1271 | C    |
| 78  | S2    | 1274 | G    |
| 78  | S2    | 1275 | G    |
| 78  | S2    | 1285 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 78  | S2    | 1287 | A    |
| 78  | S2    | 1301 | A    |
| 78  | S2    | 1302 | G    |
| 78  | S2    | 1303 | C    |
| 78  | S2    | 1308 | U    |
| 78  | S2    | 1313 | A    |
| 78  | S2    | 1315 | U    |
| 78  | S2    | 1341 | C    |
| 78  | S2    | 1342 | U    |
| 78  | S2    | 1348 | G    |
| 78  | S2    | 1358 | U    |
| 78  | S2    | 1364 | U    |
| 78  | S2    | 1371 | U    |
| 78  | S2    | 1372 | U    |
| 78  | S2    | 1373 | C    |
| 78  | S2    | 1375 | G    |
| 78  | S2    | 1378 | A    |
| 78  | S2    | 1402 | A    |
| 78  | S2    | 1406 | G    |
| 78  | S2    | 1417 | C    |
| 78  | S2    | 1424 | G    |
| 78  | S2    | 1433 | C    |
| 78  | S2    | 1435 | C    |
| 78  | S2    | 1436 | C    |
| 78  | S2    | 1438 | A    |
| 78  | S2    | 1442 | U    |
| 78  | S2    | 1452 | A    |
| 78  | S2    | 1454 | A    |
| 78  | S2    | 1463 | U    |
| 78  | S2    | 1466 | G    |
| 78  | S2    | 1487 | A    |
| 78  | S2    | 1489 | A    |
| 78  | S2    | 1490 | OMG  |
| 78  | S2    | 1494 | U    |
| 78  | S2    | 1495 | G    |
| 78  | S2    | 1498 | A    |
| 78  | S2    | 1521 | C    |
| 78  | S2    | 1531 | A    |
| 78  | S2    | 1533 | A    |
| 78  | S2    | 1544 | C    |
| 78  | S2    | 1553 | C    |
| 78  | S2    | 1555 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 78  | S2    | 1557 | C    |
| 78  | S2    | 1560 | U    |
| 78  | S2    | 1563 | G    |
| 78  | S2    | 1579 | A    |
| 78  | S2    | 1580 | A    |
| 78  | S2    | 1585 | U    |
| 78  | S2    | 1586 | U    |
| 78  | S2    | 1587 | G    |
| 78  | S2    | 1588 | A    |
| 78  | S2    | 1601 | A    |
| 78  | S2    | 1606 | G    |
| 78  | S2    | 1621 | U    |
| 78  | S2    | 1623 | A    |
| 78  | S2    | 1639 | G7M  |
| 78  | S2    | 1648 | G    |
| 78  | S2    | 1654 | G    |
| 78  | S2    | 1661 | A    |
| 78  | S2    | 1664 | A    |
| 78  | S2    | 1665 | G    |
| 78  | S2    | 1671 | G    |
| 78  | S2    | 1680 | G    |
| 78  | S2    | 1695 | A    |
| 78  | S2    | 1698 | C    |
| 78  | S2    | 1699 | A    |
| 78  | S2    | 1721 | U    |
| 78  | S2    | 1722 | G    |
| 78  | S2    | 1744 | G    |
| 78  | S2    | 1784 | G    |
| 78  | S2    | 1825 | A    |
| 78  | S2    | 1826 | G    |
| 78  | S2    | 1829 | G    |
| 78  | S2    | 1831 | A    |
| 78  | S2    | 1835 | A    |
| 78  | S2    | 1838 | U    |
| 78  | S2    | 1849 | G    |
| 78  | S2    | 1851 | MA6  |
| 78  | S2    | 1861 | G    |
| 78  | S2    | 1862 | G    |
| 78  | S2    | 1863 | A    |
| 78  | S2    | 1865 | C    |
| 79  | L5    | 2    | G    |
| 79  | L5    | 21   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | L5    | 25  | A    |
| 79  | L5    | 39  | A    |
| 79  | L5    | 42  | A    |
| 79  | L5    | 48  | G    |
| 79  | L5    | 59  | A    |
| 79  | L5    | 64  | A    |
| 79  | L5    | 65  | A    |
| 79  | L5    | 66  | A    |
| 79  | L5    | 73  | A    |
| 79  | L5    | 74  | G    |
| 79  | L5    | 75  | G    |
| 79  | L5    | 85  | G    |
| 79  | L5    | 91  | G    |
| 79  | L5    | 108 | A    |
| 79  | L5    | 109 | G    |
| 79  | L5    | 110 | C    |
| 79  | L5    | 119 | G    |
| 79  | L5    | 120 | A    |
| 79  | L5    | 132 | G    |
| 79  | L5    | 133 | C    |
| 79  | L5    | 134 | G    |
| 79  | L5    | 136 | C    |
| 79  | L5    | 140 | G    |
| 79  | L5    | 141 | C    |
| 79  | L5    | 143 | C    |
| 79  | L5    | 159 | C    |
| 79  | L5    | 178 | C    |
| 79  | L5    | 181 | C    |
| 79  | L5    | 184 | U    |
| 79  | L5    | 186 | G    |
| 79  | L5    | 187 | U    |
| 79  | L5    | 189 | G    |
| 79  | L5    | 200 | U    |
| 79  | L5    | 209 | U    |
| 79  | L5    | 210 | C    |
| 79  | L5    | 234 | G    |
| 79  | L5    | 253 | G    |
| 79  | L5    | 257 | C    |
| 79  | L5    | 259 | C    |
| 79  | L5    | 262 | G    |
| 79  | L5    | 266 | C    |
| 79  | L5    | 278 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | L5    | 280 | G    |
| 79  | L5    | 297 | U    |
| 79  | L5    | 306 | A    |
| 79  | L5    | 315 | G    |
| 79  | L5    | 316 | U    |
| 79  | L5    | 328 | A    |
| 79  | L5    | 340 | C    |
| 79  | L5    | 387 | G    |
| 79  | L5    | 398 | A2M  |
| 79  | L5    | 409 | G    |
| 79  | L5    | 410 | A    |
| 79  | L5    | 412 | G    |
| 79  | L5    | 413 | G    |
| 79  | L5    | 440 | U    |
| 79  | L5    | 449 | C    |
| 79  | L5    | 450 | G    |
| 79  | L5    | 451 | C    |
| 79  | L5    | 453 | G    |
| 79  | L5    | 454 | U    |
| 79  | L5    | 461 | G    |
| 79  | L5    | 467 | U    |
| 79  | L5    | 496 | G    |
| 79  | L5    | 498 | C    |
| 79  | L5    | 504 | G    |
| 79  | L5    | 509 | A    |
| 79  | L5    | 510 | U    |
| 79  | L5    | 644 | G    |
| 79  | L5    | 669 | C    |
| 79  | L5    | 686 | A    |
| 79  | L5    | 687 | U    |
| 79  | L5    | 692 | A    |
| 79  | L5    | 696 | C    |
| 79  | L5    | 705 | G    |
| 79  | L5    | 708 | G    |
| 79  | L5    | 731 | G    |
| 79  | L5    | 738 | C    |
| 79  | L5    | 739 | G    |
| 79  | L5    | 740 | G    |
| 79  | L5    | 747 | A    |
| 79  | L5    | 757 | G    |
| 79  | L5    | 759 | G    |
| 79  | L5    | 904 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 915  | A    |
| 79  | L5    | 916  | C    |
| 79  | L5    | 917  | A    |
| 79  | L5    | 925  | C    |
| 79  | L5    | 926  | G    |
| 79  | L5    | 932  | A    |
| 79  | L5    | 933  | G    |
| 79  | L5    | 936  | C    |
| 79  | L5    | 937  | U    |
| 79  | L5    | 944  | A    |
| 79  | L5    | 945  | U    |
| 79  | L5    | 956  | A    |
| 79  | L5    | 958  | G    |
| 79  | L5    | 959  | G    |
| 79  | L5    | 960  | A    |
| 79  | L5    | 961  | G    |
| 79  | L5    | 962  | C    |
| 79  | L5    | 964  | A    |
| 79  | L5    | 965  | G    |
| 79  | L5    | 967  | C    |
| 79  | L5    | 968  | C    |
| 79  | L5    | 969  | C    |
| 79  | L5    | 970  | G    |
| 79  | L5    | 1070 | G    |
| 79  | L5    | 1072 | C    |
| 79  | L5    | 1092 | G    |
| 79  | L5    | 1094 | G    |
| 79  | L5    | 1101 | C    |
| 79  | L5    | 1168 | G    |
| 79  | L5    | 1171 | G    |
| 79  | L5    | 1182 | C    |
| 79  | L5    | 1183 | C    |
| 79  | L5    | 1187 | G    |
| 79  | L5    | 1199 | G    |
| 79  | L5    | 1200 | G    |
| 79  | L5    | 1211 | G    |
| 79  | L5    | 1215 | C    |
| 79  | L5    | 1216 | C    |
| 79  | L5    | 1241 | C    |
| 79  | L5    | 1253 | G    |
| 79  | L5    | 1254 | A    |
| 79  | L5    | 1257 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 1262 | G    |
| 79  | L5    | 1266 | G    |
| 79  | L5    | 1270 | A    |
| 79  | L5    | 1272 | C    |
| 79  | L5    | 1273 | G    |
| 79  | L5    | 1284 | G    |
| 79  | L5    | 1287 | G    |
| 79  | L5    | 1293 | G    |
| 79  | L5    | 1302 | U    |
| 79  | L5    | 1303 | A    |
| 79  | L5    | 1326 | A2M  |
| 79  | L5    | 1354 | A    |
| 79  | L5    | 1359 | G    |
| 79  | L5    | 1366 | G    |
| 79  | L5    | 1379 | C    |
| 79  | L5    | 1381 | U    |
| 79  | L5    | 1387 | A    |
| 79  | L5    | 1397 | A    |
| 79  | L5    | 1398 | A    |
| 79  | L5    | 1403 | G    |
| 79  | L5    | 1408 | G    |
| 79  | L5    | 1410 | U    |
| 79  | L5    | 1411 | C    |
| 79  | L5    | 1417 | C    |
| 79  | L5    | 1420 | A    |
| 79  | L5    | 1435 | G    |
| 79  | L5    | 1439 | C    |
| 79  | L5    | 1442 | C    |
| 79  | L5    | 1443 | A    |
| 79  | L5    | 1444 | G    |
| 79  | L5    | 1446 | C    |
| 79  | L5    | 1457 | G    |
| 79  | L5    | 1484 | G    |
| 79  | L5    | 1498 | G    |
| 79  | L5    | 1502 | G    |
| 79  | L5    | 1516 | G    |
| 79  | L5    | 1518 | A    |
| 79  | L5    | 1525 | A    |
| 79  | L5    | 1534 | A2M  |
| 79  | L5    | 1547 | A    |
| 79  | L5    | 1566 | C    |
| 79  | L5    | 1578 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 1591 | U    |
| 79  | L5    | 1596 | U    |
| 79  | L5    | 1612 | G    |
| 79  | L5    | 1614 | C    |
| 79  | L5    | 1624 | G    |
| 79  | L5    | 1625 | OMG  |
| 79  | L5    | 1631 | A    |
| 79  | L5    | 1633 | G    |
| 79  | L5    | 1634 | A    |
| 79  | L5    | 1638 | A    |
| 79  | L5    | 1640 | C    |
| 79  | L5    | 1641 | G    |
| 79  | L5    | 1642 | A    |
| 79  | L5    | 1654 | G    |
| 79  | L5    | 1661 | C    |
| 79  | L5    | 1676 | C    |
| 79  | L5    | 1677 | PSU  |
| 79  | L5    | 1680 | G    |
| 79  | L5    | 1691 | G    |
| 79  | L5    | 1699 | A    |
| 79  | L5    | 1701 | A    |
| 79  | L5    | 1703 | C    |
| 79  | L5    | 1721 | G    |
| 79  | L5    | 1741 | G    |
| 79  | L5    | 1755 | C    |
| 79  | L5    | 1761 | G    |
| 79  | L5    | 1766 | A    |
| 79  | L5    | 1767 | A    |
| 79  | L5    | 1768 | C    |
| 79  | L5    | 1785 | C    |
| 79  | L5    | 1787 | A    |
| 79  | L5    | 1789 | C    |
| 79  | L5    | 1792 | PSU  |
| 79  | L5    | 1804 | A    |
| 79  | L5    | 1806 | G    |
| 79  | L5    | 1815 | G    |
| 79  | L5    | 1821 | G    |
| 79  | L5    | 1833 | G    |
| 79  | L5    | 1834 | U    |
| 79  | L5    | 1836 | G    |
| 79  | L5    | 1837 | A    |
| 79  | L5    | 1842 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 1855 | G    |
| 79  | L5    | 1869 | G    |
| 79  | L5    | 1882 | U    |
| 79  | L5    | 1892 | A    |
| 79  | L5    | 1897 | A    |
| 79  | L5    | 1918 | U    |
| 79  | L5    | 1919 | G    |
| 79  | L5    | 1920 | C    |
| 79  | L5    | 1921 | C    |
| 79  | L5    | 1922 | G    |
| 79  | L5    | 1925 | G    |
| 79  | L5    | 1931 | C    |
| 79  | L5    | 1932 | A    |
| 79  | L5    | 1940 | G    |
| 79  | L5    | 1941 | A    |
| 79  | L5    | 1945 | G    |
| 79  | L5    | 1948 | G    |
| 79  | L5    | 1955 | G    |
| 79  | L5    | 1960 | A    |
| 79  | L5    | 1961 | G    |
| 79  | L5    | 1966 | C    |
| 79  | L5    | 1967 | A    |
| 79  | L5    | 1969 | G    |
| 79  | L5    | 2018 | C    |
| 79  | L5    | 2019 | C    |
| 79  | L5    | 2025 | A    |
| 79  | L5    | 2026 | A    |
| 79  | L5    | 2044 | U    |
| 79  | L5    | 2046 | G    |
| 79  | L5    | 2048 | U    |
| 79  | L5    | 2055 | G    |
| 79  | L5    | 2056 | G    |
| 79  | L5    | 2069 | A    |
| 79  | L5    | 2071 | A    |
| 79  | L5    | 2084 | C    |
| 79  | L5    | 2090 | U    |
| 79  | L5    | 2092 | G    |
| 79  | L5    | 2093 | A    |
| 79  | L5    | 2095 | A    |
| 79  | L5    | 2096 | G    |
| 79  | L5    | 2097 | U    |
| 79  | L5    | 2098 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 2099 | G    |
| 79  | L5    | 2100 | A    |
| 79  | L5    | 2102 | G    |
| 79  | L5    | 2105 | A    |
| 79  | L5    | 2106 | G    |
| 79  | L5    | 2107 | C    |
| 79  | L5    | 2289 | C    |
| 79  | L5    | 2300 | A    |
| 79  | L5    | 2301 | G    |
| 79  | L5    | 2306 | G    |
| 79  | L5    | 2313 | A    |
| 79  | L5    | 2316 | G    |
| 79  | L5    | 2331 | G    |
| 79  | L5    | 2333 | G    |
| 79  | L5    | 2345 | G    |
| 79  | L5    | 2348 | G    |
| 79  | L5    | 2351 | OMC  |
| 79  | L5    | 2360 | A    |
| 79  | L5    | 2395 | A    |
| 79  | L5    | 2397 | G    |
| 79  | L5    | 2402 | G    |
| 79  | L5    | 2408 | U    |
| 79  | L5    | 2417 | A    |
| 79  | L5    | 2421 | G    |
| 79  | L5    | 2450 | G    |
| 79  | L5    | 2469 | C    |
| 79  | L5    | 2470 | C    |
| 79  | L5    | 2471 | G    |
| 79  | L5    | 2474 | G    |
| 79  | L5    | 2478 | C    |
| 79  | L5    | 2483 | G    |
| 79  | L5    | 2488 | C    |
| 79  | L5    | 2492 | C    |
| 79  | L5    | 2496 | G    |
| 79  | L5    | 2503 | G    |
| 79  | L5    | 2504 | C    |
| 79  | L5    | 2505 | C    |
| 79  | L5    | 2506 | G    |
| 79  | L5    | 2513 | A    |
| 79  | L5    | 2519 | U    |
| 79  | L5    | 2520 | C    |
| 79  | L5    | 2554 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 2566 | G    |
| 79  | L5    | 2567 | G    |
| 79  | L5    | 2573 | A    |
| 79  | L5    | 2583 | C    |
| 79  | L5    | 2586 | G    |
| 79  | L5    | 2587 | A    |
| 79  | L5    | 2589 | C    |
| 79  | L5    | 2601 | A    |
| 79  | L5    | 2612 | G    |
| 79  | L5    | 2627 | C    |
| 79  | L5    | 2653 | C    |
| 79  | L5    | 2660 | A    |
| 79  | L5    | 2662 | G    |
| 79  | L5    | 2669 | C    |
| 79  | L5    | 2687 | U    |
| 79  | L5    | 2694 | G    |
| 79  | L5    | 2695 | A    |
| 79  | L5    | 2696 | A    |
| 79  | L5    | 2705 | G    |
| 79  | L5    | 2708 | U    |
| 79  | L5    | 2711 | G    |
| 79  | L5    | 2724 | G    |
| 79  | L5    | 2735 | G    |
| 79  | L5    | 2739 | C    |
| 79  | L5    | 2743 | A    |
| 79  | L5    | 2754 | G    |
| 79  | L5    | 2759 | G    |
| 79  | L5    | 2761 | U    |
| 79  | L5    | 2764 | A    |
| 79  | L5    | 2770 | C    |
| 79  | L5    | 2787 | A    |
| 79  | L5    | 2788 | U    |
| 79  | L5    | 2790 | U    |
| 79  | L5    | 2814 | C    |
| 79  | L5    | 2815 | A2M  |
| 79  | L5    | 2826 | U    |
| 79  | L5    | 2827 | G    |
| 79  | L5    | 2842 | G    |
| 79  | L5    | 2855 | G    |
| 79  | L5    | 2856 | C    |
| 79  | L5    | 2877 | G    |
| 79  | L5    | 3597 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 3605 | C    |
| 79  | L5    | 3615 | G    |
| 79  | L5    | 3616 | U    |
| 79  | L5    | 3619 | G    |
| 79  | L5    | 3626 | G    |
| 79  | L5    | 3635 | A    |
| 79  | L5    | 3644 | U    |
| 79  | L5    | 3648 | A    |
| 79  | L5    | 3662 | A    |
| 79  | L5    | 3664 | G    |
| 79  | L5    | 3672 | G    |
| 79  | L5    | 3673 | C    |
| 79  | L5    | 3710 | G    |
| 79  | L5    | 3711 | A    |
| 79  | L5    | 3712 | A    |
| 79  | L5    | 3729 | PSU  |
| 79  | L5    | 3748 | A    |
| 79  | L5    | 3753 | G    |
| 79  | L5    | 3754 | G    |
| 79  | L5    | 3760 | A    |
| 79  | L5    | 3776 | G    |
| 79  | L5    | 3777 | G    |
| 79  | L5    | 3784 | A    |
| 79  | L5    | 3785 | A2M  |
| 79  | L5    | 3788 | C    |
| 79  | L5    | 3811 | G    |
| 79  | L5    | 3812 | C    |
| 79  | L5    | 3814 | U    |
| 79  | L5    | 3817 | A    |
| 79  | L5    | 3819 | G    |
| 79  | L5    | 3838 | U    |
| 79  | L5    | 3839 | G    |
| 79  | L5    | 3840 | U    |
| 79  | L5    | 3877 | A    |
| 79  | L5    | 3878 | C    |
| 79  | L5    | 3879 | G    |
| 79  | L5    | 3892 | U    |
| 79  | L5    | 3897 | G    |
| 79  | L5    | 3901 | A    |
| 79  | L5    | 3906 | A    |
| 79  | L5    | 3907 | G    |
| 79  | L5    | 3915 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 3938 | G    |
| 79  | L5    | 3946 | G    |
| 79  | L5    | 4066 | U    |
| 79  | L5    | 4076 | G    |
| 79  | L5    | 4096 | C    |
| 79  | L5    | 4097 | G    |
| 79  | L5    | 4111 | U    |
| 79  | L5    | 4119 | C    |
| 79  | L5    | 4121 | G    |
| 79  | L5    | 4122 | G    |
| 79  | L5    | 4127 | A    |
| 79  | L5    | 4139 | G    |
| 79  | L5    | 4140 | C    |
| 79  | L5    | 4141 | G    |
| 79  | L5    | 4142 | C    |
| 79  | L5    | 4145 | C    |
| 79  | L5    | 4158 | C    |
| 79  | L5    | 4162 | C    |
| 79  | L5    | 4163 | U    |
| 79  | L5    | 4164 | C    |
| 79  | L5    | 4170 | A    |
| 79  | L5    | 4183 | G    |
| 79  | L5    | 4184 | G    |
| 79  | L5    | 4191 | G    |
| 79  | L5    | 4203 | A    |
| 79  | L5    | 4212 | A    |
| 79  | L5    | 4222 | G    |
| 79  | L5    | 4225 | G    |
| 79  | L5    | 4228 | OMG  |
| 79  | L5    | 4229 | U    |
| 79  | L5    | 4233 | A    |
| 79  | L5    | 4235 | G    |
| 79  | L5    | 4251 | A    |
| 79  | L5    | 4254 | G    |
| 79  | L5    | 4266 | G    |
| 79  | L5    | 4268 | A    |
| 79  | L5    | 4273 | A    |
| 79  | L5    | 4281 | A    |
| 79  | L5    | 4282 | A    |
| 79  | L5    | 4291 | G    |
| 79  | L5    | 4304 | A    |
| 79  | L5    | 4305 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 4314 | C    |
| 79  | L5    | 4329 | G    |
| 79  | L5    | 4330 | G    |
| 79  | L5    | 4332 | C    |
| 79  | L5    | 4338 | G    |
| 79  | L5    | 4354 | U    |
| 79  | L5    | 4373 | G    |
| 79  | L5    | 4376 | A    |
| 79  | L5    | 4377 | G    |
| 79  | L5    | 4378 | A    |
| 79  | L5    | 4380 | A    |
| 79  | L5    | 4387 | C    |
| 79  | L5    | 4391 | G    |
| 79  | L5    | 4394 | A    |
| 79  | L5    | 4415 | A    |
| 79  | L5    | 4416 | G    |
| 79  | L5    | 4420 | PSU  |
| 79  | L5    | 4421 | C    |
| 79  | L5    | 4422 | A    |
| 79  | L5    | 4437 | U    |
| 79  | L5    | 4440 | G    |
| 79  | L5    | 4448 | G    |
| 79  | L5    | 4453 | C    |
| 79  | L5    | 4464 | A    |
| 79  | L5    | 4465 | U    |
| 79  | L5    | 4466 | C    |
| 79  | L5    | 4475 | G    |
| 79  | L5    | 4500 | PSU  |
| 79  | L5    | 4510 | A    |
| 79  | L5    | 4512 | U    |
| 79  | L5    | 4513 | A    |
| 79  | L5    | 4515 | G    |
| 79  | L5    | 4519 | C    |
| 79  | L5    | 4524 | G    |
| 79  | L5    | 4529 | G    |
| 79  | L5    | 4532 | PSU  |
| 79  | L5    | 4548 | A    |
| 79  | L5    | 4560 | C    |
| 79  | L5    | 4567 | G    |
| 79  | L5    | 4573 | G    |
| 79  | L5    | 4574 | U    |
| 79  | L5    | 4575 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 4590 | A2M  |
| 79  | L5    | 4600 | G    |
| 79  | L5    | 4627 | U    |
| 79  | L5    | 4636 | PSU  |
| 79  | L5    | 4637 | OMG  |
| 79  | L5    | 4652 | G    |
| 79  | L5    | 4656 | A    |
| 79  | L5    | 4657 | U    |
| 79  | L5    | 4670 | C    |
| 79  | L5    | 4672 | A    |
| 79  | L5    | 4677 | U    |
| 79  | L5    | 4700 | A    |
| 79  | L5    | 4708 | A    |
| 79  | L5    | 4709 | U    |
| 79  | L5    | 4720 | C    |
| 79  | L5    | 4730 | C    |
| 79  | L5    | 4731 | G    |
| 79  | L5    | 4732 | G    |
| 79  | L5    | 4733 | C    |
| 79  | L5    | 4740 | G    |
| 79  | L5    | 4741 | C    |
| 79  | L5    | 4742 | G    |
| 79  | L5    | 4743 | G    |
| 79  | L5    | 4745 | G    |
| 79  | L5    | 4750 | G    |
| 79  | L5    | 4754 | G    |
| 79  | L5    | 4757 | C    |
| 79  | L5    | 4759 | C    |
| 79  | L5    | 4761 | G    |
| 79  | L5    | 4765 | G    |
| 79  | L5    | 4771 | C    |
| 79  | L5    | 4772 | C    |
| 79  | L5    | 4860 | G    |
| 79  | L5    | 4870 | G    |
| 79  | L5    | 4871 | C    |
| 79  | L5    | 4875 | G    |
| 79  | L5    | 4882 | U    |
| 79  | L5    | 4883 | C    |
| 79  | L5    | 4889 | G    |
| 79  | L5    | 4895 | C    |
| 79  | L5    | 4896 | G    |
| 79  | L5    | 4900 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 4901 | G    |
| 79  | L5    | 4903 | G    |
| 79  | L5    | 4910 | G    |
| 79  | L5    | 4912 | G    |
| 79  | L5    | 4913 | G    |
| 79  | L5    | 4914 | C    |
| 79  | L5    | 4922 | C    |
| 79  | L5    | 4928 | C    |
| 79  | L5    | 4934 | A    |
| 79  | L5    | 4938 | A    |
| 79  | L5    | 4941 | G    |
| 79  | L5    | 4943 | A    |
| 79  | L5    | 4944 | C    |
| 79  | L5    | 4949 | G    |
| 79  | L5    | 4975 | G    |
| 79  | L5    | 4976 | U    |
| 79  | L5    | 4985 | U    |
| 79  | L5    | 4990 | C    |
| 79  | L5    | 4991 | U    |
| 79  | L5    | 4994 | G    |
| 79  | L5    | 5017 | G    |
| 79  | L5    | 5041 | G    |
| 79  | L5    | 5050 | C    |
| 79  | L5    | 5062 | G    |
| 79  | L5    | 5069 | U    |
| 80  | Et    | 17   | C    |
| 80  | Et    | 20   | A    |
| 80  | Et    | 21   | A    |
| 80  | Et    | 22   | G    |
| 80  | Et    | 30   | G    |
| 80  | Et    | 35   | A    |
| 80  | Et    | 36   | U    |
| 80  | Et    | 37   | A    |
| 80  | Et    | 38   | A    |
| 80  | Et    | 46   | G    |
| 80  | Et    | 48   | C    |
| 80  | Et    | 50   | A    |
| 80  | Et    | 52   | G    |
| 80  | Et    | 59   | A    |
| 80  | Et    | 67   | U    |
| 80  | Et    | 73   | A    |
| 80  | Et    | 76   | A    |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | L5    | 132  | G    |
| 79  | L5    | 1633 | G    |
| 79  | L5    | 1754 | U    |
| 79  | L5    | 1765 | A    |
| 79  | L5    | 4699 | U    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

225 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 |
| 78  | A2M  | S2    | 99   | -    | 22,25,26     | 3.93 | 11 (50%) | 31,36,39    | 3.70 | 15 (48%) |
| 78  | PSU  | S2    | 1625 | -    | 18,21,22     | 1.10 | 1 (5%)   | 22,30,33    | 1.71 | 4 (18%)  |
| 78  | OMC  | S2    | 1391 | -    | 19,22,23     | 0.53 | 0        | 26,31,34    | 0.65 | 0        |
| 79  | OMC  | L5    | 2824 | -    | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.75 | 1 (3%)   |
| 78  | OMU  | S2    | 354  | -    | 19,22,23     | 2.96 | 8 (42%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 79  | A2M  | L5    | 3723 | -    | 22,25,26     | 3.93 | 10 (45%) | 31,36,39    | 3.74 | 14 (45%) |
| 79  | A2M  | L5    | 3825 | -    | 22,25,26     | 3.92 | 10 (45%) | 31,36,39    | 3.65 | 14 (45%) |
| 76  | 4SU  | Pt    | 8    | -    | 18,21,22     | 3.74 | 8 (44%)  | 26,30,33    | 2.22 | 4 (15%)  |
| 79  | OMC  | L5    | 4536 | -    | 19,22,23     | 0.57 | 0        | 26,31,34    | 0.76 | 0        |
| 78  | PSU  | S2    | 918  | -    | 18,21,22     | 1.09 | 2 (11%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 78  | OMU  | S2    | 1804 | -    | 19,22,23     | 2.99 | 8 (42%)  | 26,31,34    | 1.77 | 5 (19%)  |
| 79  | PSU  | L5    | 3884 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 78  | PSU  | S2    | 815  | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 79  | PSU  | L5    | 4299 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.70 | 4 (18%)  |
| 79  | PSU  | L5    | 4312 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 79  | PSU  | L5    | 3851 | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 78  | PSU  | S2    | 1004 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 79  | A2M  | L5    | 4571 | -    | 22,25,26     | 3.93 | 10 (45%) | 31,36,39    | 3.74 | 14 (45%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 79  | PSU  | L5    | 1862 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 79  | PSU  | L5    | 3734 | -    | 18,21,22     | 1.01 | 1 (5%)   | 22,30,33    | 1.63 | 4 (18%)  |
| 78  | OMG  | S2    | 436  | -    | 23,26,27     | 0.53 | 0        | 33,38,41    | 0.54 | 0        |
| 78  | A2M  | S2    | 484  | -    | 22,25,26     | 3.85 | 11 (50%) | 31,36,39    | 3.68 | 13 (41%) |
| 78  | PSU  | S2    | 651  | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 61  | MLZ  | Lb    | 5    | -    | 8,9,10       | 0.78 | 0        | 4,9,11      | 0.68 | 0        |
| 78  | PSU  | S2    | 1056 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 79  | OMG  | L5    | 4196 | -    | 23,26,27     | 0.52 | 0        | 33,38,41    | 0.54 | 0        |
| 78  | PSU  | S2    | 119  | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.61 | 4 (18%)  |
| 78  | 6MZ  | S2    | 1832 | -    | 22,25,26     | 2.54 | 3 (13%)  | 30,36,39    | 3.51 | 12 (40%) |
| 79  | OMG  | L5    | 3944 | -    | 23,26,27     | 0.49 | 0        | 33,38,41    | 0.55 | 0        |
| 79  | OMG  | L5    | 2364 | -    | 23,26,27     | 0.51 | 0        | 33,38,41    | 0.47 | 0        |
| 79  | PSU  | L5    | 3695 | -    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 79  | OMC  | L5    | 2861 | -    | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.83 | 1 (3%)   |
| 79  | PSU  | L5    | 1860 | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 78  | PSU  | S2    | 34   | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 78  | OMG  | S2    | 509  | -    | 23,26,27     | 0.51 | 0        | 33,38,41    | 0.53 | 0        |
| 78  | PSU  | S2    | 572  | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.71 | 4 (18%)  |
| 79  | PSU  | L5    | 1744 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 79  | A2M  | L5    | 2363 | -    | 22,25,26     | 3.93 | 10 (45%) | 31,36,39    | 3.73 | 14 (45%) |
| 78  | A2M  | S2    | 1678 | -    | 22,25,26     | 3.94 | 10 (45%) | 31,36,39    | 3.82 | 14 (45%) |
| 79  | OMC  | L5    | 2422 | -    | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.77 | 1 (3%)   |
| 79  | A2M  | L5    | 3830 | -    | 22,25,26     | 3.92 | 10 (45%) | 31,36,39    | 3.63 | 14 (45%) |
| 79  | PSU  | L5    | 4442 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.77 | 5 (22%)  |
| 78  | 4AC  | S2    | 1842 | -    | 21,24,25     | 3.45 | 10 (47%) | 29,34,37    | 1.11 | 4 (13%)  |
| 78  | OMG  | S2    | 601  | -    | 23,26,27     | 0.49 | 0        | 33,38,41    | 0.46 | 0        |
| 79  | PSU  | L5    | 4423 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 78  | PSU  | S2    | 649  | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.76 | 4 (18%)  |
| 79  | OMG  | L5    | 1625 | -    | 23,26,27     | 0.54 | 0        | 33,38,41    | 0.54 | 0        |
| 79  | OMG  | L5    | 4623 | -    | 23,26,27     | 0.53 | 0        | 33,38,41    | 0.59 | 0        |
| 79  | 5MC  | L5    | 4447 | -    | 18,22,23     | 0.73 | 0        | 26,32,35    | 0.67 | 0        |
| 79  | PSU  | L5    | 4552 | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 79  | PSU  | L5    | 4361 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 78  | PSU  | S2    | 863  | -    | 18,21,22     | 1.10 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 79  | 1MA  | L5    | 1322 | -    | 21,25,26     | 0.51 | 0        | 31,37,40    | 0.76 | 1 (3%)   |
| 79  | PSU  | L5    | 1782 | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 79  | OMG  | L5    | 4499 | -    | 23,26,27     | 0.52 | 0        | 33,38,41    | 0.47 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 78  | PSU  | S2    | 406  | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 79  | PSU  | L5    | 3758 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.76 | 4 (18%)  |
| 78  | PSU  | S2    | 1643 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.78 | 6 (27%)  |
| 79  | OMC  | L5    | 2804 | -    | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.71 | 0        |
| 79  | PSU  | L5    | 5010 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.69 | 4 (18%)  |
| 79  | OMG  | L5    | 4494 | -    | 23,26,27     | 0.53 | 0        | 33,38,41    | 0.49 | 0        |
| 79  | OMC  | L5    | 3887 | -    | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.66 | 0        |
| 79  | PSU  | L5    | 4579 | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.70 | 4 (18%)  |
| 78  | OMU  | S2    | 1288 | -    | 19,22,23     | 3.02 | 8 (42%)  | 26,31,34    | 1.65 | 4 (15%)  |
| 78  | A2M  | S2    | 512  | -    | 22,25,26     | 3.92 | 10 (45%) | 31,36,39    | 3.70 | 15 (48%) |
| 5   | PSU  | L8    | 69   | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.75 | 5 (22%)  |
| 79  | A2M  | L5    | 1534 | -    | 22,25,26     | 3.93 | 11 (50%) | 31,36,39    | 3.81 | 15 (48%) |
| 78  | A2M  | S2    | 1031 | -    | 22,25,26     | 3.92 | 10 (45%) | 31,36,39    | 3.71 | 15 (48%) |
| 78  | PSU  | S2    | 36   | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 79  | OMC  | L5    | 1340 | -    | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.66 | 0        |
| 79  | A2M  | L5    | 3724 | -    | 22,25,26     | 3.94 | 11 (50%) | 31,36,39    | 3.72 | 14 (45%) |
| 79  | PSU  | L5    | 1781 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.65 | 4 (18%)  |
| 79  | A2M  | L5    | 1524 | -    | 22,25,26     | 3.97 | 9 (40%)  | 31,36,39    | 3.94 | 14 (45%) |
| 74  | MLZ  | Lo    | 53   | -    | 8,9,10       | 0.75 | 0        | 4,9,11      | 0.61 | 0        |
| 79  | PSU  | L5    | 3639 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 78  | A2M  | S2    | 576  | -    | 22,25,26     | 3.93 | 11 (50%) | 31,36,39    | 3.71 | 15 (48%) |
| 78  | PSU  | S2    | 296  | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.68 | 4 (18%)  |
| 78  | PSU  | S2    | 1692 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 79  | PSU  | L5    | 3920 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.76 | 4 (18%)  |
| 79  | PSU  | L5    | 4457 | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.80 | 5 (22%)  |
| 78  | OMC  | S2    | 517  | -    | 19,22,23     | 0.54 | 0        | 26,31,34    | 0.64 | 0        |
| 79  | A2M  | L5    | 3867 | -    | 22,25,26     | 3.94 | 10 (45%) | 31,36,39    | 3.75 | 14 (45%) |
| 78  | PSU  | S2    | 814  | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.69 | 4 (18%)  |
| 79  | A2M  | L5    | 2401 | -    | 22,25,26     | 3.94 | 10 (45%) | 31,36,39    | 3.74 | 16 (51%) |
| 1   | V5N  | LA    | 216  | -    | 9,11,12      | 2.71 | 2 (22%)  | 9,14,16     | 1.25 | 1 (11%)  |
| 79  | PSU  | L5    | 1536 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 79  | OMC  | L5    | 1881 | -    | 19,22,23     | 0.57 | 0        | 26,31,34    | 0.67 | 0        |
| 79  | OMG  | L5    | 3792 | -    | 23,26,27     | 0.51 | 0        | 33,38,41    | 0.47 | 0        |
| 79  | OMU  | L5    | 2837 | -    | 19,22,23     | 3.01 | 8 (42%)  | 26,31,34    | 1.77 | 5 (19%)  |
| 78  | PSU  | S2    | 1136 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.83 | 5 (22%)  |
| 78  | PSU  | S2    | 1244 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 79  | PSU  | L5    | 5001 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 78  | PSU  | S2    | 686  | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 79  | PSU  | L5    | 3764 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.74 | 5 (22%)  |
| 79  | A2M  | L5    | 1326 | -    | 22,25,26     | 3.92 | 10 (45%) | 31,36,39    | 3.69 | 14 (45%) |
| 79  | PSU  | L5    | 4431 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 79  | OMU  | L5    | 4620 | -    | 19,22,23     | 2.94 | 8 (42%)  | 26,31,34    | 1.69 | 5 (19%)  |
| 78  | A2M  | S2    | 166  | -    | 22,25,26     | 3.93 | 9 (40%)  | 31,36,39    | 3.74 | 16 (51%) |
| 78  | OMG  | S2    | 1447 | -    | 23,26,27     | 0.48 | 0        | 33,38,41    | 0.50 | 0        |
| 79  | OMU  | L5    | 2415 | -    | 19,22,23     | 3.00 | 8 (42%)  | 26,31,34    | 1.70 | 4 (15%)  |
| 79  | PSU  | L5    | 4493 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.71 | 4 (18%)  |
| 79  | PSU  | L5    | 4532 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.73 | 4 (18%)  |
| 78  | A2M  | S2    | 468  | -    | 22,25,26     | 3.92 | 11 (50%) | 31,36,39    | 3.65 | 15 (48%) |
| 79  | PSU  | L5    | 2508 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 78  | PSU  | S2    | 93   | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.65 | 4 (18%)  |
| 78  | OMU  | S2    | 172  | -    | 19,22,23     | 3.02 | 8 (42%)  | 26,31,34    | 1.76 | 5 (19%)  |
| 79  | PSU  | L5    | 2839 | -    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.73 | 4 (18%)  |
| 78  | PSU  | S2    | 1174 | -    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 79  | A2M  | L5    | 400  | -    | 22,25,26     | 3.93 | 10 (45%) | 31,36,39    | 3.71 | 14 (45%) |
| 78  | PSU  | S2    | 866  | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.73 | 4 (18%)  |
| 78  | G7M  | S2    | 1639 | -    | 23,26,27     | 2.76 | 8 (34%)  | 35,39,42    | 2.32 | 10 (28%) |
| 78  | PSU  | S2    | 1232 | -    | 18,21,22     | 1.11 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 79  | PSU  | L5    | 2632 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.66 | 4 (18%)  |
| 79  | PSU  | L5    | 3762 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 78  | PSU  | S2    | 822  | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.76 | 5 (22%)  |
| 79  | PSU  | L5    | 4293 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 79  | PSU  | L5    | 4689 | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.71 | 4 (18%)  |
| 79  | OMG  | L5    | 4370 | -    | 23,26,27     | 0.51 | 0        | 33,38,41    | 0.51 | 0        |
| 79  | OMC  | L5    | 3841 | -    | 19,22,23     | 0.57 | 0        | 26,31,34    | 0.65 | 0        |
| 78  | PSU  | S2    | 801  | -    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 46  | V5N  | La    | 39   | -    | 9,11,12      | 2.66 | 2 (22%)  | 9,14,16     | 1.23 | 1 (11%)  |
| 79  | PSU  | L5    | 4420 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.60 | 5 (22%)  |
| 79  | PSU  | L5    | 1683 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.71 | 4 (18%)  |
| 79  | A2M  | L5    | 3785 | -    | 22,25,26     | 3.94 | 11 (50%) | 31,36,39    | 3.76 | 14 (45%) |
| 79  | OMC  | L5    | 3701 | -    | 19,22,23     | 0.53 | 0        | 26,31,34    | 0.57 | 0        |
| 79  | A2M  | L5    | 4590 | -    | 22,25,26     | 3.94 | 9 (40%)  | 31,36,39    | 3.76 | 16 (51%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 79  | OMU  | L5    | 4227 | -    | 19,22,23     | 2.99 | 8 (42%)  | 26,31,34    | 1.73 | 5 (19%)  |
| 76  | H2U  | Pt    | 21   | -    | 18,21,22     | 0.45 | 0        | 21,30,33    | 1.02 | 1 (4%)   |
| 79  | PSU  | L5    | 3844 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 78  | A2M  | S2    | 159  | -    | 22,25,26     | 3.89 | 10 (45%) | 31,36,39    | 3.69 | 13 (41%) |
| 78  | OMC  | S2    | 1703 | -    | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.62 | 0        |
| 78  | B8N  | S2    | 1248 | -    | 24,29,30     | 3.02 | 6 (25%)  | 29,42,45    | 1.75 | 5 (17%)  |
| 79  | PSU  | L5    | 3853 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 78  | PSU  | S2    | 966  | -    | 18,21,22     | 1.01 | 1 (5%)   | 22,30,33    | 1.67 | 4 (18%)  |
| 79  | OMG  | L5    | 3744 | -    | 23,26,27     | 0.50 | 0        | 33,38,41    | 0.48 | 0        |
| 79  | PSU  | L5    | 4569 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.66 | 4 (18%)  |
| 78  | A2M  | S2    | 1383 | -    | 22,25,26     | 3.95 | 10 (45%) | 31,36,39    | 3.69 | 15 (48%) |
| 79  | PSU  | L5    | 1779 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 79  | OMG  | L5    | 3627 | -    | 23,26,27     | 0.52 | 0        | 33,38,41    | 0.64 | 0        |
| 79  | PSU  | L5    | 4296 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 76  | G7M  | Pt    | 47   | -    | 23,26,27     | 2.79 | 8 (34%)  | 35,39,42    | 2.29 | 10 (28%) |
| 79  | PSU  | L5    | 4972 | -    | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 79  | PSU  | L5    | 1677 | -    | 18,21,22     | 1.13 | 1 (5%)   | 22,30,33    | 1.79 | 5 (22%)  |
| 78  | OMU  | S2    | 116  | -    | 19,22,23     | 2.97 | 8 (42%)  | 26,31,34    | 1.64 | 5 (19%)  |
| 78  | PSU  | S2    | 1243 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 79  | A2M  | L5    | 398  | -    | 22,25,26     | 3.88 | 10 (45%) | 31,36,39    | 3.69 | 13 (41%) |
| 79  | 6MZ  | L5    | 4220 | -    | 22,25,26     | 2.61 | 3 (13%)  | 30,36,39    | 3.46 | 9 (30%)  |
| 79  | PSU  | L5    | 1792 | -    | 18,21,22     | 1.01 | 1 (5%)   | 22,30,33    | 1.70 | 4 (18%)  |
| 79  | 5MC  | L5    | 3782 | -    | 18,22,23     | 0.57 | 0        | 26,32,35    | 0.72 | 0        |
| 76  | PSU  | Pt    | 56   | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 78  | OMG  | S2    | 644  | -    | 23,26,27     | 0.49 | 0        | 33,38,41    | 0.52 | 0        |
| 79  | OMG  | L5    | 2876 | -    | 23,26,27     | 0.57 | 0        | 33,38,41    | 0.74 | 1 (3%)   |
| 79  | OMG  | L5    | 4228 | -    | 23,26,27     | 0.50 | 0        | 33,38,41    | 0.55 | 0        |
| 79  | UY1  | L5    | 3818 | -    | 19,22,23     | 4.18 | 8 (42%)  | 22,31,34    | 1.80 | 5 (22%)  |
| 78  | OMU  | S2    | 627  | -    | 19,22,23     | 3.04 | 8 (42%)  | 26,31,34    | 1.67 | 4 (15%)  |
| 79  | A2M  | L5    | 2815 | -    | 22,25,26     | 3.93 | 10 (45%) | 31,36,39    | 3.78 | 14 (45%) |
| 78  | PSU  | S2    | 1177 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 79  | PSU  | L5    | 4353 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 78  | OMU  | S2    | 121  | -    | 19,22,23     | 2.99 | 8 (42%)  | 26,31,34    | 1.66 | 5 (19%)  |
| 79  | OMC  | L5    | 2351 | -    | 19,22,23     | 0.59 | 0        | 26,31,34    | 1.23 | 2 (7%)   |
| 79  | PSU  | L5    | 4471 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.67 | 4 (18%)  |
| 79  | PSU  | L5    | 4531 | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.81 | 5 (22%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 78  | PSU  | S2    | 609  | -    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 3   | HIC  | LB    | 245  | -    | 10,11,12     | 0.53 | 0        | 8,14,16     | 0.45 | 0        |
| 5   | OMG  | L8    | 75   | -    | 23,26,27     | 0.49 | 0        | 33,38,41    | 0.49 | 0        |
| 78  | A2M  | S2    | 27   | -    | 22,25,26     | 3.91 | 10 (45%) | 31,36,39    | 3.68 | 13 (41%) |
| 78  | PSU  | S2    | 105  | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.70 | 4 (18%)  |
| 79  | OMC  | L5    | 2365 | -    | 19,22,23     | 0.56 | 0        | 26,31,34    | 0.65 | 0        |
| 79  | OMG  | L5    | 3899 | -    | 23,26,27     | 0.56 | 0        | 33,38,41    | 0.60 | 0        |
| 79  | PSU  | L5    | 4628 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.88 | 5 (22%)  |
| 78  | A2M  | S2    | 590  | -    | 22,25,26     | 3.97 | 9 (40%)  | 31,36,39    | 3.93 | 13 (41%) |
| 78  | PSU  | S2    | 681  | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.72 | 4 (18%)  |
| 79  | PSU  | L5    | 3770 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 79  | A2M  | L5    | 4523 | -    | 22,25,26     | 3.91 | 11 (50%) | 31,36,39    | 3.70 | 15 (48%) |
| 78  | PSU  | S2    | 1238 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.76 | 4 (18%)  |
| 79  | PSU  | L5    | 3715 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.75 | 5 (22%)  |
| 79  | PSU  | L5    | 3637 | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.83 | 4 (18%)  |
| 78  | PSU  | S2    | 1081 | -    | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.70 | 5 (22%)  |
| 79  | OMG  | L5    | 1316 | -    | 23,26,27     | 0.54 | 0        | 33,38,41    | 0.58 | 0        |
| 79  | PSU  | L5    | 4521 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 79  | OMU  | L5    | 4306 | -    | 19,22,23     | 2.99 | 8 (42%)  | 26,31,34    | 1.70 | 5 (19%)  |
| 78  | A2M  | S2    | 668  | -    | 22,25,26     | 3.91 | 11 (50%) | 31,36,39    | 3.63 | 14 (45%) |
| 79  | OMU  | L5    | 3925 | -    | 19,22,23     | 2.99 | 8 (42%)  | 26,31,34    | 1.74 | 5 (19%)  |
| 19  | HY3  | SX    | 62   | -    | 6,8,9        | 7.80 | 3 (50%)  | 5,10,12     | 0.98 | 0        |
| 78  | MA6  | S2    | 1850 | -    | 23,26,27     | 1.48 | 4 (17%)  | 34,38,41    | 3.28 | 11 (32%) |
| 79  | PSU  | L5    | 4636 | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.71 | 5 (22%)  |
| 78  | MA6  | S2    | 1851 | -    | 23,26,27     | 1.46 | 4 (17%)  | 34,38,41    | 3.48 | 12 (35%) |
| 78  | OMC  | S2    | 174  | -    | 19,22,23     | 0.52 | 0        | 26,31,34    | 0.65 | 0        |
| 78  | PSU  | S2    | 218  | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.69 | 5 (22%)  |
| 79  | OMG  | L5    | 4637 | -    | 23,26,27     | 0.53 | 0        | 33,38,41    | 0.50 | 0        |
| 79  | PSU  | L5    | 4500 | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.87 | 5 (22%)  |
| 5   | PSU  | L8    | 55   | -    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.73 | 4 (18%)  |
| 78  | PSU  | S2    | 573  | -    | 18,21,22     | 1.11 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 79  | PSU  | L5    | 1582 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.70 | 4 (18%)  |
| 72  | M3L  | Lm    | 98   | -    | 10,11,12     | 0.40 | 0        | 9,14,16     | 0.28 | 0        |
| 78  | 4AC  | S2    | 1337 | -    | 21,24,25     | 3.46 | 10 (47%) | 29,34,37    | 1.09 | 3 (10%)  |
| 78  | PSU  | S2    | 1347 | -    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 79  | OMC  | L5    | 3869 | -    | 19,22,23     | 0.58 | 0        | 26,31,34    | 0.74 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 79  | OMC  | L5    | 3808 | -    | 19,22,23     | 0.64 | 0        | 26,31,34    | 0.90 | 2 (7%)   |
| 79  | OMG  | L5    | 1522 | -    | 23,26,27     | 0.51 | 0        | 33,38,41    | 0.61 | 0        |
| 78  | OMU  | S2    | 428  | -    | 19,22,23     | 3.05 | 8 (42%)  | 26,31,34    | 1.71 | 4 (15%)  |
| 79  | OMC  | L5    | 4456 | -    | 19,22,23     | 0.60 | 0        | 26,31,34    | 0.79 | 1 (3%)   |
| 79  | PSU  | L5    | 4576 | -    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 78  | PSU  | S2    | 1367 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 78  | OMG  | S2    | 1490 | -    | 23,26,27     | 0.54 | 0        | 33,38,41    | 0.51 | 0        |
| 78  | OMG  | S2    | 1328 | -    | 23,26,27     | 0.49 | 0        | 33,38,41    | 0.48 | 0        |
| 79  | A2M  | L5    | 3718 | -    | 22,25,26     | 3.90 | 11 (50%) | 31,36,39    | 3.66 | 14 (45%) |
| 79  | PSU  | L5    | 3768 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.69 | 4 (18%)  |
| 78  | PSU  | S2    | 1445 | -    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.78 | 5 (22%)  |
| 79  | A2M  | L5    | 1871 | -    | 22,25,26     | 3.93 | 10 (45%) | 31,36,39    | 3.67 | 15 (48%) |
| 79  | OMG  | L5    | 4392 | -    | 23,26,27     | 0.50 | 0        | 33,38,41    | 0.45 | 0        |
| 79  | PSU  | L5    | 3729 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.71 | 4 (18%)  |
| 78  | OMC  | S2    | 462  | -    | 19,22,23     | 0.53 | 0        | 26,31,34    | 0.68 | 0        |
| 79  | OMU  | L5    | 4498 | -    | 19,22,23     | 2.99 | 8 (42%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 79  | PSU  | L5    | 2843 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.73 | 4 (18%)  |
| 78  | UY1  | S2    | 1326 | -    | 19,22,23     | 4.20 | 8 (42%)  | 22,31,34    | 1.81 | 5 (22%)  |
| 78  | PSU  | S2    | 1239 | -    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.73 | 4 (18%)  |
| 79  | PSU  | L5    | 4403 | -    | 18,21,22     | 1.00 | 1 (5%)   | 22,30,33    | 1.82 | 5 (22%)  |
| 76  | OMC  | Pt    | 33   | -    | 19,22,23     | 0.57 | 0        | 26,31,34    | 1.01 | 2 (7%)   |
| 78  | OMG  | S2    | 683  | -    | 23,26,27     | 0.51 | 0        | 33,38,41    | 0.57 | 0        |
| 79  | PSU  | L5    | 4673 | -    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 79  | OMG  | L5    | 2424 | -    | 23,26,27     | 0.52 | 0        | 33,38,41    | 0.44 | 0        |
| 79  | UR3  | L5    | 4530 | -    | 19,22,23     | 2.76 | 8 (42%)  | 26,32,35    | 1.29 | 2 (7%)   |
| 78  | PSU  | S2    | 109  | -    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 79  | OMG  | L5    | 4618 | -    | 23,26,27     | 0.50 | 0        | 33,38,41    | 0.54 | 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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 78  | A2M  | S2    | 99   | -    | -       | 3/9/27/28 | 0/3/3/3 |
| 78  | PSU  | S2    | 1625 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | OMC  | S2    | 1391 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | OMC  | L5    | 2824 | -    | -       | 1/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 78  | OMU  | S2    | 354  | -    | -       | 1/9/27/28  | 0/2/2/2 |
| 79  | A2M  | L5    | 3723 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | A2M  | L5    | 3825 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 76  | 4SU  | Pt    | 8    | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMC  | L5    | 4536 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 78  | PSU  | S2    | 918  | -    | -       | 2/7/25/26  | 0/2/2/2 |
| 78  | OMU  | S2    | 1804 | -    | -       | 1/9/27/28  | 0/2/2/2 |
| 79  | PSU  | L5    | 3884 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 815  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 4299 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 4312 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 3851 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 1004 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | A2M  | L5    | 4571 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 1862 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 3734 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | OMG  | S2    | 436  | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 78  | A2M  | S2    | 484  | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 78  | PSU  | S2    | 651  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 61  | MLZ  | Lb    | 5    | -    | -       | 4/7/8/10   | -       |
| 78  | PSU  | S2    | 1056 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMG  | L5    | 4196 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 78  | PSU  | S2    | 119  | -    | -       | 1/7/25/26  | 0/2/2/2 |
| 78  | 6MZ  | S2    | 1832 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | OMG  | L5    | 3944 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | OMG  | L5    | 2364 | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 3695 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMC  | L5    | 2861 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | PSU  | L5    | 1860 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 34   | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | OMG  | S2    | 509  | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 78  | PSU  | S2    | 572  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 1744 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | A2M  | L5    | 2363 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 78  | A2M  | S2    | 1678 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | OMC  | L5    | 2422 | -    | -       | 2/9/27/28  | 0/2/2/2 |
| 79  | A2M  | L5    | 3830 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 4442 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | 4AC  | S2    | 1842 | -    | -       | 0/11/29/30 | 0/2/2/2 |
| 78  | OMG  | S2    | 601  | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 4423 | -    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 78  | PSU  | S2    | 649  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMG  | L5    | 1625 | -    | -       | 1/9/27/28 | 0/3/3/3 |
| 79  | OMG  | L5    | 4623 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | 5MC  | L5    | 4447 | -    | -       | 4/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 4552 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 4361 | -    | -       | 1/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 863  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | 1MA  | L5    | 1322 | -    | -       | 2/7/25/26 | 0/3/3/3 |
| 79  | PSU  | L5    | 1782 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMG  | L5    | 4499 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 78  | PSU  | S2    | 406  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 3758 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 1643 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMC  | L5    | 2804 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | PSU  | L5    | 5010 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMG  | L5    | 4494 | -    | -       | 1/9/27/28 | 0/3/3/3 |
| 79  | OMC  | L5    | 3887 | -    | -       | 1/9/27/28 | 0/2/2/2 |
| 79  | PSU  | L5    | 4579 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | OMU  | S2    | 1288 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 78  | A2M  | S2    | 512  | -    | -       | 3/9/27/28 | 0/3/3/3 |
| 5   | PSU  | L8    | 69   | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | A2M  | L5    | 1534 | -    | -       | 2/9/27/28 | 0/3/3/3 |
| 78  | A2M  | S2    | 1031 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 78  | PSU  | S2    | 36   | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMC  | L5    | 1340 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | A2M  | L5    | 3724 | -    | -       | 1/9/27/28 | 0/3/3/3 |
| 79  | PSU  | L5    | 1781 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | A2M  | L5    | 1524 | -    | -       | 2/9/27/28 | 0/3/3/3 |
| 74  | MLZ  | Lo    | 53   | -    | -       | 2/7/8/10  | -       |
| 79  | PSU  | L5    | 3639 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | A2M  | S2    | 576  | -    | -       | 3/9/27/28 | 0/3/3/3 |
| 78  | PSU  | S2    | 296  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 1692 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 3920 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 4457 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | OMC  | S2    | 517  | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | A2M  | L5    | 3867 | -    | -       | 3/9/27/28 | 0/3/3/3 |
| 78  | PSU  | S2    | 814  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | A2M  | L5    | 2401 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | V5N  | LA    | 216  | -    | -       | 1/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 79  | PSU  | L5    | 1536 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMC  | L5    | 1881 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | OMG  | L5    | 3792 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | OMU  | L5    | 2837 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 78  | PSU  | S2    | 1136 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 1244 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 5001 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 686  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 3764 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | A2M  | L5    | 1326 | -    | -       | 1/9/27/28 | 0/3/3/3 |
| 79  | PSU  | L5    | 4431 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMU  | L5    | 4620 | -    | -       | 1/9/27/28 | 0/2/2/2 |
| 78  | A2M  | S2    | 166  | -    | -       | 1/9/27/28 | 0/3/3/3 |
| 78  | OMG  | S2    | 1447 | -    | -       | 2/9/27/28 | 0/3/3/3 |
| 79  | OMU  | L5    | 2415 | -    | -       | 1/9/27/28 | 0/2/2/2 |
| 79  | PSU  | L5    | 4493 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 4532 | -    | -       | 2/7/25/26 | 0/2/2/2 |
| 78  | A2M  | S2    | 468  | -    | -       | 2/9/27/28 | 0/3/3/3 |
| 79  | PSU  | L5    | 2508 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 93   | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | OMU  | S2    | 172  | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | PSU  | L5    | 2839 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 1174 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | A2M  | L5    | 400  | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 78  | PSU  | S2    | 866  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | G7M  | S2    | 1639 | -    | -       | 2/7/25/26 | 0/3/3/3 |
| 78  | PSU  | S2    | 1232 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 2632 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 3762 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 822  | -    | -       | 2/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 4293 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 4689 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMG  | L5    | 4370 | -    | -       | 2/9/27/28 | 0/3/3/3 |
| 79  | OMC  | L5    | 3841 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 78  | PSU  | S2    | 801  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | V5N  | La    | 39   | -    | -       | 1/9/10/12 | 0/1/1/1 |
| 79  | PSU  | L5    | 4420 | -    | -       | 4/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 1683 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | A2M  | L5    | 3785 | -    | -       | 4/9/27/28 | 0/3/3/3 |
| 79  | OMC  | L5    | 3701 | -    | -       | 4/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 79  | A2M  | L5    | 4590 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | OMU  | L5    | 4227 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 76  | H2U  | Pt    | 21   | -    | -       | 6/7/38/39  | 0/2/2/2 |
| 79  | PSU  | L5    | 3844 | -    | -       | 1/7/25/26  | 0/2/2/2 |
| 78  | A2M  | S2    | 159  | -    | -       | 3/9/27/28  | 0/3/3/3 |
| 78  | OMC  | S2    | 1703 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 78  | B8N  | S2    | 1248 | -    | -       | 6/16/34/35 | 0/2/2/2 |
| 79  | PSU  | L5    | 3853 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 966  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMG  | L5    | 3744 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 4569 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | A2M  | S2    | 1383 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 1779 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMG  | L5    | 3627 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 4296 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 76  | G7M  | Pt    | 47   | -    | -       | 2/7/25/26  | 0/3/3/3 |
| 79  | PSU  | L5    | 4972 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 1677 | -    | -       | 1/7/25/26  | 0/2/2/2 |
| 78  | OMU  | S2    | 116  | -    | -       | 1/9/27/28  | 0/2/2/2 |
| 78  | PSU  | S2    | 1243 | -    | -       | 2/7/25/26  | 0/2/2/2 |
| 79  | A2M  | L5    | 398  | -    | -       | 3/9/27/28  | 0/3/3/3 |
| 79  | 6MZ  | L5    | 4220 | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 1792 | -    | -       | 2/7/25/26  | 0/2/2/2 |
| 79  | 5MC  | L5    | 3782 | -    | -       | 1/7/25/26  | 0/2/2/2 |
| 76  | PSU  | Pt    | 56   | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | OMG  | S2    | 644  | -    | -       | 3/9/27/28  | 0/3/3/3 |
| 79  | OMG  | L5    | 2876 | -    | -       | 3/9/27/28  | 0/3/3/3 |
| 79  | OMG  | L5    | 4228 | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 79  | UY1  | L5    | 3818 | -    | -       | 3/9/27/28  | 0/2/2/2 |
| 78  | OMU  | S2    | 627  | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | A2M  | L5    | 2815 | -    | -       | 3/9/27/28  | 0/3/3/3 |
| 78  | PSU  | S2    | 1177 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 4353 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | OMU  | S2    | 121  | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | OMC  | L5    | 2351 | -    | -       | 4/9/27/28  | 0/2/2/2 |
| 79  | PSU  | L5    | 4471 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 4531 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 609  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | HIC  | LB    | 245  | -    | -       | 0/5/6/8    | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 5   | OMG  | L8    | 75   | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 78  | A2M  | S2    | 27   | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 78  | PSU  | S2    | 105  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMC  | L5    | 2365 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | OMG  | L5    | 3899 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 4628 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | A2M  | S2    | 590  | -    | -       | 6/9/27/28  | 0/3/3/3 |
| 78  | PSU  | S2    | 681  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 3770 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | A2M  | L5    | 4523 | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 78  | PSU  | S2    | 1238 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 3715 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 3637 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 1081 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMG  | L5    | 1316 | -    | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 4521 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMU  | L5    | 4306 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 78  | A2M  | S2    | 668  | -    | -       | 2/9/27/28  | 0/3/3/3 |
| 79  | OMU  | L5    | 3925 | -    | -       | 1/9/27/28  | 0/2/2/2 |
| 19  | HY3  | SX    | 62   | -    | -       | 0/1/12/14  | 0/1/1/1 |
| 78  | MA6  | S2    | 1850 | -    | -       | 0/11/29/30 | 0/3/3/3 |
| 79  | PSU  | L5    | 4636 | -    | -       | 2/7/25/26  | 0/2/2/2 |
| 78  | MA6  | S2    | 1851 | -    | -       | 3/11/29/30 | 0/3/3/3 |
| 78  | OMC  | S2    | 174  | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 78  | PSU  | S2    | 218  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMG  | L5    | 4637 | -    | -       | 3/9/27/28  | 0/3/3/3 |
| 79  | PSU  | L5    | 4500 | -    | -       | 1/7/25/26  | 0/2/2/2 |
| 5   | PSU  | L8    | 55   | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 573  | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | PSU  | L5    | 1582 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 72  | M3L  | Lm    | 98   | -    | -       | 0/9/10/12  | -       |
| 78  | 4AC  | S2    | 1337 | -    | -       | 0/11/29/30 | 0/2/2/2 |
| 78  | PSU  | S2    | 1347 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 79  | OMC  | L5    | 3869 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | OMC  | L5    | 3808 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | OMG  | L5    | 1522 | -    | -       | 0/9/27/28  | 0/3/3/3 |
| 78  | OMU  | S2    | 428  | -    | -       | 6/9/27/28  | 0/2/2/2 |
| 79  | OMC  | L5    | 4456 | -    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | PSU  | L5    | 4576 | -    | -       | 0/7/25/26  | 0/2/2/2 |
| 78  | PSU  | S2    | 1367 | -    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 78  | OMG  | S2    | 1490 | -    | -       | 2/9/27/28 | 0/3/3/3 |
| 78  | OMG  | S2    | 1328 | -    | -       | 1/9/27/28 | 0/3/3/3 |
| 79  | A2M  | L5    | 3718 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | PSU  | L5    | 3768 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 1445 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | A2M  | L5    | 1871 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | OMG  | L5    | 4392 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | PSU  | L5    | 3729 | -    | -       | 2/7/25/26 | 0/2/2/2 |
| 78  | OMC  | S2    | 462  | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | OMU  | L5    | 4498 | -    | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | PSU  | L5    | 2843 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | UY1  | S2    | 1326 | -    | -       | 2/9/27/28 | 0/2/2/2 |
| 78  | PSU  | S2    | 1239 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | PSU  | L5    | 4403 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 76  | OMC  | Pt    | 33   | -    | -       | 1/9/27/28 | 0/2/2/2 |
| 78  | OMG  | S2    | 683  | -    | -       | 2/9/27/28 | 0/3/3/3 |
| 79  | PSU  | L5    | 4673 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMG  | L5    | 2424 | -    | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | UR3  | L5    | 4530 | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 78  | PSU  | S2    | 109  | -    | -       | 0/7/25/26 | 0/2/2/2 |
| 79  | OMG  | L5    | 4618 | -    | -       | 0/9/27/28 | 0/3/3/3 |

All (646) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 19  | SX    | 62   | HY3  | C3-CA   | -17.99 | 1.37        | 1.55     |
| 78  | S2    | 590  | A2M  | C3'-C2' | -12.71 | 1.24        | 1.52     |
| 78  | S2    | 1383 | A2M  | C3'-C2' | -12.67 | 1.24        | 1.52     |
| 79  | L5    | 4590 | A2M  | C3'-C2' | -12.67 | 1.24        | 1.52     |
| 79  | L5    | 3785 | A2M  | C3'-C2' | -12.67 | 1.24        | 1.52     |
| 79  | L5    | 3867 | A2M  | C3'-C2' | -12.66 | 1.24        | 1.52     |
| 79  | L5    | 1534 | A2M  | C3'-C2' | -12.64 | 1.24        | 1.52     |
| 79  | L5    | 2363 | A2M  | C3'-C2' | -12.62 | 1.24        | 1.52     |
| 79  | L5    | 1871 | A2M  | C3'-C2' | -12.62 | 1.24        | 1.52     |
| 78  | S2    | 99   | A2M  | C3'-C2' | -12.58 | 1.24        | 1.52     |
| 78  | S2    | 27   | A2M  | C3'-C2' | -12.56 | 1.24        | 1.52     |
| 78  | S2    | 468  | A2M  | C3'-C2' | -12.56 | 1.24        | 1.52     |
| 79  | L5    | 3825 | A2M  | C3'-C2' | -12.56 | 1.24        | 1.52     |
| 79  | L5    | 3830 | A2M  | C3'-C2' | -12.56 | 1.24        | 1.52     |
| 79  | L5    | 1524 | A2M  | C3'-C2' | -12.55 | 1.25        | 1.52     |
| 79  | L5    | 3724 | A2M  | C3'-C2' | -12.55 | 1.25        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 79  | L5    | 4571 | A2M  | C3'-C2' | -12.55 | 1.25        | 1.52     |
| 79  | L5    | 2815 | A2M  | C3'-C2' | -12.55 | 1.25        | 1.52     |
| 79  | L5    | 400  | A2M  | C3'-C2' | -12.54 | 1.25        | 1.52     |
| 79  | L5    | 2401 | A2M  | C3'-C2' | -12.54 | 1.25        | 1.52     |
| 78  | S2    | 166  | A2M  | C3'-C2' | -12.54 | 1.25        | 1.52     |
| 79  | L5    | 1326 | A2M  | C3'-C2' | -12.53 | 1.25        | 1.52     |
| 78  | S2    | 1031 | A2M  | C3'-C2' | -12.53 | 1.25        | 1.52     |
| 78  | S2    | 512  | A2M  | C3'-C2' | -12.52 | 1.25        | 1.52     |
| 79  | L5    | 3723 | A2M  | C3'-C2' | -12.50 | 1.25        | 1.52     |
| 78  | S2    | 1678 | A2M  | C3'-C2' | -12.50 | 1.25        | 1.52     |
| 78  | S2    | 576  | A2M  | C3'-C2' | -12.47 | 1.25        | 1.52     |
| 79  | L5    | 3718 | A2M  | C3'-C2' | -12.45 | 1.25        | 1.52     |
| 79  | L5    | 398  | A2M  | C3'-C2' | -12.43 | 1.25        | 1.52     |
| 79  | L5    | 4523 | A2M  | C3'-C2' | -12.39 | 1.25        | 1.52     |
| 78  | S2    | 159  | A2M  | C3'-C2' | -12.34 | 1.25        | 1.52     |
| 78  | S2    | 668  | A2M  | C3'-C2' | -12.11 | 1.25        | 1.52     |
| 78  | S2    | 484  | A2M  | C3'-C2' | -12.11 | 1.26        | 1.52     |
| 78  | S2    | 1326 | UY1  | C6-C5   | 11.06  | 1.48        | 1.35     |
| 79  | L5    | 3818 | UY1  | C6-C5   | 10.99  | 1.48        | 1.35     |
| 79  | L5    | 4220 | 6MZ  | C6-N6   | 10.85  | 1.45        | 1.34     |
| 78  | S2    | 1832 | 6MZ  | C6-N6   | 10.47  | 1.45        | 1.34     |
| 78  | S2    | 1326 | UY1  | C2-N1   | 9.59   | 1.49        | 1.36     |
| 79  | L5    | 3818 | UY1  | C2-N1   | 9.51   | 1.49        | 1.36     |
| 76  | Pt    | 8    | 4SU  | C4-N3   | 7.96   | 1.46        | 1.37     |
| 78  | S2    | 1248 | B8N  | C4-N3   | -7.84  | 1.25        | 1.40     |
| 78  | S2    | 1248 | B8N  | C6-N1   | 7.57   | 1.55        | 1.36     |
| 78  | S2    | 1326 | UY1  | C2-N3   | 7.36   | 1.50        | 1.37     |
| 79  | L5    | 3818 | UY1  | C2-N3   | 7.29   | 1.50        | 1.37     |
| 79  | L5    | 4530 | UR3  | C2-N1   | 7.21   | 1.48        | 1.38     |
| 78  | S2    | 428  | OMU  | C2-N1   | 7.19   | 1.50        | 1.38     |
| 79  | L5    | 2415 | OMU  | C2-N1   | 7.12   | 1.49        | 1.38     |
| 78  | S2    | 627  | OMU  | C2-N1   | 7.07   | 1.49        | 1.38     |
| 78  | S2    | 1842 | 4AC  | C4-N3   | 7.06   | 1.45        | 1.32     |
| 79  | L5    | 4227 | OMU  | C2-N1   | 7.03   | 1.49        | 1.38     |
| 78  | S2    | 1337 | 4AC  | C4-N3   | 7.02   | 1.45        | 1.32     |
| 78  | S2    | 172  | OMU  | C2-N1   | 7.02   | 1.49        | 1.38     |
| 78  | S2    | 1288 | OMU  | C2-N1   | 7.01   | 1.49        | 1.38     |
| 79  | L5    | 2837 | OMU  | C2-N1   | 7.01   | 1.49        | 1.38     |
| 76  | Pt    | 8    | 4SU  | C2-N3   | 6.97   | 1.50        | 1.38     |
| 78  | S2    | 668  | A2M  | O4'-C4' | -6.96  | 1.29        | 1.45     |
| 79  | L5    | 4498 | OMU  | C2-N1   | 6.93   | 1.49        | 1.38     |
| 78  | S2    | 1804 | OMU  | C2-N1   | 6.90   | 1.49        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 78  | S2    | 121  | OMU  | C2-N1   | 6.89  | 1.49        | 1.38     |
| 79  | L5    | 4306 | OMU  | C2-N1   | 6.88  | 1.49        | 1.38     |
| 79  | L5    | 3925 | OMU  | C2-N1   | 6.88  | 1.49        | 1.38     |
| 78  | S2    | 627  | OMU  | C2-N3   | 6.86  | 1.50        | 1.38     |
| 78  | S2    | 172  | OMU  | C2-N3   | 6.83  | 1.50        | 1.38     |
| 78  | S2    | 428  | OMU  | C2-N3   | 6.82  | 1.50        | 1.38     |
| 78  | S2    | 116  | OMU  | C2-N3   | 6.79  | 1.50        | 1.38     |
| 78  | S2    | 121  | OMU  | C2-N3   | 6.79  | 1.50        | 1.38     |
| 76  | Pt    | 8    | 4SU  | C2-N1   | 6.77  | 1.49        | 1.38     |
| 78  | S2    | 354  | OMU  | C2-N1   | 6.77  | 1.49        | 1.38     |
| 79  | L5    | 1524 | A2M  | O4'-C4' | -6.76 | 1.29        | 1.45     |
| 78  | S2    | 116  | OMU  | C2-N1   | 6.76  | 1.49        | 1.38     |
| 79  | L5    | 4620 | OMU  | C2-N1   | 6.76  | 1.49        | 1.38     |
| 79  | L5    | 2837 | OMU  | C2-N3   | 6.75  | 1.50        | 1.38     |
| 78  | S2    | 1288 | OMU  | C2-N3   | 6.75  | 1.50        | 1.38     |
| 78  | S2    | 1337 | 4AC  | C2-N3   | 6.74  | 1.50        | 1.36     |
| 78  | S2    | 1842 | 4AC  | C2-N3   | 6.73  | 1.50        | 1.36     |
| 79  | L5    | 3867 | A2M  | O4'-C4' | -6.73 | 1.30        | 1.45     |
| 79  | L5    | 2415 | OMU  | C2-N3   | 6.72  | 1.49        | 1.38     |
| 79  | L5    | 4306 | OMU  | C2-N3   | 6.72  | 1.49        | 1.38     |
| 78  | S2    | 354  | OMU  | C2-N3   | 6.71  | 1.49        | 1.38     |
| 78  | S2    | 1804 | OMU  | C2-N3   | 6.71  | 1.49        | 1.38     |
| 76  | Pt    | 47   | G7M  | C4-N3   | 6.70  | 1.50        | 1.34     |
| 78  | S2    | 1678 | A2M  | O4'-C4' | -6.70 | 1.30        | 1.45     |
| 79  | L5    | 3925 | OMU  | C2-N3   | 6.68  | 1.49        | 1.38     |
| 79  | L5    | 4227 | OMU  | C2-N3   | 6.66  | 1.49        | 1.38     |
| 79  | L5    | 4498 | OMU  | C2-N3   | 6.63  | 1.49        | 1.38     |
| 79  | L5    | 4620 | OMU  | C2-N3   | 6.63  | 1.49        | 1.38     |
| 79  | L5    | 400  | A2M  | O4'-C4' | -6.62 | 1.30        | 1.45     |
| 78  | S2    | 1639 | G7M  | C4-N3   | 6.61  | 1.50        | 1.34     |
| 79  | L5    | 4571 | A2M  | O4'-C4' | -6.60 | 1.30        | 1.45     |
| 79  | L5    | 2815 | A2M  | O4'-C4' | -6.60 | 1.30        | 1.45     |
| 79  | L5    | 1326 | A2M  | O4'-C4' | -6.59 | 1.30        | 1.45     |
| 79  | L5    | 4523 | A2M  | O4'-C4' | -6.58 | 1.30        | 1.45     |
| 78  | S2    | 512  | A2M  | O4'-C4' | -6.56 | 1.30        | 1.45     |
| 79  | L5    | 2363 | A2M  | O4'-C4' | -6.56 | 1.30        | 1.45     |
| 1   | LA    | 216  | V5N  | CG-ND1  | -6.55 | 1.31        | 1.37     |
| 79  | L5    | 3724 | A2M  | O4'-C4' | -6.54 | 1.30        | 1.45     |
| 78  | S2    | 159  | A2M  | O4'-C4' | -6.53 | 1.30        | 1.45     |
| 78  | S2    | 27   | A2M  | O4'-C4' | -6.52 | 1.30        | 1.45     |
| 79  | L5    | 4590 | A2M  | O4'-C4' | -6.52 | 1.30        | 1.45     |
| 79  | L5    | 3723 | A2M  | O4'-C4' | -6.51 | 1.30        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 78  | S2    | 590  | A2M  | O4'-C4' | -6.50 | 1.30        | 1.45     |
| 79  | L5    | 3825 | A2M  | O4'-C4' | -6.50 | 1.30        | 1.45     |
| 78  | S2    | 576  | A2M  | O4'-C4' | -6.50 | 1.30        | 1.45     |
| 78  | S2    | 484  | A2M  | O4'-C4' | -6.47 | 1.30        | 1.45     |
| 79  | L5    | 1871 | A2M  | O4'-C4' | -6.46 | 1.30        | 1.45     |
| 78  | S2    | 166  | A2M  | O4'-C4' | -6.46 | 1.30        | 1.45     |
| 46  | La    | 39   | V5N  | CG-ND1  | -6.45 | 1.31        | 1.37     |
| 78  | S2    | 99   | A2M  | O4'-C4' | -6.44 | 1.30        | 1.45     |
| 78  | S2    | 1031 | A2M  | O4'-C4' | -6.43 | 1.30        | 1.45     |
| 79  | L5    | 2401 | A2M  | O4'-C4' | -6.42 | 1.30        | 1.45     |
| 79  | L5    | 398  | A2M  | O4'-C4' | -6.40 | 1.30        | 1.45     |
| 78  | S2    | 1383 | A2M  | O4'-C4' | -6.39 | 1.30        | 1.45     |
| 78  | S2    | 468  | A2M  | O4'-C4' | -6.39 | 1.30        | 1.45     |
| 79  | L5    | 3718 | A2M  | O4'-C4' | -6.35 | 1.30        | 1.45     |
| 78  | S2    | 1337 | 4AC  | C6-C5   | 6.34  | 1.49        | 1.35     |
| 79  | L5    | 3785 | A2M  | O4'-C4' | -6.34 | 1.30        | 1.45     |
| 79  | L5    | 3830 | A2M  | O4'-C4' | -6.34 | 1.30        | 1.45     |
| 79  | L5    | 1534 | A2M  | O4'-C4' | -6.30 | 1.30        | 1.45     |
| 78  | S2    | 1842 | 4AC  | C6-C5   | 6.26  | 1.49        | 1.35     |
| 79  | L5    | 4530 | UR3  | C6-C5   | 6.08  | 1.49        | 1.35     |
| 78  | S2    | 1248 | B8N  | C6-C5   | 5.90  | 1.43        | 1.34     |
| 78  | S2    | 1248 | B8N  | C2-N1   | 5.89  | 1.56        | 1.39     |
| 76  | Pt    | 47   | G7M  | C2-N2   | 5.86  | 1.48        | 1.34     |
| 78  | S2    | 1639 | G7M  | C2-N2   | 5.82  | 1.48        | 1.34     |
| 76  | Pt    | 8    | 4SU  | C6-C5   | 5.81  | 1.48        | 1.35     |
| 78  | S2    | 627  | OMU  | C6-C5   | 5.72  | 1.48        | 1.35     |
| 78  | S2    | 1288 | OMU  | C6-C5   | 5.70  | 1.48        | 1.35     |
| 78  | S2    | 172  | OMU  | C6-C5   | 5.68  | 1.48        | 1.35     |
| 79  | L5    | 4498 | OMU  | C6-C5   | 5.68  | 1.48        | 1.35     |
| 78  | S2    | 428  | OMU  | C6-C5   | 5.68  | 1.48        | 1.35     |
| 79  | L5    | 2837 | OMU  | C6-C5   | 5.67  | 1.48        | 1.35     |
| 79  | L5    | 4227 | OMU  | C6-C5   | 5.66  | 1.48        | 1.35     |
| 79  | L5    | 3925 | OMU  | C6-C5   | 5.63  | 1.48        | 1.35     |
| 79  | L5    | 4306 | OMU  | C6-C5   | 5.62  | 1.48        | 1.35     |
| 78  | S2    | 121  | OMU  | C6-C5   | 5.61  | 1.48        | 1.35     |
| 78  | S2    | 354  | OMU  | C6-C5   | 5.60  | 1.48        | 1.35     |
| 78  | S2    | 1804 | OMU  | C6-C5   | 5.60  | 1.48        | 1.35     |
| 79  | L5    | 3785 | A2M  | C3'-C4' | 5.59  | 1.67        | 1.53     |
| 79  | L5    | 2415 | OMU  | C6-C5   | 5.58  | 1.48        | 1.35     |
| 79  | L5    | 4620 | OMU  | C6-C5   | 5.58  | 1.48        | 1.35     |
| 78  | S2    | 116  | OMU  | C6-C5   | 5.58  | 1.48        | 1.35     |
| 76  | Pt    | 47   | G7M  | C2-N3   | 5.52  | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 79  | L5    | 4571 | A2M  | C6-N6   | 5.48 | 1.47        | 1.34     |
| 78  | S2    | 1337 | 4AC  | C4-N4   | 5.45 | 1.47        | 1.39     |
| 78  | S2    | 1842 | 4AC  | C4-N4   | 5.44 | 1.47        | 1.39     |
| 78  | S2    | 576  | A2M  | C6-N6   | 5.43 | 1.47        | 1.34     |
| 78  | S2    | 468  | A2M  | C6-N6   | 5.43 | 1.47        | 1.34     |
| 78  | S2    | 590  | A2M  | C6-N6   | 5.43 | 1.47        | 1.34     |
| 78  | S2    | 1383 | A2M  | C6-N6   | 5.42 | 1.47        | 1.34     |
| 79  | L5    | 3724 | A2M  | C6-N6   | 5.42 | 1.47        | 1.34     |
| 78  | S2    | 166  | A2M  | C6-N6   | 5.42 | 1.47        | 1.34     |
| 79  | L5    | 3723 | A2M  | C6-N6   | 5.42 | 1.47        | 1.34     |
| 78  | S2    | 484  | A2M  | C6-N6   | 5.41 | 1.47        | 1.34     |
| 78  | S2    | 159  | A2M  | C6-N6   | 5.41 | 1.47        | 1.34     |
| 78  | S2    | 1031 | A2M  | C6-N6   | 5.41 | 1.47        | 1.34     |
| 78  | S2    | 512  | A2M  | C6-N6   | 5.41 | 1.47        | 1.34     |
| 78  | S2    | 27   | A2M  | C6-N6   | 5.41 | 1.47        | 1.34     |
| 78  | S2    | 668  | A2M  | C6-N6   | 5.41 | 1.47        | 1.34     |
| 78  | S2    | 1639 | G7M  | C2-N3   | 5.41 | 1.46        | 1.33     |
| 79  | L5    | 1871 | A2M  | C6-N6   | 5.40 | 1.47        | 1.34     |
| 79  | L5    | 3867 | A2M  | C6-N6   | 5.40 | 1.47        | 1.34     |
| 79  | L5    | 400  | A2M  | C6-N6   | 5.39 | 1.47        | 1.34     |
| 78  | S2    | 1678 | A2M  | C6-N6   | 5.39 | 1.47        | 1.34     |
| 79  | L5    | 1524 | A2M  | C6-N6   | 5.39 | 1.47        | 1.34     |
| 79  | L5    | 3718 | A2M  | C6-N6   | 5.39 | 1.47        | 1.34     |
| 79  | L5    | 4590 | A2M  | C6-N6   | 5.38 | 1.47        | 1.34     |
| 79  | L5    | 4523 | A2M  | C6-N6   | 5.38 | 1.47        | 1.34     |
| 79  | L5    | 2401 | A2M  | C6-N6   | 5.38 | 1.47        | 1.34     |
| 79  | L5    | 398  | A2M  | C6-N6   | 5.37 | 1.47        | 1.34     |
| 79  | L5    | 2815 | A2M  | C6-N6   | 5.36 | 1.47        | 1.34     |
| 79  | L5    | 3825 | A2M  | C6-N6   | 5.35 | 1.47        | 1.34     |
| 79  | L5    | 3830 | A2M  | C6-N6   | 5.35 | 1.47        | 1.34     |
| 79  | L5    | 1326 | A2M  | C6-N6   | 5.34 | 1.47        | 1.34     |
| 79  | L5    | 2363 | A2M  | C6-N6   | 5.33 | 1.47        | 1.34     |
| 78  | S2    | 99   | A2M  | C6-N6   | 5.33 | 1.47        | 1.34     |
| 79  | L5    | 3785 | A2M  | C6-N6   | 5.33 | 1.47        | 1.34     |
| 79  | L5    | 1534 | A2M  | C3'-C4' | 5.32 | 1.66        | 1.53     |
| 78  | S2    | 668  | A2M  | C3'-C4' | 5.28 | 1.66        | 1.53     |
| 79  | L5    | 1534 | A2M  | C6-N6   | 5.27 | 1.47        | 1.34     |
| 78  | S2    | 159  | A2M  | C3'-C4' | 5.27 | 1.66        | 1.53     |
| 78  | S2    | 468  | A2M  | C3'-C4' | 5.27 | 1.66        | 1.53     |
| 79  | L5    | 3830 | A2M  | C3'-C4' | 5.25 | 1.66        | 1.53     |
| 78  | S2    | 1326 | UY1  | C6-N1   | 5.24 | 1.44        | 1.36     |
| 78  | S2    | 1678 | A2M  | C3'-C4' | 5.24 | 1.66        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 78  | S2    | 484  | A2M  | C3'-C4' | 5.22  | 1.66        | 1.53     |
| 79  | L5    | 3724 | A2M  | C3'-C4' | 5.22  | 1.66        | 1.53     |
| 78  | S2    | 99   | A2M  | C3'-C4' | 5.20  | 1.66        | 1.53     |
| 79  | L5    | 1326 | A2M  | C3'-C4' | 5.20  | 1.66        | 1.53     |
| 79  | L5    | 3723 | A2M  | C3'-C4' | 5.20  | 1.66        | 1.53     |
| 79  | L5    | 3818 | UY1  | C6-N1   | 5.19  | 1.44        | 1.36     |
| 79  | L5    | 4523 | A2M  | C3'-C4' | 5.17  | 1.66        | 1.53     |
| 78  | S2    | 1031 | A2M  | C3'-C4' | 5.17  | 1.66        | 1.53     |
| 79  | L5    | 2363 | A2M  | C3'-C4' | 5.17  | 1.66        | 1.53     |
| 78  | S2    | 590  | A2M  | C3'-C4' | 5.16  | 1.66        | 1.53     |
| 79  | L5    | 4571 | A2M  | C3'-C4' | 5.16  | 1.66        | 1.53     |
| 79  | L5    | 3718 | A2M  | C3'-C4' | 5.15  | 1.66        | 1.53     |
| 79  | L5    | 3825 | A2M  | C3'-C4' | 5.15  | 1.66        | 1.53     |
| 79  | L5    | 398  | A2M  | C3'-C4' | 5.13  | 1.66        | 1.53     |
| 79  | L5    | 400  | A2M  | C3'-C4' | 5.13  | 1.66        | 1.53     |
| 79  | L5    | 1871 | A2M  | C3'-C4' | 5.11  | 1.66        | 1.53     |
| 78  | S2    | 576  | A2M  | C3'-C4' | 5.09  | 1.66        | 1.53     |
| 79  | L5    | 2401 | A2M  | C3'-C4' | 5.09  | 1.66        | 1.53     |
| 78  | S2    | 27   | A2M  | C3'-C4' | 5.08  | 1.66        | 1.53     |
| 78  | S2    | 1383 | A2M  | C3'-C4' | 5.07  | 1.66        | 1.53     |
| 79  | L5    | 2815 | A2M  | C3'-C4' | 5.07  | 1.65        | 1.53     |
| 79  | L5    | 4590 | A2M  | C3'-C4' | 5.06  | 1.65        | 1.53     |
| 78  | S2    | 166  | A2M  | C3'-C4' | 5.04  | 1.65        | 1.53     |
| 78  | S2    | 512  | A2M  | C3'-C4' | 5.04  | 1.65        | 1.53     |
| 79  | L5    | 1524 | A2M  | C1'-N9  | -5.03 | 1.32        | 1.46     |
| 79  | L5    | 1524 | A2M  | C3'-C4' | 5.02  | 1.65        | 1.53     |
| 79  | L5    | 3867 | A2M  | C3'-C4' | 5.02  | 1.65        | 1.53     |
| 79  | L5    | 4530 | UR3  | C2-N3   | 5.01  | 1.48        | 1.39     |
| 76  | Pt    | 8    | 4SU  | C5-C4   | 4.96  | 1.49        | 1.42     |
| 78  | S2    | 590  | A2M  | C1'-N9  | -4.91 | 1.32        | 1.46     |
| 78  | S2    | 1850 | MA6  | C6-N6   | 4.69  | 1.50        | 1.36     |
| 78  | S2    | 1851 | MA6  | C6-N6   | 4.66  | 1.50        | 1.36     |
| 78  | S2    | 576  | A2M  | C1'-N9  | -4.61 | 1.33        | 1.46     |
| 76  | Pt    | 8    | 4SU  | C4-S4   | -4.60 | 1.59        | 1.68     |
| 79  | L5    | 4590 | A2M  | C1'-N9  | -4.56 | 1.33        | 1.46     |
| 78  | S2    | 1383 | A2M  | O4'-C1' | 4.53  | 1.52        | 1.42     |
| 78  | S2    | 1337 | 4AC  | C5-C4   | 4.53  | 1.50        | 1.40     |
| 79  | L5    | 2401 | A2M  | C1'-N9  | -4.50 | 1.33        | 1.46     |
| 79  | L5    | 3718 | A2M  | O4'-C1' | 4.49  | 1.52        | 1.42     |
| 79  | L5    | 1534 | A2M  | C1'-N9  | -4.48 | 1.33        | 1.46     |
| 78  | S2    | 166  | A2M  | O4'-C1' | 4.47  | 1.52        | 1.42     |
| 79  | L5    | 1871 | A2M  | C1'-N9  | -4.46 | 1.33        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 79  | L5    | 3724 | A2M  | O4'-C1' | 4.46  | 1.52        | 1.42     |
| 79  | L5    | 3830 | A2M  | O4'-C1' | 4.46  | 1.52        | 1.42     |
| 79  | L5    | 398  | A2M  | O4'-C1' | 4.46  | 1.52        | 1.42     |
| 78  | S2    | 99   | A2M  | O4'-C1' | 4.46  | 1.52        | 1.42     |
| 79  | L5    | 2401 | A2M  | O4'-C1' | 4.44  | 1.52        | 1.42     |
| 78  | S2    | 1031 | A2M  | O4'-C1' | 4.44  | 1.52        | 1.42     |
| 79  | L5    | 3785 | A2M  | C1'-N9  | -4.44 | 1.33        | 1.46     |
| 78  | S2    | 166  | A2M  | C1'-N9  | -4.44 | 1.33        | 1.46     |
| 79  | L5    | 4590 | A2M  | O4'-C1' | 4.44  | 1.52        | 1.42     |
| 78  | S2    | 1842 | 4AC  | C5-C4   | 4.44  | 1.50        | 1.40     |
| 79  | L5    | 3723 | A2M  | O4'-C1' | 4.43  | 1.52        | 1.42     |
| 79  | L5    | 2815 | A2M  | C1'-N9  | -4.42 | 1.33        | 1.46     |
| 79  | L5    | 2815 | A2M  | O4'-C1' | 4.42  | 1.52        | 1.42     |
| 78  | S2    | 1678 | A2M  | O4'-C1' | 4.42  | 1.52        | 1.42     |
| 78  | S2    | 576  | A2M  | O4'-C1' | 4.42  | 1.52        | 1.42     |
| 78  | S2    | 1842 | 4AC  | C2-N1   | 4.41  | 1.49        | 1.40     |
| 78  | S2    | 1678 | A2M  | C1'-N9  | -4.41 | 1.33        | 1.46     |
| 79  | L5    | 1871 | A2M  | O4'-C1' | 4.40  | 1.52        | 1.42     |
| 78  | S2    | 1031 | A2M  | C1'-N9  | -4.39 | 1.33        | 1.46     |
| 78  | S2    | 512  | A2M  | C1'-N9  | -4.39 | 1.33        | 1.46     |
| 78  | S2    | 468  | A2M  | O4'-C1' | 4.39  | 1.52        | 1.42     |
| 79  | L5    | 3724 | A2M  | C1'-N9  | -4.38 | 1.33        | 1.46     |
| 79  | L5    | 1326 | A2M  | C1'-N9  | -4.38 | 1.33        | 1.46     |
| 79  | L5    | 2363 | A2M  | C1'-N9  | -4.38 | 1.33        | 1.46     |
| 78  | S2    | 1337 | 4AC  | C2-N1   | 4.38  | 1.49        | 1.40     |
| 78  | S2    | 99   | A2M  | C1'-N9  | -4.38 | 1.33        | 1.46     |
| 79  | L5    | 4571 | A2M  | O4'-C1' | 4.38  | 1.52        | 1.42     |
| 78  | S2    | 1383 | A2M  | C1'-N9  | -4.37 | 1.33        | 1.46     |
| 79  | L5    | 3825 | A2M  | O4'-C1' | 4.37  | 1.52        | 1.42     |
| 79  | L5    | 2363 | A2M  | O4'-C1' | 4.36  | 1.52        | 1.42     |
| 78  | S2    | 27   | A2M  | C1'-N9  | -4.35 | 1.34        | 1.46     |
| 78  | S2    | 668  | A2M  | C1'-N9  | -4.35 | 1.34        | 1.46     |
| 79  | L5    | 3830 | A2M  | C1'-N9  | -4.35 | 1.34        | 1.46     |
| 79  | L5    | 1534 | A2M  | O4'-C1' | 4.35  | 1.52        | 1.42     |
| 79  | L5    | 3723 | A2M  | C1'-N9  | -4.34 | 1.34        | 1.46     |
| 79  | L5    | 3867 | A2M  | O4'-C1' | 4.34  | 1.52        | 1.42     |
| 79  | L5    | 400  | A2M  | C1'-N9  | -4.34 | 1.34        | 1.46     |
| 78  | S2    | 468  | A2M  | C1'-N9  | -4.34 | 1.34        | 1.46     |
| 79  | L5    | 400  | A2M  | O4'-C1' | 4.34  | 1.52        | 1.42     |
| 78  | S2    | 512  | A2M  | O4'-C1' | 4.33  | 1.52        | 1.42     |
| 79  | L5    | 4523 | A2M  | O4'-C1' | 4.32  | 1.52        | 1.42     |
| 79  | L5    | 3825 | A2M  | C1'-N9  | -4.31 | 1.34        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 79  | L5    | 3867 | A2M  | C1'-N9  | -4.31 | 1.34        | 1.46     |
| 79  | L5    | 1326 | A2M  | O4'-C1' | 4.31  | 1.52        | 1.42     |
| 79  | L5    | 4523 | A2M  | C1'-N9  | -4.31 | 1.34        | 1.46     |
| 78  | S2    | 159  | A2M  | C1'-N9  | -4.30 | 1.34        | 1.46     |
| 79  | L5    | 4571 | A2M  | C1'-N9  | -4.29 | 1.34        | 1.46     |
| 78  | S2    | 27   | A2M  | O4'-C1' | 4.29  | 1.52        | 1.42     |
| 78  | S2    | 590  | A2M  | O4'-C1' | 4.26  | 1.52        | 1.42     |
| 78  | S2    | 1337 | 4AC  | C7-N4   | 4.22  | 1.45        | 1.37     |
| 79  | L5    | 398  | A2M  | C1'-N9  | -4.21 | 1.34        | 1.46     |
| 1   | LA    | 216  | V5N  | CD2-NE2 | -4.20 | 1.31        | 1.37     |
| 78  | S2    | 159  | A2M  | O4'-C1' | 4.19  | 1.51        | 1.42     |
| 78  | S2    | 484  | A2M  | O4'-C1' | 4.19  | 1.51        | 1.42     |
| 78  | S2    | 1842 | 4AC  | C7-N4   | 4.19  | 1.44        | 1.37     |
| 78  | S2    | 484  | A2M  | C1'-N9  | -4.18 | 1.34        | 1.46     |
| 78  | S2    | 627  | OMU  | C4-N3   | 4.18  | 1.46        | 1.38     |
| 78  | S2    | 428  | OMU  | C4-N3   | 4.14  | 1.46        | 1.38     |
| 79  | L5    | 3718 | A2M  | C1'-N9  | -4.14 | 1.34        | 1.46     |
| 78  | S2    | 1639 | G7M  | C5-N7   | -4.13 | 1.34        | 1.39     |
| 19  | SX    | 62   | HY3  | C4-C5   | 4.13  | 1.59        | 1.53     |
| 78  | S2    | 1288 | OMU  | C4-N3   | 4.12  | 1.45        | 1.38     |
| 19  | SX    | 62   | HY3  | C5-N    | -4.11 | 1.34        | 1.49     |
| 78  | S2    | 1804 | OMU  | C4-N3   | 4.11  | 1.45        | 1.38     |
| 76  | Pt    | 47   | G7M  | C5-C6   | 4.10  | 1.54        | 1.43     |
| 79  | L5    | 1524 | A2M  | O4'-C1' | 4.09  | 1.51        | 1.42     |
| 78  | S2    | 172  | OMU  | C4-N3   | 4.09  | 1.45        | 1.38     |
| 78  | S2    | 121  | OMU  | C4-N3   | 4.07  | 1.45        | 1.38     |
| 78  | S2    | 116  | OMU  | C4-N3   | 4.07  | 1.45        | 1.38     |
| 46  | La    | 39   | V5N  | CD2-NE2 | -4.06 | 1.31        | 1.37     |
| 79  | L5    | 4306 | OMU  | C4-N3   | 4.05  | 1.45        | 1.38     |
| 78  | S2    | 1639 | G7M  | C5-C6   | 4.04  | 1.54        | 1.43     |
| 78  | S2    | 354  | OMU  | C4-N3   | 4.03  | 1.45        | 1.38     |
| 79  | L5    | 2837 | OMU  | C4-N3   | 4.02  | 1.45        | 1.38     |
| 79  | L5    | 3925 | OMU  | C4-N3   | 4.02  | 1.45        | 1.38     |
| 79  | L5    | 2415 | OMU  | C4-N3   | 3.97  | 1.45        | 1.38     |
| 79  | L5    | 3785 | A2M  | O4'-C1' | 3.94  | 1.51        | 1.42     |
| 79  | L5    | 4620 | OMU  | C4-N3   | 3.93  | 1.45        | 1.38     |
| 76  | Pt    | 47   | G7M  | C5-N7   | -3.91 | 1.34        | 1.39     |
| 78  | S2    | 668  | A2M  | O4'-C1' | 3.91  | 1.51        | 1.42     |
| 79  | L5    | 4498 | OMU  | C4-N3   | 3.91  | 1.45        | 1.38     |
| 79  | L5    | 4227 | OMU  | C4-N3   | 3.91  | 1.45        | 1.38     |
| 78  | S2    | 1326 | UY1  | C4-N3   | 3.84  | 1.46        | 1.38     |
| 79  | L5    | 3818 | UY1  | C4-N3   | 3.75  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 78  | S2    | 1232 | PSU  | C6-C5 | 3.62 | 1.39        | 1.35     |
| 78  | S2    | 573  | PSU  | C6-C5 | 3.59 | 1.39        | 1.35     |
| 79  | L5    | 1677 | PSU  | C6-C5 | 3.59 | 1.39        | 1.35     |
| 78  | S2    | 1842 | 4AC  | C6-N1 | 3.59 | 1.46        | 1.38     |
| 78  | S2    | 1625 | PSU  | C6-C5 | 3.58 | 1.39        | 1.35     |
| 78  | S2    | 1337 | 4AC  | C6-N1 | 3.58 | 1.46        | 1.38     |
| 78  | S2    | 609  | PSU  | C6-C5 | 3.57 | 1.39        | 1.35     |
| 79  | L5    | 4420 | PSU  | C6-C5 | 3.57 | 1.39        | 1.35     |
| 76  | Pt    | 47   | G7M  | C2-N1 | 3.56 | 1.46        | 1.37     |
| 79  | L5    | 1781 | PSU  | C6-C5 | 3.56 | 1.39        | 1.35     |
| 78  | S2    | 801  | PSU  | C6-C5 | 3.56 | 1.39        | 1.35     |
| 78  | S2    | 863  | PSU  | C6-C5 | 3.53 | 1.39        | 1.35     |
| 78  | S2    | 119  | PSU  | C6-C5 | 3.52 | 1.39        | 1.35     |
| 76  | Pt    | 56   | PSU  | C6-C5 | 3.49 | 1.39        | 1.35     |
| 78  | S2    | 1177 | PSU  | C6-C5 | 3.48 | 1.39        | 1.35     |
| 79  | L5    | 4471 | PSU  | C6-C5 | 3.48 | 1.39        | 1.35     |
| 78  | S2    | 1004 | PSU  | C6-C5 | 3.48 | 1.39        | 1.35     |
| 78  | S2    | 1239 | PSU  | C6-C5 | 3.48 | 1.39        | 1.35     |
| 79  | L5    | 1779 | PSU  | C6-C5 | 3.47 | 1.39        | 1.35     |
| 79  | L5    | 3758 | PSU  | C6-C5 | 3.47 | 1.39        | 1.35     |
| 79  | L5    | 3762 | PSU  | C6-C5 | 3.46 | 1.39        | 1.35     |
| 79  | L5    | 1744 | PSU  | C6-C5 | 3.46 | 1.39        | 1.35     |
| 78  | S2    | 1639 | G7M  | C2-N1 | 3.45 | 1.46        | 1.37     |
| 79  | L5    | 5010 | PSU  | C6-C5 | 3.45 | 1.39        | 1.35     |
| 78  | S2    | 649  | PSU  | C6-C5 | 3.45 | 1.39        | 1.35     |
| 79  | L5    | 2632 | PSU  | C6-C5 | 3.44 | 1.39        | 1.35     |
| 79  | L5    | 2839 | PSU  | C6-C5 | 3.43 | 1.39        | 1.35     |
| 78  | S2    | 93   | PSU  | C6-C5 | 3.43 | 1.39        | 1.35     |
| 78  | S2    | 1174 | PSU  | C6-C5 | 3.43 | 1.39        | 1.35     |
| 79  | L5    | 4293 | PSU  | C6-C5 | 3.43 | 1.39        | 1.35     |
| 78  | S2    | 36   | PSU  | C6-C5 | 3.43 | 1.39        | 1.35     |
| 79  | L5    | 3844 | PSU  | C6-C5 | 3.42 | 1.39        | 1.35     |
| 79  | L5    | 4531 | PSU  | C6-C5 | 3.42 | 1.39        | 1.35     |
| 78  | S2    | 1244 | PSU  | C6-C5 | 3.41 | 1.39        | 1.35     |
| 78  | S2    | 1238 | PSU  | C6-C5 | 3.41 | 1.39        | 1.35     |
| 79  | L5    | 2843 | PSU  | C6-C5 | 3.41 | 1.39        | 1.35     |
| 78  | S2    | 1692 | PSU  | C6-C5 | 3.40 | 1.39        | 1.35     |
| 79  | L5    | 1582 | PSU  | C6-C5 | 3.40 | 1.39        | 1.35     |
| 79  | L5    | 3764 | PSU  | C6-C5 | 3.40 | 1.39        | 1.35     |
| 78  | S2    | 406  | PSU  | C6-C5 | 3.40 | 1.39        | 1.35     |
| 79  | L5    | 1862 | PSU  | C6-C5 | 3.40 | 1.39        | 1.35     |
| 79  | L5    | 4296 | PSU  | C6-C5 | 3.39 | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 79  | L5    | 3768 | PSU  | C6-C5 | 3.39 | 1.39        | 1.35     |
| 78  | S2    | 34   | PSU  | C6-C5 | 3.39 | 1.39        | 1.35     |
| 79  | L5    | 4532 | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 79  | L5    | 4312 | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 78  | S2    | 686  | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 78  | S2    | 1367 | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 5   | L8    | 69   | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 79  | L5    | 3884 | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 78  | S2    | 109  | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 79  | L5    | 4493 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 79  | L5    | 4423 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 79  | L5    | 2508 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 78  | S2    | 822  | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 79  | L5    | 1683 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 79  | L5    | 4431 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 79  | L5    | 4636 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 79  | L5    | 4673 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 79  | L5    | 5001 | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 78  | S2    | 866  | PSU  | C6-C5 | 3.36 | 1.39        | 1.35     |
| 78  | S2    | 218  | PSU  | C6-C5 | 3.36 | 1.39        | 1.35     |
| 79  | L5    | 1536 | PSU  | C6-C5 | 3.35 | 1.39        | 1.35     |
| 79  | L5    | 4361 | PSU  | C6-C5 | 3.35 | 1.39        | 1.35     |
| 78  | S2    | 1347 | PSU  | C6-C5 | 3.35 | 1.39        | 1.35     |
| 78  | S2    | 814  | PSU  | C6-C5 | 3.34 | 1.39        | 1.35     |
| 79  | L5    | 1792 | PSU  | C6-C5 | 3.34 | 1.39        | 1.35     |
| 79  | L5    | 3639 | PSU  | C6-C5 | 3.34 | 1.39        | 1.35     |
| 78  | S2    | 1643 | PSU  | C6-C5 | 3.34 | 1.39        | 1.35     |
| 78  | S2    | 815  | PSU  | C6-C5 | 3.34 | 1.39        | 1.35     |
| 78  | S2    | 105  | PSU  | C6-C5 | 3.33 | 1.39        | 1.35     |
| 79  | L5    | 3715 | PSU  | C6-C5 | 3.33 | 1.39        | 1.35     |
| 78  | S2    | 1243 | PSU  | C6-C5 | 3.33 | 1.39        | 1.35     |
| 79  | L5    | 4299 | PSU  | C6-C5 | 3.33 | 1.39        | 1.35     |
| 79  | L5    | 3695 | PSU  | C6-C5 | 3.32 | 1.39        | 1.35     |
| 79  | L5    | 4569 | PSU  | C6-C5 | 3.32 | 1.39        | 1.35     |
| 78  | S2    | 651  | PSU  | C6-C5 | 3.32 | 1.39        | 1.35     |
| 78  | S2    | 966  | PSU  | C6-C5 | 3.31 | 1.39        | 1.35     |
| 78  | S2    | 918  | PSU  | C6-C5 | 3.30 | 1.39        | 1.35     |
| 79  | L5    | 3729 | PSU  | C6-C5 | 3.30 | 1.39        | 1.35     |
| 79  | L5    | 4521 | PSU  | C6-C5 | 3.30 | 1.39        | 1.35     |
| 5   | L8    | 55   | PSU  | C6-C5 | 3.30 | 1.39        | 1.35     |
| 79  | L5    | 3853 | PSU  | C6-C5 | 3.30 | 1.39        | 1.35     |
| 79  | L5    | 4353 | PSU  | C6-C5 | 3.30 | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 78  | S2    | 572  | PSU  | C6-C5   | 3.28  | 1.39        | 1.35     |
| 79  | L5    | 3851 | PSU  | C6-C5   | 3.28  | 1.39        | 1.35     |
| 79  | L5    | 1782 | PSU  | C6-C5   | 3.28  | 1.39        | 1.35     |
| 79  | L5    | 4442 | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 78  | S2    | 296  | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 79  | L5    | 3734 | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 79  | L5    | 4576 | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 79  | L5    | 4628 | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 78  | S2    | 1445 | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 79  | L5    | 3637 | PSU  | C6-C5   | 3.26  | 1.39        | 1.35     |
| 79  | L5    | 1860 | PSU  | C6-C5   | 3.26  | 1.39        | 1.35     |
| 78  | S2    | 1056 | PSU  | C6-C5   | 3.25  | 1.39        | 1.35     |
| 78  | S2    | 681  | PSU  | C6-C5   | 3.25  | 1.39        | 1.35     |
| 79  | L5    | 3920 | PSU  | C6-C5   | 3.23  | 1.39        | 1.35     |
| 79  | L5    | 4972 | PSU  | C6-C5   | 3.22  | 1.39        | 1.35     |
| 78  | S2    | 1081 | PSU  | C6-C5   | 3.21  | 1.39        | 1.35     |
| 79  | L5    | 4689 | PSU  | C6-C5   | 3.21  | 1.39        | 1.35     |
| 78  | S2    | 1136 | PSU  | C6-C5   | 3.21  | 1.39        | 1.35     |
| 79  | L5    | 3770 | PSU  | C6-C5   | 3.20  | 1.39        | 1.35     |
| 79  | L5    | 4579 | PSU  | C6-C5   | 3.17  | 1.39        | 1.35     |
| 79  | L5    | 4457 | PSU  | C6-C5   | 3.16  | 1.39        | 1.35     |
| 79  | L5    | 4552 | PSU  | C6-C5   | 3.11  | 1.38        | 1.35     |
| 79  | L5    | 4530 | UR3  | C6-N1   | 3.10  | 1.45        | 1.38     |
| 78  | S2    | 668  | A2M  | C2'-C1' | 3.10  | 1.61        | 1.53     |
| 76  | Pt    | 8    | 4SU  | C6-N1   | 3.09  | 1.45        | 1.38     |
| 79  | L5    | 3723 | A2M  | O2'-C2' | 3.04  | 1.50        | 1.42     |
| 78  | S2    | 1639 | G7M  | O6-C6   | -3.04 | 1.17        | 1.23     |
| 79  | L5    | 4500 | PSU  | C6-C5   | 3.02  | 1.38        | 1.35     |
| 79  | L5    | 3724 | A2M  | O2'-C2' | 3.01  | 1.50        | 1.42     |
| 79  | L5    | 4620 | OMU  | O4-C4   | -3.01 | 1.18        | 1.24     |
| 79  | L5    | 1524 | A2M  | O2'-C2' | 3.00  | 1.50        | 1.42     |
| 79  | L5    | 2401 | A2M  | O2'-C2' | 3.00  | 1.50        | 1.42     |
| 78  | S2    | 1678 | A2M  | O2'-C2' | 3.00  | 1.50        | 1.42     |
| 76  | Pt    | 47   | G7M  | O6-C6   | -2.99 | 1.17        | 1.23     |
| 79  | L5    | 4227 | OMU  | O4-C4   | -2.99 | 1.18        | 1.24     |
| 79  | L5    | 2415 | OMU  | O4-C4   | -2.98 | 1.18        | 1.24     |
| 79  | L5    | 3718 | A2M  | O2'-C2' | 2.98  | 1.50        | 1.42     |
| 78  | S2    | 590  | A2M  | O2'-C2' | 2.98  | 1.50        | 1.42     |
| 79  | L5    | 400  | A2M  | O2'-C2' | 2.98  | 1.50        | 1.42     |
| 78  | S2    | 1383 | A2M  | O2'-C2' | 2.98  | 1.50        | 1.42     |
| 78  | S2    | 484  | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 78  | S2    | 159  | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 78  | S2    | 1804 | OMU  | O4-C4   | -2.97 | 1.18        | 1.24     |
| 78  | S2    | 116  | OMU  | O4-C4   | -2.97 | 1.18        | 1.24     |
| 79  | L5    | 4571 | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 79  | L5    | 1326 | A2M  | O2'-C2' | 2.96  | 1.50        | 1.42     |
| 78  | S2    | 354  | OMU  | O4-C4   | -2.95 | 1.18        | 1.24     |
| 79  | L5    | 4523 | A2M  | O2'-C2' | 2.95  | 1.50        | 1.42     |
| 78  | S2    | 668  | A2M  | O2'-C2' | 2.95  | 1.50        | 1.42     |
| 78  | S2    | 166  | A2M  | O2'-C2' | 2.95  | 1.50        | 1.42     |
| 78  | S2    | 468  | A2M  | O2'-C2' | 2.95  | 1.50        | 1.42     |
| 79  | L5    | 3825 | A2M  | O2'-C2' | 2.95  | 1.50        | 1.42     |
| 79  | L5    | 4498 | OMU  | O4-C4   | -2.95 | 1.18        | 1.24     |
| 78  | S2    | 484  | A2M  | C2'-C1' | 2.95  | 1.60        | 1.53     |
| 78  | S2    | 1031 | A2M  | O2'-C2' | 2.94  | 1.50        | 1.42     |
| 78  | S2    | 428  | OMU  | O4-C4   | -2.94 | 1.18        | 1.24     |
| 79  | L5    | 4306 | OMU  | O4-C4   | -2.94 | 1.18        | 1.24     |
| 78  | S2    | 576  | A2M  | O2'-C2' | 2.94  | 1.50        | 1.42     |
| 79  | L5    | 3925 | OMU  | O4-C4   | -2.94 | 1.18        | 1.24     |
| 79  | L5    | 2837 | OMU  | O4-C4   | -2.93 | 1.18        | 1.24     |
| 79  | L5    | 2363 | A2M  | O2'-C2' | 2.92  | 1.50        | 1.42     |
| 78  | S2    | 1832 | 6MZ  | C5-C4   | -2.92 | 1.33        | 1.39     |
| 79  | L5    | 4590 | A2M  | O2'-C2' | 2.92  | 1.50        | 1.42     |
| 78  | S2    | 172  | OMU  | O4-C4   | -2.92 | 1.18        | 1.24     |
| 79  | L5    | 3830 | A2M  | O2'-C2' | 2.92  | 1.50        | 1.42     |
| 78  | S2    | 1383 | A2M  | C2'-C1' | 2.92  | 1.60        | 1.53     |
| 79  | L5    | 3785 | A2M  | O2'-C2' | 2.92  | 1.50        | 1.42     |
| 78  | S2    | 27   | A2M  | O2'-C2' | 2.91  | 1.50        | 1.42     |
| 78  | S2    | 121  | OMU  | O4-C4   | -2.91 | 1.18        | 1.24     |
| 78  | S2    | 512  | A2M  | O2'-C2' | 2.91  | 1.50        | 1.42     |
| 79  | L5    | 2815 | A2M  | O2'-C2' | 2.90  | 1.50        | 1.42     |
| 79  | L5    | 2401 | A2M  | C2'-C1' | 2.90  | 1.60        | 1.53     |
| 79  | L5    | 1871 | A2M  | O2'-C2' | 2.90  | 1.50        | 1.42     |
| 78  | S2    | 99   | A2M  | O2'-C2' | 2.89  | 1.50        | 1.42     |
| 78  | S2    | 1288 | OMU  | O4-C4   | -2.88 | 1.18        | 1.24     |
| 78  | S2    | 627  | OMU  | O4-C4   | -2.88 | 1.18        | 1.24     |
| 79  | L5    | 1534 | A2M  | O2'-C2' | 2.88  | 1.50        | 1.42     |
| 79  | L5    | 4220 | 6MZ  | C5-C4   | -2.86 | 1.33        | 1.39     |
| 79  | L5    | 3867 | A2M  | O2'-C2' | 2.85  | 1.49        | 1.42     |
| 78  | S2    | 166  | A2M  | C2'-C1' | 2.85  | 1.60        | 1.53     |
| 79  | L5    | 4403 | PSU  | C6-C5   | 2.84  | 1.38        | 1.35     |
| 79  | L5    | 398  | A2M  | O2'-C2' | 2.84  | 1.49        | 1.42     |
| 78  | S2    | 1288 | OMU  | C6-N1   | 2.84  | 1.44        | 1.38     |
| 78  | S2    | 627  | OMU  | C6-N1   | 2.84  | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 78  | S2    | 428  | OMU  | C6-N1   | 2.83  | 1.44        | 1.38     |
| 79  | L5    | 4306 | OMU  | C6-N1   | 2.82  | 1.44        | 1.38     |
| 78  | S2    | 159  | A2M  | C2'-C1' | 2.81  | 1.60        | 1.53     |
| 79  | L5    | 3723 | A2M  | C2'-C1' | 2.81  | 1.60        | 1.53     |
| 79  | L5    | 4220 | 6MZ  | C5-N7   | -2.81 | 1.33        | 1.39     |
| 78  | S2    | 1804 | OMU  | C6-N1   | 2.80  | 1.44        | 1.38     |
| 79  | L5    | 3718 | A2M  | C2'-C1' | 2.80  | 1.60        | 1.53     |
| 78  | S2    | 576  | A2M  | C2'-C1' | 2.80  | 1.60        | 1.53     |
| 79  | L5    | 3785 | A2M  | C2'-C1' | 2.80  | 1.60        | 1.53     |
| 78  | S2    | 121  | OMU  | C6-N1   | 2.79  | 1.44        | 1.38     |
| 78  | S2    | 468  | A2M  | C2'-C1' | 2.79  | 1.60        | 1.53     |
| 79  | L5    | 3785 | A2M  | C5-C4   | -2.78 | 1.33        | 1.39     |
| 79  | L5    | 3925 | OMU  | C6-N1   | 2.78  | 1.44        | 1.38     |
| 79  | L5    | 1524 | A2M  | C2'-C1' | 2.78  | 1.60        | 1.53     |
| 79  | L5    | 398  | A2M  | C2'-C1' | 2.77  | 1.60        | 1.53     |
| 79  | L5    | 3830 | A2M  | C2'-C1' | 2.77  | 1.60        | 1.53     |
| 79  | L5    | 4523 | A2M  | C2'-C1' | 2.77  | 1.60        | 1.53     |
| 79  | L5    | 2837 | OMU  | C6-N1   | 2.76  | 1.44        | 1.38     |
| 78  | S2    | 1326 | UY1  | C1'-C5  | 2.76  | 1.56        | 1.50     |
| 78  | S2    | 512  | A2M  | C2'-C1' | 2.76  | 1.60        | 1.53     |
| 78  | S2    | 1851 | MA6  | C5-C4   | -2.76 | 1.33        | 1.39     |
| 79  | L5    | 4498 | OMU  | C6-N1   | 2.76  | 1.44        | 1.38     |
| 79  | L5    | 2815 | A2M  | C2'-C1' | 2.75  | 1.60        | 1.53     |
| 78  | S2    | 172  | OMU  | C6-N1   | 2.74  | 1.44        | 1.38     |
| 79  | L5    | 3818 | UY1  | C1'-C5  | 2.74  | 1.56        | 1.50     |
| 79  | L5    | 4227 | OMU  | C6-N1   | 2.74  | 1.44        | 1.38     |
| 79  | L5    | 1871 | A2M  | C5-C4   | -2.74 | 1.33        | 1.39     |
| 78  | S2    | 1031 | A2M  | C2'-C1' | 2.74  | 1.60        | 1.53     |
| 79  | L5    | 3724 | A2M  | C2'-C1' | 2.73  | 1.60        | 1.53     |
| 79  | L5    | 400  | A2M  | C2'-C1' | 2.73  | 1.60        | 1.53     |
| 79  | L5    | 2415 | OMU  | C6-N1   | 2.73  | 1.44        | 1.38     |
| 79  | L5    | 4523 | A2M  | C5-C4   | -2.72 | 1.33        | 1.39     |
| 78  | S2    | 1031 | A2M  | C5-C4   | -2.72 | 1.33        | 1.39     |
| 78  | S2    | 99   | A2M  | C2'-C1' | 2.72  | 1.60        | 1.53     |
| 78  | S2    | 116  | OMU  | C6-N1   | 2.71  | 1.44        | 1.38     |
| 78  | S2    | 354  | OMU  | C6-N1   | 2.71  | 1.44        | 1.38     |
| 78  | S2    | 1832 | 6MZ  | C5-N7   | -2.71 | 1.33        | 1.39     |
| 78  | S2    | 27   | A2M  | C2'-C1' | 2.70  | 1.60        | 1.53     |
| 79  | L5    | 1326 | A2M  | C2'-C1' | 2.69  | 1.60        | 1.53     |
| 79  | L5    | 1534 | A2M  | C5-C4   | -2.69 | 1.34        | 1.39     |
| 76  | Pt    | 47   | G7M  | C6-N1   | 2.69  | 1.43        | 1.38     |
| 78  | S2    | 1678 | A2M  | C5-C4   | -2.68 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 79  | L5    | 2401 | A2M  | C5-C4   | -2.68 | 1.34        | 1.39     |
| 79  | L5    | 3867 | A2M  | C2'-C1' | 2.68  | 1.60        | 1.53     |
| 79  | L5    | 4590 | A2M  | C5-C4   | -2.67 | 1.34        | 1.39     |
| 79  | L5    | 1326 | A2M  | C5-C4   | -2.67 | 1.34        | 1.39     |
| 79  | L5    | 3825 | A2M  | C2'-C1' | 2.67  | 1.59        | 1.53     |
| 78  | S2    | 668  | A2M  | C5-C4   | -2.67 | 1.34        | 1.39     |
| 79  | L5    | 1524 | A2M  | C5-C4   | -2.67 | 1.34        | 1.39     |
| 78  | S2    | 1850 | MA6  | C5-C4   | -2.67 | 1.34        | 1.39     |
| 78  | S2    | 99   | A2M  | C5-C4   | -2.66 | 1.34        | 1.39     |
| 79  | L5    | 4571 | A2M  | C2'-C1' | 2.66  | 1.59        | 1.53     |
| 78  | S2    | 590  | A2M  | C2'-C1' | 2.66  | 1.59        | 1.53     |
| 79  | L5    | 4590 | A2M  | C2'-C1' | 2.66  | 1.59        | 1.53     |
| 78  | S2    | 512  | A2M  | C5-C4   | -2.66 | 1.34        | 1.39     |
| 79  | L5    | 4620 | OMU  | C6-N1   | 2.64  | 1.44        | 1.38     |
| 79  | L5    | 2815 | A2M  | C5-C4   | -2.64 | 1.34        | 1.39     |
| 79  | L5    | 2363 | A2M  | C5-C4   | -2.64 | 1.34        | 1.39     |
| 79  | L5    | 3830 | A2M  | C5-C4   | -2.64 | 1.34        | 1.39     |
| 79  | L5    | 3724 | A2M  | C5-C4   | -2.63 | 1.34        | 1.39     |
| 78  | S2    | 1383 | A2M  | C5-C4   | -2.63 | 1.34        | 1.39     |
| 78  | S2    | 166  | A2M  | C5-C4   | -2.63 | 1.34        | 1.39     |
| 78  | S2    | 576  | A2M  | C5-C4   | -2.62 | 1.34        | 1.39     |
| 78  | S2    | 27   | A2M  | C5-C4   | -2.62 | 1.34        | 1.39     |
| 79  | L5    | 2363 | A2M  | C2'-C1' | 2.62  | 1.59        | 1.53     |
| 79  | L5    | 1871 | A2M  | C2'-C1' | 2.61  | 1.59        | 1.53     |
| 78  | S2    | 590  | A2M  | C5-C4   | -2.61 | 1.34        | 1.39     |
| 79  | L5    | 400  | A2M  | C5-C4   | -2.61 | 1.34        | 1.39     |
| 79  | L5    | 3825 | A2M  | C5-C4   | -2.60 | 1.34        | 1.39     |
| 79  | L5    | 398  | A2M  | C5-C4   | -2.59 | 1.34        | 1.39     |
| 79  | L5    | 3867 | A2M  | C5-C4   | -2.59 | 1.34        | 1.39     |
| 79  | L5    | 3723 | A2M  | C5-C4   | -2.58 | 1.34        | 1.39     |
| 79  | L5    | 4571 | A2M  | C5-C4   | -2.58 | 1.34        | 1.39     |
| 78  | S2    | 1639 | G7M  | C6-N1   | 2.58  | 1.43        | 1.38     |
| 78  | S2    | 1326 | UY1  | O4-C4   | -2.56 | 1.18        | 1.23     |
| 78  | S2    | 468  | A2M  | C5-C4   | -2.55 | 1.34        | 1.39     |
| 79  | L5    | 3718 | A2M  | C5-C4   | -2.54 | 1.34        | 1.39     |
| 78  | S2    | 159  | A2M  | C5-C4   | -2.53 | 1.34        | 1.39     |
| 78  | S2    | 484  | A2M  | C5-C4   | -2.53 | 1.34        | 1.39     |
| 79  | L5    | 3818 | UY1  | O4-C4   | -2.53 | 1.18        | 1.23     |
| 78  | S2    | 1678 | A2M  | C2'-C1' | 2.52  | 1.59        | 1.53     |
| 79  | L5    | 1534 | A2M  | C2'-C1' | 2.49  | 1.59        | 1.53     |
| 78  | S2    | 1842 | 4AC  | O2-C2   | -2.48 | 1.19        | 1.23     |
| 78  | S2    | 627  | OMU  | C5-C4   | 2.46  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 78  | S2    | 1337 | 4AC  | O2-C2 | -2.46 | 1.19        | 1.23     |
| 79  | L5    | 2837 | OMU  | C5-C4 | 2.44  | 1.49        | 1.43     |
| 78  | S2    | 1288 | OMU  | C5-C4 | 2.44  | 1.49        | 1.43     |
| 78  | S2    | 428  | OMU  | C5-C4 | 2.40  | 1.48        | 1.43     |
| 79  | L5    | 4498 | OMU  | O2-C2 | -2.40 | 1.18        | 1.23     |
| 78  | S2    | 172  | OMU  | C5-C4 | 2.39  | 1.48        | 1.43     |
| 79  | L5    | 4498 | OMU  | C5-C4 | 2.38  | 1.48        | 1.43     |
| 79  | L5    | 4227 | OMU  | C5-C4 | 2.37  | 1.48        | 1.43     |
| 78  | S2    | 1850 | MA6  | C5-N7 | -2.36 | 1.34        | 1.39     |
| 79  | L5    | 3925 | OMU  | C5-C4 | 2.36  | 1.48        | 1.43     |
| 79  | L5    | 3925 | OMU  | O2-C2 | -2.34 | 1.18        | 1.23     |
| 78  | S2    | 1804 | OMU  | C5-C4 | 2.33  | 1.48        | 1.43     |
| 78  | S2    | 1804 | OMU  | O2-C2 | -2.32 | 1.18        | 1.23     |
| 79  | L5    | 4306 | OMU  | C5-C4 | 2.31  | 1.48        | 1.43     |
| 78  | S2    | 121  | OMU  | C5-C4 | 2.29  | 1.48        | 1.43     |
| 78  | S2    | 354  | OMU  | C5-C4 | 2.28  | 1.48        | 1.43     |
| 79  | L5    | 3718 | A2M  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 79  | L5    | 4306 | OMU  | O2-C2 | -2.27 | 1.18        | 1.23     |
| 79  | L5    | 4620 | OMU  | O2-C2 | -2.27 | 1.18        | 1.23     |
| 79  | L5    | 4227 | OMU  | O2-C2 | -2.27 | 1.18        | 1.23     |
| 78  | S2    | 116  | OMU  | C5-C4 | 2.27  | 1.48        | 1.43     |
| 79  | L5    | 2415 | OMU  | C5-C4 | 2.27  | 1.48        | 1.43     |
| 79  | L5    | 2837 | OMU  | O2-C2 | -2.25 | 1.18        | 1.23     |
| 78  | S2    | 116  | OMU  | O2-C2 | -2.24 | 1.18        | 1.23     |
| 78  | S2    | 1842 | 4AC  | O7-C7 | -2.24 | 1.18        | 1.23     |
| 78  | S2    | 428  | OMU  | O2-C2 | -2.24 | 1.19        | 1.23     |
| 78  | S2    | 354  | OMU  | O2-C2 | -2.23 | 1.19        | 1.23     |
| 79  | L5    | 4530 | UR3  | O4-C4 | -2.21 | 1.18        | 1.23     |
| 79  | L5    | 4620 | OMU  | C5-C4 | 2.21  | 1.48        | 1.43     |
| 79  | L5    | 2415 | OMU  | O2-C2 | -2.21 | 1.19        | 1.23     |
| 78  | S2    | 121  | OMU  | O2-C2 | -2.21 | 1.19        | 1.23     |
| 78  | S2    | 172  | OMU  | O2-C2 | -2.21 | 1.19        | 1.23     |
| 79  | L5    | 4530 | UR3  | C5-C4 | 2.19  | 1.49        | 1.43     |
| 78  | S2    | 1326 | UY1  | O2-C2 | -2.18 | 1.18        | 1.23     |
| 79  | L5    | 4530 | UR3  | O2-C2 | -2.18 | 1.18        | 1.22     |
| 78  | S2    | 1850 | MA6  | C8-N9 | -2.17 | 1.33        | 1.37     |
| 78  | S2    | 627  | OMU  | O2-C2 | -2.16 | 1.19        | 1.23     |
| 78  | S2    | 1337 | 4AC  | O7-C7 | -2.16 | 1.18        | 1.23     |
| 78  | S2    | 1851 | MA6  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 78  | S2    | 1288 | OMU  | O2-C2 | -2.16 | 1.19        | 1.23     |
| 79  | L5    | 3830 | A2M  | C5-N7 | -2.15 | 1.35        | 1.39     |
| 79  | L5    | 4530 | UR3  | C4-N3 | 2.15  | 1.45        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 79  | L5    | 3818 | UY1  | O2-C2   | -2.15 | 1.18        | 1.23     |
| 79  | L5    | 3867 | A2M  | C5-N7   | -2.15 | 1.35        | 1.39     |
| 78  | S2    | 1248 | B8N  | O2-C2   | -2.15 | 1.18        | 1.22     |
| 78  | S2    | 484  | A2M  | C5-N7   | -2.14 | 1.35        | 1.39     |
| 78  | S2    | 668  | A2M  | C5-N7   | -2.13 | 1.35        | 1.39     |
| 79  | L5    | 2401 | A2M  | C5-N7   | -2.13 | 1.35        | 1.39     |
| 79  | L5    | 398  | A2M  | C5-N7   | -2.13 | 1.35        | 1.39     |
| 78  | S2    | 512  | A2M  | C5-N7   | -2.12 | 1.35        | 1.39     |
| 78  | S2    | 918  | PSU  | O4'-C1' | -2.12 | 1.40        | 1.43     |
| 79  | L5    | 1871 | A2M  | C5-N7   | -2.11 | 1.35        | 1.39     |
| 79  | L5    | 400  | A2M  | C5-N7   | -2.10 | 1.35        | 1.39     |
| 78  | S2    | 668  | A2M  | O3'-C3' | 2.09  | 1.47        | 1.43     |
| 79  | L5    | 4571 | A2M  | C5-N7   | -2.09 | 1.35        | 1.39     |
| 79  | L5    | 4523 | A2M  | C5-N7   | -2.09 | 1.35        | 1.39     |
| 79  | L5    | 3724 | A2M  | C5-N7   | -2.08 | 1.35        | 1.39     |
| 78  | S2    | 1678 | A2M  | C5-N7   | -2.08 | 1.35        | 1.39     |
| 78  | S2    | 484  | A2M  | O3'-C3' | 2.08  | 1.47        | 1.43     |
| 78  | S2    | 1383 | A2M  | C5-N7   | -2.08 | 1.35        | 1.39     |
| 79  | L5    | 3785 | A2M  | C5-N7   | -2.07 | 1.35        | 1.39     |
| 78  | S2    | 27   | A2M  | C5-N7   | -2.07 | 1.35        | 1.39     |
| 78  | S2    | 1851 | MA6  | C8-N9   | -2.06 | 1.33        | 1.37     |
| 78  | S2    | 159  | A2M  | C5-N7   | -2.06 | 1.35        | 1.39     |
| 78  | S2    | 576  | A2M  | C5-N7   | -2.06 | 1.35        | 1.39     |
| 79  | L5    | 1326 | A2M  | C5-N7   | -2.06 | 1.35        | 1.39     |
| 79  | L5    | 1534 | A2M  | O3'-C3' | 2.06  | 1.47        | 1.43     |
| 78  | S2    | 468  | A2M  | C5-N7   | -2.06 | 1.35        | 1.39     |
| 78  | S2    | 99   | A2M  | C5-N7   | -2.05 | 1.35        | 1.39     |
| 79  | L5    | 3785 | A2M  | O3'-C3' | 2.05  | 1.47        | 1.43     |
| 79  | L5    | 3825 | A2M  | C5-N7   | -2.05 | 1.35        | 1.39     |
| 76  | Pt    | 8    | 4SU  | O2-C2   | -2.05 | 1.19        | 1.23     |
| 79  | L5    | 1534 | A2M  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 79  | L5    | 2363 | A2M  | C5-N7   | -2.03 | 1.35        | 1.39     |
| 79  | L5    | 4523 | A2M  | O3'-C3' | 2.03  | 1.47        | 1.43     |
| 79  | L5    | 2815 | A2M  | C5-N7   | -2.03 | 1.35        | 1.39     |
| 78  | S2    | 1031 | A2M  | C5-N7   | -2.02 | 1.35        | 1.39     |
| 78  | S2    | 99   | A2M  | O3'-C3' | 2.02  | 1.47        | 1.43     |
| 79  | L5    | 3723 | A2M  | C5-N7   | -2.02 | 1.35        | 1.39     |
| 78  | S2    | 576  | A2M  | O3'-C3' | 2.01  | 1.47        | 1.43     |
| 78  | S2    | 1248 | B8N  | C32-C31 | 2.01  | 1.56        | 1.52     |
| 79  | L5    | 3724 | A2M  | O3'-C3' | 2.00  | 1.47        | 1.43     |
| 79  | L5    | 3718 | A2M  | O3'-C3' | 2.00  | 1.47        | 1.43     |
| 78  | S2    | 468  | A2M  | O3'-C3' | 2.00  | 1.47        | 1.43     |

All (1072) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 78  | S2    | 1851 | MA6  | N1-C6-N6  | -14.02 | 101.76      | 117.08   |
| 78  | S2    | 1850 | MA6  | N1-C6-N6  | -12.80 | 103.09      | 117.08   |
| 79  | L5    | 1524 | A2M  | C1'-N9-C8 | -12.49 | 98.93       | 127.14   |
| 78  | S2    | 590  | A2M  | C1'-N9-C8 | -12.39 | 99.15       | 127.14   |
| 78  | S2    | 1678 | A2M  | C1'-N9-C8 | -11.53 | 101.09      | 127.14   |
| 79  | L5    | 1534 | A2M  | C1'-N9-C8 | -11.46 | 101.26      | 127.14   |
| 79  | L5    | 3867 | A2M  | C1'-N9-C8 | -11.41 | 101.36      | 127.14   |
| 79  | L5    | 2815 | A2M  | C1'-N9-C8 | -11.31 | 101.59      | 127.14   |
| 79  | L5    | 3785 | A2M  | C1'-N9-C8 | -11.20 | 101.85      | 127.14   |
| 79  | L5    | 4571 | A2M  | C1'-N9-C8 | -11.19 | 101.87      | 127.14   |
| 79  | L5    | 3723 | A2M  | C1'-N9-C8 | -11.11 | 102.04      | 127.14   |
| 79  | L5    | 4220 | 6MZ  | C1'-N9-C8 | -11.11 | 102.06      | 127.14   |
| 79  | L5    | 3724 | A2M  | C1'-N9-C8 | -11.05 | 102.19      | 127.14   |
| 79  | L5    | 400  | A2M  | C1'-N9-C8 | -11.03 | 102.22      | 127.14   |
| 79  | L5    | 2401 | A2M  | C1'-N9-C8 | -11.02 | 102.25      | 127.14   |
| 79  | L5    | 2363 | A2M  | C1'-N9-C8 | -11.01 | 102.27      | 127.14   |
| 79  | L5    | 1326 | A2M  | C1'-N9-C8 | -11.01 | 102.27      | 127.14   |
| 79  | L5    | 4590 | A2M  | C1'-N9-C8 | -10.98 | 102.35      | 127.14   |
| 78  | S2    | 1832 | 6MZ  | C1'-N9-C8 | -10.96 | 102.38      | 127.14   |
| 78  | S2    | 159  | A2M  | C1'-N9-C8 | -10.90 | 102.53      | 127.14   |
| 78  | S2    | 1031 | A2M  | C1'-N9-C8 | -10.88 | 102.56      | 127.14   |
| 78  | S2    | 484  | A2M  | C1'-N9-C8 | -10.87 | 102.58      | 127.14   |
| 79  | L5    | 398  | A2M  | C1'-N9-C8 | -10.87 | 102.60      | 127.14   |
| 78  | S2    | 576  | A2M  | C1'-N9-C8 | -10.83 | 102.68      | 127.14   |
| 78  | S2    | 166  | A2M  | C1'-N9-C8 | -10.81 | 102.72      | 127.14   |
| 78  | S2    | 99   | A2M  | C1'-N9-C8 | -10.77 | 102.81      | 127.14   |
| 79  | L5    | 4523 | A2M  | C1'-N9-C8 | -10.76 | 102.85      | 127.14   |
| 78  | S2    | 27   | A2M  | C1'-N9-C8 | -10.75 | 102.86      | 127.14   |
| 78  | S2    | 512  | A2M  | C1'-N9-C8 | -10.75 | 102.87      | 127.14   |
| 79  | L5    | 3718 | A2M  | C1'-N9-C8 | -10.71 | 102.95      | 127.14   |
| 78  | S2    | 1383 | A2M  | C1'-N9-C8 | -10.66 | 103.07      | 127.14   |
| 79  | L5    | 1524 | A2M  | C4-N9-C1' | 10.64  | 151.94      | 126.59   |
| 78  | S2    | 468  | A2M  | C1'-N9-C8 | -10.62 | 103.16      | 127.14   |
| 78  | S2    | 590  | A2M  | C4-N9-C1' | 10.62  | 151.89      | 126.59   |
| 79  | L5    | 3825 | A2M  | C1'-N9-C8 | -10.55 | 103.32      | 127.14   |
| 79  | L5    | 1871 | A2M  | C1'-N9-C8 | -10.52 | 103.39      | 127.14   |
| 78  | S2    | 668  | A2M  | C1'-N9-C8 | -10.51 | 103.40      | 127.14   |
| 79  | L5    | 3830 | A2M  | C1'-N9-C8 | -10.48 | 103.46      | 127.14   |
| 79  | L5    | 3867 | A2M  | C4-N9-C1' | 10.23  | 150.96      | 126.59   |
| 79  | L5    | 4220 | 6MZ  | C4-N9-C1' | 10.16  | 150.81      | 126.59   |
| 78  | S2    | 1678 | A2M  | C4-N9-C1' | 10.11  | 150.67      | 126.59   |
| 79  | L5    | 1534 | A2M  | C4-N9-C1' | 10.06  | 150.57      | 126.59   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 79  | L5    | 2815 | A2M  | C4-N9-C1' | 10.05 | 150.53      | 126.59   |
| 79  | L5    | 4571 | A2M  | C4-N9-C1' | 9.98  | 150.38      | 126.59   |
| 78  | S2    | 1832 | 6MZ  | C4-N9-C1' | 9.94  | 150.26      | 126.59   |
| 78  | S2    | 484  | A2M  | C4-N9-C1' | 9.90  | 150.18      | 126.59   |
| 79  | L5    | 3718 | A2M  | C4-N9-C1' | 9.88  | 150.14      | 126.59   |
| 79  | L5    | 3723 | A2M  | C4-N9-C1' | 9.86  | 150.08      | 126.59   |
| 79  | L5    | 3785 | A2M  | C4-N9-C1' | 9.84  | 150.04      | 126.59   |
| 79  | L5    | 400  | A2M  | C4-N9-C1' | 9.83  | 150.02      | 126.59   |
| 79  | L5    | 1326 | A2M  | C4-N9-C1' | 9.81  | 149.97      | 126.59   |
| 79  | L5    | 3724 | A2M  | C4-N9-C1' | 9.80  | 149.95      | 126.59   |
| 78  | S2    | 159  | A2M  | C4-N9-C1' | 9.79  | 149.91      | 126.59   |
| 79  | L5    | 2363 | A2M  | C4-N9-C1' | 9.78  | 149.91      | 126.59   |
| 79  | L5    | 398  | A2M  | C4-N9-C1' | 9.76  | 149.85      | 126.59   |
| 79  | L5    | 2401 | A2M  | C4-N9-C1' | 9.75  | 149.83      | 126.59   |
| 78  | S2    | 1031 | A2M  | C4-N9-C1' | 9.64  | 149.56      | 126.59   |
| 78  | S2    | 512  | A2M  | C4-N9-C1' | 9.61  | 149.49      | 126.59   |
| 79  | L5    | 4590 | A2M  | C4-N9-C1' | 9.59  | 149.45      | 126.59   |
| 78  | S2    | 27   | A2M  | C4-N9-C1' | 9.59  | 149.44      | 126.59   |
| 78  | S2    | 576  | A2M  | C4-N9-C1' | 9.57  | 149.39      | 126.59   |
| 78  | S2    | 99   | A2M  | C4-N9-C1' | 9.55  | 149.34      | 126.59   |
| 78  | S2    | 1383 | A2M  | C4-N9-C1' | 9.54  | 149.31      | 126.59   |
| 78  | S2    | 166  | A2M  | C4-N9-C1' | 9.53  | 149.31      | 126.59   |
| 79  | L5    | 4523 | A2M  | C4-N9-C1' | 9.53  | 149.30      | 126.59   |
| 78  | S2    | 468  | A2M  | C4-N9-C1' | 9.48  | 149.19      | 126.59   |
| 79  | L5    | 3825 | A2M  | C4-N9-C1' | 9.45  | 149.11      | 126.59   |
| 79  | L5    | 3830 | A2M  | C4-N9-C1' | 9.38  | 148.93      | 126.59   |
| 78  | S2    | 668  | A2M  | C4-N9-C1' | 9.32  | 148.81      | 126.59   |
| 79  | L5    | 1871 | A2M  | C4-N9-C1' | 9.32  | 148.79      | 126.59   |
| 76  | Pt    | 8    | 4SU  | C4-N3-C2  | -7.80 | 119.77      | 127.34   |
| 78  | S2    | 1851 | MA6  | C5-C6-N6  | 7.62  | 138.58      | 125.30   |
| 78  | S2    | 1850 | MA6  | C5-C6-N6  | 6.94  | 137.38      | 125.30   |
| 79  | L5    | 1534 | A2M  | N6-C6-N1  | -6.17 | 104.84      | 118.35   |
| 79  | L5    | 4590 | A2M  | N6-C6-N1  | -6.08 | 105.03      | 118.35   |
| 79  | L5    | 3825 | A2M  | N6-C6-N1  | -6.08 | 105.04      | 118.35   |
| 79  | L5    | 2363 | A2M  | N6-C6-N1  | -6.08 | 105.04      | 118.35   |
| 78  | S2    | 590  | A2M  | N6-C6-N1  | -6.06 | 105.07      | 118.35   |
| 78  | S2    | 668  | A2M  | N6-C6-N1  | -6.04 | 105.12      | 118.35   |
| 76  | Pt    | 47   | G7M  | CN7-N7-C5 | 6.03  | 134.26      | 126.77   |
| 79  | L5    | 2815 | A2M  | N6-C6-N1  | -5.99 | 105.23      | 118.35   |
| 78  | S2    | 166  | A2M  | N6-C6-N1  | -5.99 | 105.24      | 118.35   |
| 78  | S2    | 1639 | G7M  | CN7-N7-C5 | 5.99  | 134.21      | 126.77   |
| 78  | S2    | 27   | A2M  | N6-C6-N1  | -5.96 | 105.30      | 118.35   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 78  | S2    | 159  | A2M  | N6-C6-N1 | -5.96 | 105.31      | 118.35   |
| 79  | L5    | 400  | A2M  | N6-C6-N1 | -5.95 | 105.31      | 118.35   |
| 79  | L5    | 1524 | A2M  | N6-C6-N1 | -5.95 | 105.33      | 118.35   |
| 79  | L5    | 3718 | A2M  | N6-C6-N1 | -5.94 | 105.34      | 118.35   |
| 79  | L5    | 1871 | A2M  | N6-C6-N1 | -5.93 | 105.35      | 118.35   |
| 78  | S2    | 512  | A2M  | N6-C6-N1 | -5.90 | 105.42      | 118.35   |
| 79  | L5    | 3830 | A2M  | N6-C6-N1 | -5.89 | 105.45      | 118.35   |
| 78  | S2    | 99   | A2M  | N6-C6-N1 | -5.88 | 105.46      | 118.35   |
| 78  | S2    | 1031 | A2M  | N6-C6-N1 | -5.88 | 105.47      | 118.35   |
| 79  | L5    | 1326 | A2M  | N6-C6-N1 | -5.88 | 105.48      | 118.35   |
| 79  | L5    | 4523 | A2M  | N6-C6-N1 | -5.87 | 105.49      | 118.35   |
| 79  | L5    | 2401 | A2M  | N6-C6-N1 | -5.87 | 105.50      | 118.35   |
| 79  | L5    | 3723 | A2M  | N6-C6-N1 | -5.86 | 105.51      | 118.35   |
| 78  | S2    | 1678 | A2M  | N6-C6-N1 | -5.86 | 105.52      | 118.35   |
| 79  | L5    | 4571 | A2M  | N6-C6-N1 | -5.84 | 105.55      | 118.35   |
| 79  | L5    | 398  | A2M  | N6-C6-N1 | -5.84 | 105.56      | 118.35   |
| 78  | S2    | 484  | A2M  | N6-C6-N1 | -5.82 | 105.60      | 118.35   |
| 78  | S2    | 1383 | A2M  | N6-C6-N1 | -5.81 | 105.62      | 118.35   |
| 79  | L5    | 3867 | A2M  | N6-C6-N1 | -5.81 | 105.63      | 118.35   |
| 79  | L5    | 3724 | A2M  | N6-C6-N1 | -5.80 | 105.64      | 118.35   |
| 78  | S2    | 468  | A2M  | N6-C6-N1 | -5.79 | 105.66      | 118.35   |
| 78  | S2    | 576  | A2M  | N6-C6-N1 | -5.77 | 105.71      | 118.35   |
| 79  | L5    | 1871 | A2M  | N3-C2-N1 | -5.74 | 119.62      | 128.60   |
| 79  | L5    | 3785 | A2M  | N6-C6-N1 | -5.74 | 105.79      | 118.35   |
| 78  | S2    | 1851 | MA6  | N1-C2-N3 | -5.72 | 119.65      | 128.60   |
| 79  | L5    | 3724 | A2M  | N3-C2-N1 | -5.64 | 119.79      | 128.60   |
| 78  | S2    | 512  | A2M  | N3-C2-N1 | -5.61 | 119.83      | 128.60   |
| 78  | S2    | 166  | A2M  | N3-C2-N1 | -5.61 | 119.83      | 128.60   |
| 79  | L5    | 4590 | A2M  | N3-C2-N1 | -5.60 | 119.83      | 128.60   |
| 78  | S2    | 27   | A2M  | N3-C2-N1 | -5.60 | 119.84      | 128.60   |
| 79  | L5    | 4220 | 6MZ  | N1-C2-N3 | -5.60 | 119.85      | 128.60   |
| 79  | L5    | 400  | A2M  | N3-C2-N1 | -5.59 | 119.85      | 128.60   |
| 78  | S2    | 1383 | A2M  | N3-C2-N1 | -5.59 | 119.85      | 128.60   |
| 79  | L5    | 3830 | A2M  | N3-C2-N1 | -5.59 | 119.86      | 128.60   |
| 76  | Pt    | 8    | 4SU  | C5-C4-N3 | 5.57  | 119.86      | 114.69   |
| 78  | S2    | 590  | A2M  | N3-C2-N1 | -5.57 | 119.88      | 128.60   |
| 79  | L5    | 3785 | A2M  | N3-C2-N1 | -5.57 | 119.89      | 128.60   |
| 78  | S2    | 1031 | A2M  | N3-C2-N1 | -5.56 | 119.90      | 128.60   |
| 79  | L5    | 1326 | A2M  | N3-C2-N1 | -5.55 | 119.92      | 128.60   |
| 79  | L5    | 1534 | A2M  | N3-C2-N1 | -5.54 | 119.94      | 128.60   |
| 78  | S2    | 99   | A2M  | N3-C2-N1 | -5.54 | 119.94      | 128.60   |
| 79  | L5    | 398  | A2M  | N3-C2-N1 | -5.54 | 119.94      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 79  | L5    | 4523 | A2M  | N3-C2-N1 | -5.53 | 119.94      | 128.60   |
| 79  | L5    | 2363 | A2M  | N3-C2-N1 | -5.52 | 119.97      | 128.60   |
| 78  | S2    | 1832 | 6MZ  | N1-C2-N3 | -5.51 | 119.98      | 128.60   |
| 79  | L5    | 2401 | A2M  | N3-C2-N1 | -5.51 | 119.99      | 128.60   |
| 79  | L5    | 2815 | A2M  | N3-C2-N1 | -5.49 | 120.02      | 128.60   |
| 79  | L5    | 3723 | A2M  | N3-C2-N1 | -5.47 | 120.04      | 128.60   |
| 78  | S2    | 159  | A2M  | N3-C2-N1 | -5.46 | 120.06      | 128.60   |
| 78  | S2    | 668  | A2M  | N3-C2-N1 | -5.45 | 120.07      | 128.60   |
| 79  | L5    | 1524 | A2M  | N3-C2-N1 | -5.44 | 120.09      | 128.60   |
| 78  | S2    | 468  | A2M  | N3-C2-N1 | -5.43 | 120.11      | 128.60   |
| 79  | L5    | 3718 | A2M  | C5-C4-N3 | -5.42 | 119.67      | 126.75   |
| 79  | L5    | 2837 | OMU  | C4-N3-C2 | -5.42 | 119.43      | 126.58   |
| 78  | S2    | 1678 | A2M  | N3-C2-N1 | -5.41 | 120.14      | 128.60   |
| 78  | S2    | 484  | A2M  | N3-C2-N1 | -5.41 | 120.14      | 128.60   |
| 78  | S2    | 1850 | MA6  | N1-C2-N3 | -5.40 | 120.15      | 128.60   |
| 79  | L5    | 4571 | A2M  | N3-C2-N1 | -5.40 | 120.16      | 128.60   |
| 78  | S2    | 1804 | OMU  | C4-N3-C2 | -5.39 | 119.47      | 126.58   |
| 78  | S2    | 668  | A2M  | C5-C6-N6 | 5.39  | 135.15      | 123.43   |
| 79  | L5    | 4227 | OMU  | C4-N3-C2 | -5.38 | 119.49      | 126.58   |
| 78  | S2    | 172  | OMU  | C4-N3-C2 | -5.36 | 119.51      | 126.58   |
| 79  | L5    | 3867 | A2M  | C5-C4-N3 | -5.34 | 119.78      | 126.75   |
| 79  | L5    | 4590 | A2M  | C5-C6-N6 | 5.34  | 135.04      | 123.43   |
| 79  | L5    | 2363 | A2M  | C5-C6-N6 | 5.33  | 135.03      | 123.43   |
| 78  | S2    | 484  | A2M  | C5-C4-N3 | -5.32 | 119.81      | 126.75   |
| 78  | S2    | 576  | A2M  | N3-C2-N1 | -5.32 | 120.28      | 128.60   |
| 79  | L5    | 4498 | OMU  | C4-N3-C2 | -5.32 | 119.57      | 126.58   |
| 78  | S2    | 1850 | MA6  | C5-C4-N3 | -5.30 | 119.83      | 126.75   |
| 78  | S2    | 590  | A2M  | C5-C6-N6 | 5.30  | 134.95      | 123.43   |
| 79  | L5    | 3825 | A2M  | C5-C6-N6 | 5.29  | 134.95      | 123.43   |
| 79  | L5    | 3825 | A2M  | N3-C2-N1 | -5.28 | 120.35      | 128.60   |
| 79  | L5    | 2415 | OMU  | C4-N3-C2 | -5.27 | 119.63      | 126.58   |
| 79  | L5    | 1871 | A2M  | C5-C6-N6 | 5.26  | 134.89      | 123.43   |
| 79  | L5    | 400  | A2M  | C5-C6-N6 | 5.26  | 134.88      | 123.43   |
| 79  | L5    | 1534 | A2M  | C5-C6-N6 | 5.26  | 134.88      | 123.43   |
| 78  | S2    | 159  | A2M  | C5-C6-N6 | 5.26  | 134.87      | 123.43   |
| 79  | L5    | 3925 | OMU  | C4-N3-C2 | -5.25 | 119.65      | 126.58   |
| 78  | S2    | 27   | A2M  | C5-C6-N6 | 5.25  | 134.85      | 123.43   |
| 78  | S2    | 428  | OMU  | C4-N3-C2 | -5.25 | 119.66      | 126.58   |
| 79  | L5    | 1524 | A2M  | C5-C6-N6 | 5.25  | 134.85      | 123.43   |
| 78  | S2    | 166  | A2M  | C5-C6-N6 | 5.22  | 134.80      | 123.43   |
| 78  | S2    | 1678 | A2M  | C5-C4-N3 | -5.22 | 119.94      | 126.75   |
| 78  | S2    | 354  | OMU  | C4-N3-C2 | -5.21 | 119.70      | 126.58   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 79  | L5    | 3718 | A2M  | C5-C6-N6 | 5.21  | 134.78      | 123.43   |
| 79  | L5    | 3830 | A2M  | C5-C6-N6 | 5.20  | 134.75      | 123.43   |
| 78  | S2    | 1248 | B8N  | C5-C4-N3 | 5.20  | 125.80      | 116.17   |
| 78  | S2    | 512  | A2M  | C5-C6-N6 | 5.20  | 134.75      | 123.43   |
| 79  | L5    | 398  | A2M  | C5-C4-N3 | -5.20 | 119.97      | 126.75   |
| 79  | L5    | 2815 | A2M  | C5-C4-N3 | -5.19 | 119.98      | 126.75   |
| 79  | L5    | 4571 | A2M  | C5-C4-N3 | -5.19 | 119.98      | 126.75   |
| 79  | L5    | 4306 | OMU  | C4-N3-C2 | -5.18 | 119.74      | 126.58   |
| 79  | L5    | 2815 | A2M  | C5-C6-N6 | 5.18  | 134.71      | 123.43   |
| 79  | L5    | 3867 | A2M  | N3-C2-N1 | -5.18 | 120.50      | 128.60   |
| 78  | S2    | 627  | OMU  | C4-N3-C2 | -5.16 | 119.77      | 126.58   |
| 78  | S2    | 576  | A2M  | C5-C6-N6 | 5.16  | 134.66      | 123.43   |
| 79  | L5    | 3723 | A2M  | C5-C4-N3 | -5.16 | 120.02      | 126.75   |
| 79  | L5    | 2401 | A2M  | C5-C6-N6 | 5.16  | 134.65      | 123.43   |
| 79  | L5    | 4571 | A2M  | C5-C6-N6 | 5.15  | 134.64      | 123.43   |
| 79  | L5    | 3785 | A2M  | C5-C4-N3 | -5.14 | 120.05      | 126.75   |
| 79  | L5    | 1326 | A2M  | C5-C6-N6 | 5.13  | 134.59      | 123.43   |
| 79  | L5    | 398  | A2M  | C5-C6-N6 | 5.12  | 134.57      | 123.43   |
| 79  | L5    | 4523 | A2M  | C5-C6-N6 | 5.12  | 134.57      | 123.43   |
| 78  | S2    | 1383 | A2M  | C5-C6-N6 | 5.12  | 134.56      | 123.43   |
| 78  | S2    | 1832 | 6MZ  | C5-C4-N3 | -5.11 | 120.08      | 126.75   |
| 78  | S2    | 1031 | A2M  | C5-C6-N6 | 5.10  | 134.54      | 123.43   |
| 79  | L5    | 3723 | A2M  | C5-C6-N6 | 5.10  | 134.53      | 123.43   |
| 79  | L5    | 3724 | A2M  | C5-C6-N6 | 5.10  | 134.53      | 123.43   |
| 79  | L5    | 1534 | A2M  | C5-C4-N3 | -5.09 | 120.11      | 126.75   |
| 78  | S2    | 99   | A2M  | C5-C4-N3 | -5.09 | 120.11      | 126.75   |
| 78  | S2    | 468  | A2M  | C5-C6-N6 | 5.08  | 134.50      | 123.43   |
| 78  | S2    | 159  | A2M  | C5-C4-N3 | -5.08 | 120.12      | 126.75   |
| 79  | L5    | 3724 | A2M  | C5-C4-N3 | -5.08 | 120.13      | 126.75   |
| 78  | S2    | 1678 | A2M  | C5-C6-N6 | 5.07  | 134.47      | 123.43   |
| 78  | S2    | 512  | A2M  | C5-C4-N3 | -5.07 | 120.14      | 126.75   |
| 78  | S2    | 1031 | A2M  | C5-C4-N3 | -5.06 | 120.14      | 126.75   |
| 79  | L5    | 2401 | A2M  | C5-C4-N3 | -5.06 | 120.14      | 126.75   |
| 79  | L5    | 1326 | A2M  | C5-C4-N3 | -5.06 | 120.15      | 126.75   |
| 78  | S2    | 484  | A2M  | C5-C6-N6 | 5.06  | 134.44      | 123.43   |
| 78  | S2    | 99   | A2M  | C5-C6-N6 | 5.06  | 134.44      | 123.43   |
| 78  | S2    | 1288 | OMU  | C4-N3-C2 | -5.05 | 119.92      | 126.58   |
| 79  | L5    | 3867 | A2M  | C5-C6-N6 | 5.04  | 134.40      | 123.43   |
| 79  | L5    | 3825 | A2M  | C5-C4-N3 | -5.04 | 120.17      | 126.75   |
| 79  | L5    | 400  | A2M  | C5-C4-N3 | -5.04 | 120.18      | 126.75   |
| 79  | L5    | 4523 | A2M  | C5-C4-N3 | -5.03 | 120.19      | 126.75   |
| 79  | L5    | 4220 | 6MZ  | C5-C4-N3 | -5.03 | 120.19      | 126.75   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 78  | S2    | 1383 | A2M  | C5-C4-N3  | -5.02 | 120.20      | 126.75   |
| 79  | L5    | 2363 | A2M  | C5-C4-N3  | -5.01 | 120.21      | 126.75   |
| 78  | S2    | 468  | A2M  | C5-C4-N3  | -4.99 | 120.23      | 126.75   |
| 78  | S2    | 166  | A2M  | C5-C4-N3  | -4.99 | 120.24      | 126.75   |
| 78  | S2    | 121  | OMU  | C4-N3-C2  | -4.99 | 120.00      | 126.58   |
| 79  | L5    | 4620 | OMU  | C4-N3-C2  | -4.98 | 120.01      | 126.58   |
| 78  | S2    | 27   | A2M  | C5-C4-N3  | -4.98 | 120.25      | 126.75   |
| 78  | S2    | 116  | OMU  | C4-N3-C2  | -4.97 | 120.02      | 126.58   |
| 79  | L5    | 3637 | PSU  | N1-C2-N3  | 4.97  | 120.76      | 115.13   |
| 79  | L5    | 3718 | A2M  | N3-C2-N1  | -4.93 | 120.90      | 128.60   |
| 79  | L5    | 3830 | A2M  | C5-C4-N3  | -4.88 | 120.38      | 126.75   |
| 79  | L5    | 4628 | PSU  | N1-C2-N3  | 4.87  | 120.65      | 115.13   |
| 79  | L5    | 3785 | A2M  | C5-C6-N6  | 4.86  | 134.02      | 123.43   |
| 78  | S2    | 1851 | MA6  | C5-C4-N3  | -4.85 | 120.42      | 126.75   |
| 79  | L5    | 1524 | A2M  | N9-C8-N7  | -4.84 | 107.30      | 113.91   |
| 79  | L5    | 4457 | PSU  | C4-N3-C2  | -4.83 | 119.37      | 126.34   |
| 78  | S2    | 590  | A2M  | C5-C4-N3  | -4.83 | 120.45      | 126.75   |
| 78  | S2    | 668  | A2M  | C5-C4-N3  | -4.83 | 120.45      | 126.75   |
| 79  | L5    | 4590 | A2M  | C5-C4-N3  | -4.82 | 120.47      | 126.75   |
| 78  | S2    | 590  | A2M  | N9-C8-N7  | -4.80 | 107.35      | 113.91   |
| 78  | S2    | 576  | A2M  | C5-C4-N3  | -4.80 | 120.49      | 126.75   |
| 79  | L5    | 1871 | A2M  | C5-C4-N3  | -4.79 | 120.50      | 126.75   |
| 79  | L5    | 4403 | PSU  | C4-N3-C2  | -4.78 | 119.45      | 126.34   |
| 78  | S2    | 1326 | UY1  | C4-N3-C2  | -4.70 | 119.57      | 126.34   |
| 79  | L5    | 4500 | PSU  | N1-C2-N3  | 4.69  | 120.45      | 115.13   |
| 79  | L5    | 4293 | PSU  | N1-C2-N3  | 4.69  | 120.44      | 115.13   |
| 79  | L5    | 4521 | PSU  | C4-N3-C2  | -4.68 | 119.59      | 126.34   |
| 76  | Pt    | 47   | G7M  | CN7-N7-C8 | -4.68 | 117.62      | 124.84   |
| 79  | L5    | 1524 | A2M  | C5-C4-N3  | -4.67 | 120.65      | 126.75   |
| 78  | S2    | 1136 | PSU  | C4-N3-C2  | -4.67 | 119.61      | 126.34   |
| 79  | L5    | 3695 | PSU  | C4-N3-C2  | -4.65 | 119.63      | 126.34   |
| 79  | L5    | 4500 | PSU  | C4-N3-C2  | -4.64 | 119.65      | 126.34   |
| 79  | L5    | 4296 | PSU  | C4-N3-C2  | -4.63 | 119.67      | 126.34   |
| 78  | S2    | 1851 | MA6  | N9-C8-N7  | -4.62 | 107.60      | 113.91   |
| 79  | L5    | 4531 | PSU  | N1-C2-N3  | 4.61  | 120.36      | 115.13   |
| 78  | S2    | 651  | PSU  | C4-N3-C2  | -4.61 | 119.69      | 126.34   |
| 79  | L5    | 4531 | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 78  | S2    | 1243 | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 79  | L5    | 3762 | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 79  | L5    | 4576 | PSU  | N1-C2-N3  | 4.60  | 120.34      | 115.13   |
| 78  | S2    | 1239 | PSU  | C4-N3-C2  | -4.60 | 119.71      | 126.34   |
| 79  | L5    | 3851 | PSU  | N1-C2-N3  | 4.59  | 120.33      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 78  | S2    | 1238 | PSU  | C4-N3-C2  | -4.59 | 119.72      | 126.34   |
| 79  | L5    | 3637 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 79  | L5    | 4628 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 79  | L5    | 1862 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 79  | L5    | 4293 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 79  | L5    | 4552 | PSU  | C4-N3-C2  | -4.59 | 119.73      | 126.34   |
| 79  | L5    | 5001 | PSU  | N1-C2-N3  | 4.58  | 120.32      | 115.13   |
| 78  | S2    | 1445 | PSU  | C4-N3-C2  | -4.58 | 119.74      | 126.34   |
| 78  | S2    | 815  | PSU  | C4-N3-C2  | -4.58 | 119.75      | 126.34   |
| 78  | S2    | 1639 | G7M  | CN7-N7-C8 | -4.57 | 117.78      | 124.84   |
| 79  | L5    | 4576 | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 79  | L5    | 3695 | PSU  | N1-C2-N3  | 4.57  | 120.31      | 115.13   |
| 79  | L5    | 4353 | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 78  | S2    | 1347 | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 78  | S2    | 573  | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 78  | S2    | 406  | PSU  | C4-N3-C2  | -4.56 | 119.76      | 126.34   |
| 78  | S2    | 686  | PSU  | C4-N3-C2  | -4.56 | 119.76      | 126.34   |
| 79  | L5    | 4530 | UR3  | C4-N3-C2  | -4.56 | 120.27      | 124.56   |
| 79  | L5    | 5001 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 79  | L5    | 2508 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 79  | L5    | 3758 | PSU  | C4-N3-C2  | -4.56 | 119.77      | 126.34   |
| 76  | Pt    | 56   | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 79  | L5    | 3851 | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 79  | L5    | 1536 | PSU  | N1-C2-N3  | 4.55  | 120.29      | 115.13   |
| 79  | L5    | 4457 | PSU  | N1-C2-N3  | 4.55  | 120.29      | 115.13   |
| 79  | L5    | 3770 | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 78  | S2    | 1367 | PSU  | C4-N3-C2  | -4.55 | 119.78      | 126.34   |
| 78  | S2    | 1136 | PSU  | N1-C2-N3  | 4.54  | 120.28      | 115.13   |
| 79  | L5    | 3639 | PSU  | N1-C2-N3  | 4.54  | 120.28      | 115.13   |
| 78  | S2    | 1177 | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 79  | L5    | 3884 | PSU  | N1-C2-N3  | 4.53  | 120.27      | 115.13   |
| 79  | L5    | 4296 | PSU  | N1-C2-N3  | 4.53  | 120.26      | 115.13   |
| 79  | L5    | 4521 | PSU  | N1-C2-N3  | 4.53  | 120.26      | 115.13   |
| 78  | S2    | 1056 | PSU  | C4-N3-C2  | -4.53 | 119.81      | 126.34   |
| 78  | S2    | 406  | PSU  | N1-C2-N3  | 4.53  | 120.26      | 115.13   |
| 79  | L5    | 4552 | PSU  | N1-C2-N3  | 4.53  | 120.26      | 115.13   |
| 79  | L5    | 2843 | PSU  | C4-N3-C2  | -4.53 | 119.82      | 126.34   |
| 79  | L5    | 3818 | UY1  | C4-N3-C2  | -4.52 | 119.82      | 126.34   |
| 79  | L5    | 3920 | PSU  | N1-C2-N3  | 4.52  | 120.25      | 115.13   |
| 78  | S2    | 866  | PSU  | C4-N3-C2  | -4.52 | 119.82      | 126.34   |
| 78  | S2    | 1639 | G7M  | C2-N3-C4  | 4.52  | 120.36      | 112.30   |
| 79  | L5    | 4353 | PSU  | N1-C2-N3  | 4.52  | 120.25      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 78  | S2    | 649  | PSU  | C4-N3-C2 | -4.52 | 119.83      | 126.34   |
| 79  | L5    | 1677 | PSU  | C4-N3-C2 | -4.52 | 119.83      | 126.34   |
| 78  | S2    | 1232 | PSU  | C4-N3-C2 | -4.52 | 119.83      | 126.34   |
| 78  | S2    | 1232 | PSU  | N1-C2-N3 | 4.52  | 120.25      | 115.13   |
| 78  | S2    | 1243 | PSU  | N1-C2-N3 | 4.51  | 120.24      | 115.13   |
| 79  | L5    | 1779 | PSU  | C4-N3-C2 | -4.51 | 119.84      | 126.34   |
| 78  | S2    | 1367 | PSU  | N1-C2-N3 | 4.51  | 120.24      | 115.13   |
| 78  | S2    | 801  | PSU  | C4-N3-C2 | -4.51 | 119.84      | 126.34   |
| 78  | S2    | 109  | PSU  | C4-N3-C2 | -4.51 | 119.84      | 126.34   |
| 79  | L5    | 1536 | PSU  | C4-N3-C2 | -4.51 | 119.84      | 126.34   |
| 79  | L5    | 4972 | PSU  | C4-N3-C2 | -4.51 | 119.84      | 126.34   |
| 79  | L5    | 3762 | PSU  | N1-C2-N3 | 4.51  | 120.24      | 115.13   |
| 79  | L5    | 4423 | PSU  | C4-N3-C2 | -4.51 | 119.85      | 126.34   |
| 79  | L5    | 4442 | PSU  | C4-N3-C2 | -4.51 | 119.85      | 126.34   |
| 78  | S2    | 1347 | PSU  | N1-C2-N3 | 4.50  | 120.23      | 115.13   |
| 79  | L5    | 3853 | PSU  | C4-N3-C2 | -4.50 | 119.86      | 126.34   |
| 78  | S2    | 1244 | PSU  | C4-N3-C2 | -4.50 | 119.86      | 126.34   |
| 78  | S2    | 1004 | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 79  | L5    | 3920 | PSU  | C4-N3-C2 | -4.49 | 119.87      | 126.34   |
| 78  | S2    | 34   | PSU  | C4-N3-C2 | -4.49 | 119.87      | 126.34   |
| 78  | S2    | 822  | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 79  | L5    | 4673 | PSU  | C4-N3-C2 | -4.49 | 119.87      | 126.34   |
| 78  | S2    | 1643 | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 78  | S2    | 651  | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 78  | S2    | 815  | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 78  | S2    | 1004 | PSU  | C4-N3-C2 | -4.49 | 119.87      | 126.34   |
| 78  | S2    | 1643 | PSU  | C4-N3-C2 | -4.49 | 119.88      | 126.34   |
| 79  | L5    | 1677 | PSU  | N1-C2-N3 | 4.49  | 120.21      | 115.13   |
| 79  | L5    | 3884 | PSU  | C4-N3-C2 | -4.48 | 119.88      | 126.34   |
| 79  | L5    | 4423 | PSU  | N1-C2-N3 | 4.48  | 120.21      | 115.13   |
| 78  | S2    | 1174 | PSU  | C4-N3-C2 | -4.48 | 119.88      | 126.34   |
| 78  | S2    | 218  | PSU  | C4-N3-C2 | -4.48 | 119.89      | 126.34   |
| 79  | L5    | 1744 | PSU  | C4-N3-C2 | -4.48 | 119.89      | 126.34   |
| 78  | S2    | 105  | PSU  | C4-N3-C2 | -4.48 | 119.89      | 126.34   |
| 79  | L5    | 4442 | PSU  | N1-C2-N3 | 4.48  | 120.20      | 115.13   |
| 78  | S2    | 649  | PSU  | N1-C2-N3 | 4.47  | 120.20      | 115.13   |
| 79  | L5    | 1779 | PSU  | N1-C2-N3 | 4.47  | 120.20      | 115.13   |
| 79  | L5    | 4532 | PSU  | C4-N3-C2 | -4.47 | 119.89      | 126.34   |
| 79  | L5    | 4493 | PSU  | C4-N3-C2 | -4.47 | 119.89      | 126.34   |
| 78  | S2    | 1445 | PSU  | N1-C2-N3 | 4.47  | 120.20      | 115.13   |
| 78  | S2    | 1081 | PSU  | C4-N3-C2 | -4.47 | 119.90      | 126.34   |
| 79  | L5    | 1782 | PSU  | C4-N3-C2 | -4.47 | 119.90      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 79  | L5    | 4361 | PSU  | C4-N3-C2 | -4.47 | 119.90      | 126.34   |
| 79  | L5    | 1744 | PSU  | N1-C2-N3 | 4.47  | 120.19      | 115.13   |
| 78  | S2    | 1692 | PSU  | C4-N3-C2 | -4.47 | 119.90      | 126.34   |
| 79  | L5    | 4431 | PSU  | C4-N3-C2 | -4.47 | 119.90      | 126.34   |
| 79  | L5    | 3715 | PSU  | C4-N3-C2 | -4.46 | 119.91      | 126.34   |
| 78  | S2    | 1238 | PSU  | N1-C2-N3 | 4.46  | 120.19      | 115.13   |
| 79  | L5    | 1782 | PSU  | N1-C2-N3 | 4.46  | 120.19      | 115.13   |
| 5   | L8    | 69   | PSU  | C4-N3-C2 | -4.46 | 119.92      | 126.34   |
| 79  | L5    | 1582 | PSU  | C4-N3-C2 | -4.46 | 119.92      | 126.34   |
| 79  | L5    | 3639 | PSU  | C4-N3-C2 | -4.46 | 119.92      | 126.34   |
| 5   | L8    | 69   | PSU  | N1-C2-N3 | 4.45  | 120.17      | 115.13   |
| 78  | S2    | 34   | PSU  | N1-C2-N3 | 4.45  | 120.17      | 115.13   |
| 78  | S2    | 1244 | PSU  | N1-C2-N3 | 4.45  | 120.17      | 115.13   |
| 79  | L5    | 1860 | PSU  | N1-C2-N3 | 4.45  | 120.17      | 115.13   |
| 79  | L5    | 3844 | PSU  | N1-C2-N3 | 4.45  | 120.17      | 115.13   |
| 5   | L8    | 55   | PSU  | C4-N3-C2 | -4.45 | 119.93      | 126.34   |
| 79  | L5    | 1862 | PSU  | N1-C2-N3 | 4.44  | 120.17      | 115.13   |
| 79  | L5    | 4312 | PSU  | N1-C2-N3 | 4.44  | 120.17      | 115.13   |
| 79  | L5    | 4673 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 5   | L8    | 55   | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 79  | L5    | 3715 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 79  | L5    | 2508 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 79  | L5    | 3853 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 78  | S2    | 36   | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 78  | S2    | 1177 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 79  | L5    | 3764 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 79  | L5    | 4532 | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 78  | S2    | 686  | PSU  | N1-C2-N3 | 4.44  | 120.16      | 115.13   |
| 78  | S2    | 573  | PSU  | N1-C2-N3 | 4.43  | 120.15      | 115.13   |
| 78  | S2    | 822  | PSU  | C4-N3-C2 | -4.43 | 119.95      | 126.34   |
| 79  | L5    | 3758 | PSU  | N1-C2-N3 | 4.43  | 120.15      | 115.13   |
| 79  | L5    | 2843 | PSU  | N1-C2-N3 | 4.43  | 120.15      | 115.13   |
| 79  | L5    | 4312 | PSU  | C4-N3-C2 | -4.43 | 119.96      | 126.34   |
| 79  | L5    | 4220 | 6MZ  | C4-C5-C6 | 4.43  | 120.24      | 116.81   |
| 79  | L5    | 1792 | PSU  | C4-N3-C2 | -4.42 | 119.97      | 126.34   |
| 78  | S2    | 918  | PSU  | N1-C2-N3 | 4.42  | 120.14      | 115.13   |
| 79  | L5    | 3770 | PSU  | N1-C2-N3 | 4.41  | 120.13      | 115.13   |
| 76  | Pt    | 47   | G7M  | C2-N3-C4 | 4.41  | 120.16      | 112.30   |
| 79  | L5    | 2839 | PSU  | C4-N3-C2 | -4.41 | 119.98      | 126.34   |
| 79  | L5    | 4361 | PSU  | N1-C2-N3 | 4.41  | 120.13      | 115.13   |
| 79  | L5    | 4636 | PSU  | N1-C2-N3 | 4.41  | 120.13      | 115.13   |
| 79  | L5    | 2839 | PSU  | N1-C2-N3 | 4.41  | 120.13      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 79  | L5    | 1860 | PSU  | C4-N3-C2 | -4.41 | 119.99      | 126.34   |
| 78  | S2    | 1625 | PSU  | C4-N3-C2 | -4.41 | 119.99      | 126.34   |
| 78  | S2    | 681  | PSU  | N1-C2-N3 | 4.41  | 120.12      | 115.13   |
| 78  | S2    | 681  | PSU  | C4-N3-C2 | -4.41 | 119.99      | 126.34   |
| 78  | S2    | 109  | PSU  | N1-C2-N3 | 4.40  | 120.12      | 115.13   |
| 79  | L5    | 4471 | PSU  | N1-C2-N3 | 4.40  | 120.12      | 115.13   |
| 78  | S2    | 1056 | PSU  | N1-C2-N3 | 4.40  | 120.11      | 115.13   |
| 79  | L5    | 4689 | PSU  | C4-N3-C2 | -4.40 | 120.00      | 126.34   |
| 79  | L5    | 1792 | PSU  | N1-C2-N3 | 4.39  | 120.11      | 115.13   |
| 78  | S2    | 801  | PSU  | N1-C2-N3 | 4.39  | 120.11      | 115.13   |
| 76  | Pt    | 56   | PSU  | N1-C2-N3 | 4.39  | 120.10      | 115.13   |
| 79  | L5    | 4431 | PSU  | N1-C2-N3 | 4.39  | 120.10      | 115.13   |
| 79  | L5    | 3764 | PSU  | C4-N3-C2 | -4.39 | 120.01      | 126.34   |
| 79  | L5    | 5010 | PSU  | C4-N3-C2 | -4.39 | 120.01      | 126.34   |
| 79  | L5    | 4590 | A2M  | N9-C8-N7 | -4.39 | 107.91      | 113.91   |
| 79  | L5    | 1582 | PSU  | N1-C2-N3 | 4.39  | 120.10      | 115.13   |
| 79  | L5    | 4579 | PSU  | C4-N3-C2 | -4.39 | 120.02      | 126.34   |
| 78  | S2    | 572  | PSU  | C4-N3-C2 | -4.38 | 120.02      | 126.34   |
| 78  | S2    | 1174 | PSU  | N1-C2-N3 | 4.38  | 120.09      | 115.13   |
| 79  | L5    | 4299 | PSU  | C4-N3-C2 | -4.38 | 120.03      | 126.34   |
| 78  | S2    | 36   | PSU  | C4-N3-C2 | -4.38 | 120.03      | 126.34   |
| 78  | S2    | 1239 | PSU  | N1-C2-N3 | 4.38  | 120.09      | 115.13   |
| 79  | L5    | 4972 | PSU  | N1-C2-N3 | 4.38  | 120.09      | 115.13   |
| 79  | L5    | 4299 | PSU  | N1-C2-N3 | 4.37  | 120.09      | 115.13   |
| 78  | S2    | 1625 | PSU  | N1-C2-N3 | 4.37  | 120.08      | 115.13   |
| 78  | S2    | 609  | PSU  | C4-N3-C2 | -4.37 | 120.04      | 126.34   |
| 78  | S2    | 572  | PSU  | N1-C2-N3 | 4.37  | 120.08      | 115.13   |
| 78  | S2    | 609  | PSU  | N1-C2-N3 | 4.37  | 120.08      | 115.13   |
| 78  | S2    | 863  | PSU  | N1-C2-N3 | 4.37  | 120.08      | 115.13   |
| 78  | S2    | 1692 | PSU  | N1-C2-N3 | 4.37  | 120.08      | 115.13   |
| 78  | S2    | 1678 | A2M  | N9-C8-N7 | -4.36 | 107.95      | 113.91   |
| 79  | L5    | 3768 | PSU  | C4-N3-C2 | -4.36 | 120.05      | 126.34   |
| 79  | L5    | 1683 | PSU  | C4-N3-C2 | -4.36 | 120.06      | 126.34   |
| 78  | S2    | 1248 | B8N  | C4-N3-C2 | -4.36 | 119.95      | 125.46   |
| 79  | L5    | 4493 | PSU  | N1-C2-N3 | 4.35  | 120.06      | 115.13   |
| 79  | L5    | 3785 | A2M  | N9-C8-N7 | -4.35 | 107.96      | 113.91   |
| 78  | S2    | 863  | PSU  | C4-N3-C2 | -4.35 | 120.07      | 126.34   |
| 78  | S2    | 105  | PSU  | N1-C2-N3 | 4.35  | 120.06      | 115.13   |
| 78  | S2    | 814  | PSU  | N1-C2-N3 | 4.35  | 120.06      | 115.13   |
| 79  | L5    | 5010 | PSU  | N1-C2-N3 | 4.35  | 120.06      | 115.13   |
| 78  | S2    | 918  | PSU  | C4-N3-C2 | -4.35 | 120.08      | 126.34   |
| 78  | S2    | 296  | PSU  | C4-N3-C2 | -4.34 | 120.08      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 78  | S2    | 814  | PSU  | C4-N3-C2   | -4.34 | 120.08      | 126.34   |
| 78  | S2    | 166  | A2M  | N9-C8-N7   | -4.34 | 107.98      | 113.91   |
| 78  | S2    | 1081 | PSU  | N1-C2-N3   | 4.34  | 120.05      | 115.13   |
| 79  | L5    | 1871 | A2M  | O4'-C1'-N9 | 4.34  | 116.61      | 108.06   |
| 79  | L5    | 4403 | PSU  | N1-C2-N3   | 4.33  | 120.04      | 115.13   |
| 78  | S2    | 866  | PSU  | N1-C2-N3   | 4.33  | 120.04      | 115.13   |
| 79  | L5    | 3844 | PSU  | C4-N3-C2   | -4.33 | 120.10      | 126.34   |
| 79  | L5    | 3768 | PSU  | N1-C2-N3   | 4.32  | 120.03      | 115.13   |
| 78  | S2    | 576  | A2M  | C2'-C1'-N9 | -4.32 | 106.25      | 113.53   |
| 79  | L5    | 4689 | PSU  | N1-C2-N3   | 4.32  | 120.02      | 115.13   |
| 79  | L5    | 1683 | PSU  | N1-C2-N3   | 4.32  | 120.02      | 115.13   |
| 79  | L5    | 1781 | PSU  | N1-C2-N3   | 4.31  | 120.02      | 115.13   |
| 79  | L5    | 4579 | PSU  | N1-C2-N3   | 4.31  | 120.02      | 115.13   |
| 79  | L5    | 1534 | A2M  | N9-C8-N7   | -4.31 | 108.02      | 113.91   |
| 79  | L5    | 4569 | PSU  | C4-N3-C2   | -4.31 | 120.13      | 126.34   |
| 78  | S2    | 93   | PSU  | N1-C2-N3   | 4.31  | 120.01      | 115.13   |
| 78  | S2    | 966  | PSU  | N1-C2-N3   | 4.30  | 120.01      | 115.13   |
| 79  | L5    | 2632 | PSU  | N1-C2-N3   | 4.30  | 120.00      | 115.13   |
| 79  | L5    | 3729 | PSU  | C4-N3-C2   | -4.30 | 120.14      | 126.34   |
| 78  | S2    | 966  | PSU  | C4-N3-C2   | -4.30 | 120.14      | 126.34   |
| 79  | L5    | 4569 | PSU  | N1-C2-N3   | 4.29  | 119.99      | 115.13   |
| 78  | S2    | 218  | PSU  | N1-C2-N3   | 4.29  | 119.98      | 115.13   |
| 79  | L5    | 3830 | A2M  | O4'-C1'-N9 | 4.28  | 116.50      | 108.06   |
| 78  | S2    | 93   | PSU  | C4-N3-C2   | -4.28 | 120.17      | 126.34   |
| 78  | S2    | 296  | PSU  | N1-C2-N3   | 4.27  | 119.97      | 115.13   |
| 79  | L5    | 3729 | PSU  | N1-C2-N3   | 4.27  | 119.97      | 115.13   |
| 79  | L5    | 4636 | PSU  | C4-N3-C2   | -4.26 | 120.19      | 126.34   |
| 79  | L5    | 1781 | PSU  | C4-N3-C2   | -4.24 | 120.23      | 126.34   |
| 79  | L5    | 2401 | A2M  | N9-C8-N7   | -4.23 | 108.13      | 113.91   |
| 79  | L5    | 2632 | PSU  | C4-N3-C2   | -4.22 | 120.25      | 126.34   |
| 79  | L5    | 4523 | A2M  | N9-C8-N7   | -4.22 | 108.14      | 113.91   |
| 78  | S2    | 99   | A2M  | N9-C8-N7   | -4.22 | 108.15      | 113.91   |
| 79  | L5    | 4471 | PSU  | C4-N3-C2   | -4.21 | 120.27      | 126.34   |
| 79  | L5    | 3723 | A2M  | N9-C8-N7   | -4.21 | 108.16      | 113.91   |
| 78  | S2    | 1850 | MA6  | N9-C8-N7   | -4.21 | 108.16      | 113.91   |
| 78  | S2    | 1031 | A2M  | N9-C8-N7   | -4.20 | 108.17      | 113.91   |
| 78  | S2    | 99   | A2M  | O4'-C1'-N9 | 4.20  | 116.34      | 108.06   |
| 79  | L5    | 2363 | A2M  | N9-C8-N7   | -4.20 | 108.17      | 113.91   |
| 78  | S2    | 1639 | G7M  | C1'-N9-C4  | 4.19  | 138.96      | 126.50   |
| 79  | L5    | 2815 | A2M  | N9-C8-N7   | -4.18 | 108.19      | 113.91   |
| 78  | S2    | 119  | PSU  | N1-C2-N3   | 4.18  | 119.87      | 115.13   |
| 78  | S2    | 1639 | G7M  | C1'-N9-C8  | -4.18 | 112.62      | 126.74   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 78  | S2    | 576  | A2M  | N9-C8-N7   | -4.18 | 108.19      | 113.91   |
| 79  | L5    | 3734 | PSU  | N1-C2-N3   | 4.18  | 119.86      | 115.13   |
| 78  | S2    | 468  | A2M  | O4'-C1'-N9 | 4.18  | 116.29      | 108.06   |
| 78  | S2    | 1639 | G7M  | C5-C4-N3   | -4.17 | 120.14      | 128.15   |
| 79  | L5    | 3718 | A2M  | O4'-C1'-N9 | 4.16  | 116.26      | 108.06   |
| 79  | L5    | 1871 | A2M  | N9-C8-N7   | -4.14 | 108.25      | 113.91   |
| 79  | L5    | 3734 | PSU  | C4-N3-C2   | -4.14 | 120.38      | 126.34   |
| 79  | L5    | 3724 | A2M  | N9-C8-N7   | -4.13 | 108.27      | 113.91   |
| 78  | S2    | 1326 | UY1  | N1-C2-N3   | 4.12  | 119.80      | 115.13   |
| 78  | S2    | 668  | A2M  | N9-C8-N7   | -4.12 | 108.28      | 113.91   |
| 79  | L5    | 3825 | A2M  | O4'-C1'-N9 | 4.11  | 116.17      | 108.06   |
| 78  | S2    | 27   | A2M  | N9-C8-N7   | -4.11 | 108.29      | 113.91   |
| 79  | L5    | 400  | A2M  | N9-C8-N7   | -4.10 | 108.31      | 113.91   |
| 79  | L5    | 4571 | A2M  | N9-C8-N7   | -4.09 | 108.31      | 113.91   |
| 79  | L5    | 1326 | A2M  | N9-C8-N7   | -4.08 | 108.33      | 113.91   |
| 79  | L5    | 4498 | OMU  | N3-C2-N1   | 4.08  | 120.31      | 114.89   |
| 79  | L5    | 4523 | A2M  | O4'-C1'-N9 | 4.08  | 116.10      | 108.06   |
| 78  | S2    | 512  | A2M  | N9-C8-N7   | -4.07 | 108.35      | 113.91   |
| 79  | L5    | 3825 | A2M  | N9-C8-N7   | -4.07 | 108.35      | 113.91   |
| 78  | S2    | 119  | PSU  | C4-N3-C2   | -4.07 | 120.48      | 126.34   |
| 76  | Pt    | 47   | G7M  | C5-C4-N3   | -4.05 | 120.39      | 128.15   |
| 78  | S2    | 1383 | A2M  | N9-C8-N7   | -4.05 | 108.38      | 113.91   |
| 78  | S2    | 468  | A2M  | N9-C8-N7   | -4.05 | 108.38      | 113.91   |
| 79  | L5    | 4420 | PSU  | N1-C2-N3   | 4.05  | 119.71      | 115.13   |
| 78  | S2    | 1031 | A2M  | O4'-C1'-N9 | 4.04  | 116.03      | 108.06   |
| 78  | S2    | 166  | A2M  | O4'-C1'-N9 | 4.03  | 116.00      | 108.06   |
| 78  | S2    | 1850 | MA6  | C4-C5-C6   | 4.03  | 120.39      | 115.88   |
| 79  | L5    | 3818 | UY1  | N1-C2-N3   | 4.01  | 119.68      | 115.13   |
| 79  | L5    | 4590 | A2M  | O4'-C1'-N9 | 4.00  | 115.95      | 108.06   |
| 78  | S2    | 27   | A2M  | O4'-C1'-N9 | 4.00  | 115.95      | 108.06   |
| 79  | L5    | 3830 | A2M  | N9-C8-N7   | -3.99 | 108.45      | 113.91   |
| 79  | L5    | 2837 | OMU  | N3-C2-N1   | 3.97  | 120.16      | 114.89   |
| 79  | L5    | 398  | A2M  | N9-C8-N7   | -3.97 | 108.49      | 113.91   |
| 79  | L5    | 398  | A2M  | O4'-C1'-N9 | 3.96  | 115.87      | 108.06   |
| 78  | S2    | 159  | A2M  | N9-C8-N7   | -3.96 | 108.50      | 113.91   |
| 76  | Pt    | 47   | G7M  | C1'-N9-C8  | -3.96 | 113.38      | 126.74   |
| 79  | L5    | 4420 | PSU  | C4-N3-C2   | -3.95 | 120.64      | 126.34   |
| 78  | S2    | 1383 | A2M  | O4'-C1'-N9 | 3.94  | 115.82      | 108.06   |
| 78  | S2    | 1832 | 6MZ  | N9-C8-N7   | -3.94 | 108.53      | 113.91   |
| 78  | S2    | 1639 | G7M  | C5-C6-N1   | 3.94  | 120.01      | 111.79   |
| 79  | L5    | 3867 | A2M  | N9-C8-N7   | -3.93 | 108.53      | 113.91   |
| 78  | S2    | 172  | OMU  | N3-C2-N1   | 3.90  | 120.07      | 114.89   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 78  | S2    | 512  | A2M  | O4'-C1'-N9 | 3.90  | 115.75      | 108.06   |
| 76  | Pt    | 47   | G7M  | C5-C6-N1   | 3.89  | 119.92      | 111.79   |
| 79  | L5    | 4227 | OMU  | N3-C2-N1   | 3.89  | 120.05      | 114.89   |
| 76  | Pt    | 47   | G7M  | C1'-N9-C4  | 3.89  | 138.04      | 126.50   |
| 78  | S2    | 1832 | 6MZ  | C4-C5-C6   | 3.88  | 119.82      | 116.81   |
| 79  | L5    | 3925 | OMU  | N3-C2-N1   | 3.88  | 120.04      | 114.89   |
| 79  | L5    | 3723 | A2M  | O4'-C1'-N9 | 3.88  | 115.70      | 108.06   |
| 79  | L5    | 3724 | A2M  | O4'-C1'-N9 | 3.87  | 115.69      | 108.06   |
| 79  | L5    | 2363 | A2M  | O4'-C1'-N9 | 3.86  | 115.67      | 108.06   |
| 79  | L5    | 2401 | A2M  | O4'-C1'-N9 | 3.81  | 115.57      | 108.06   |
| 78  | S2    | 428  | OMU  | N3-C2-N1   | 3.76  | 119.89      | 114.89   |
| 78  | S2    | 1804 | OMU  | N3-C2-N1   | 3.74  | 119.85      | 114.89   |
| 78  | S2    | 484  | A2M  | N9-C8-N7   | -3.73 | 108.81      | 113.91   |
| 76  | Pt    | 8    | 4SU  | N3-C2-N1   | 3.73  | 119.84      | 114.89   |
| 78  | S2    | 1851 | MA6  | C2-N1-C6   | 3.73  | 120.56      | 111.75   |
| 78  | S2    | 354  | OMU  | N3-C2-N1   | 3.72  | 119.82      | 114.89   |
| 79  | L5    | 4571 | A2M  | O4'-C1'-N9 | 3.71  | 115.37      | 108.06   |
| 79  | L5    | 4306 | OMU  | N3-C2-N1   | 3.68  | 119.78      | 114.89   |
| 79  | L5    | 2415 | OMU  | N3-C2-N1   | 3.68  | 119.77      | 114.89   |
| 78  | S2    | 1678 | A2M  | O4'-C1'-N9 | 3.66  | 115.28      | 108.06   |
| 78  | S2    | 1832 | 6MZ  | C9-N6-C6   | -3.66 | 119.72      | 122.87   |
| 78  | S2    | 627  | OMU  | N3-C2-N1   | 3.65  | 119.73      | 114.89   |
| 79  | L5    | 1534 | A2M  | C2-N3-C4   | 3.64  | 120.35      | 111.75   |
| 79  | L5    | 3785 | A2M  | C2-N3-C4   | 3.64  | 120.34      | 111.75   |
| 79  | L5    | 2815 | A2M  | C2-N3-C4   | 3.63  | 120.32      | 111.75   |
| 79  | L5    | 4620 | OMU  | N3-C2-N1   | 3.62  | 119.69      | 114.89   |
| 78  | S2    | 484  | A2M  | C2-N3-C4   | 3.61  | 120.29      | 111.75   |
| 78  | S2    | 166  | A2M  | C2-N3-C4   | 3.61  | 120.29      | 111.75   |
| 78  | S2    | 1031 | A2M  | C2-N3-C4   | 3.61  | 120.28      | 111.75   |
| 79  | L5    | 398  | A2M  | C2-N3-C4   | 3.61  | 120.27      | 111.75   |
| 78  | S2    | 99   | A2M  | C2-N3-C4   | 3.60  | 120.27      | 111.75   |
| 78  | S2    | 121  | OMU  | N3-C2-N1   | 3.60  | 119.67      | 114.89   |
| 78  | S2    | 116  | OMU  | N3-C2-N1   | 3.59  | 119.66      | 114.89   |
| 78  | S2    | 512  | A2M  | C2-N3-C4   | 3.59  | 120.23      | 111.75   |
| 79  | L5    | 3724 | A2M  | C2-N3-C4   | 3.59  | 120.23      | 111.75   |
| 78  | S2    | 159  | A2M  | O4'-C1'-N9 | 3.59  | 115.12      | 108.06   |
| 78  | S2    | 1851 | MA6  | C2-N3-C4   | 3.58  | 120.21      | 111.75   |
| 79  | L5    | 2351 | OMC  | C1'-N1-C2  | 3.58  | 126.41      | 118.42   |
| 79  | L5    | 3723 | A2M  | C2-N3-C4   | 3.58  | 120.21      | 111.75   |
| 79  | L5    | 1326 | A2M  | C2-N3-C4   | 3.57  | 120.19      | 111.75   |
| 78  | S2    | 1678 | A2M  | C2-N3-C4   | 3.57  | 120.19      | 111.75   |
| 79  | L5    | 400  | A2M  | C2-N3-C4   | 3.57  | 120.19      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 78  | S2    | 27   | A2M  | C2-N3-C4   | 3.57  | 120.18      | 111.75   |
| 78  | S2    | 1288 | OMU  | N3-C2-N1   | 3.57  | 119.62      | 114.89   |
| 78  | S2    | 1850 | MA6  | C2-N1-C6   | 3.57  | 120.17      | 111.75   |
| 79  | L5    | 4523 | A2M  | C2-N3-C4   | 3.57  | 120.17      | 111.75   |
| 79  | L5    | 4571 | A2M  | C2-N3-C4   | 3.56  | 120.16      | 111.75   |
| 78  | S2    | 1639 | G7M  | O6-C6-C5   | -3.56 | 120.03      | 128.06   |
| 79  | L5    | 2363 | A2M  | C2-N3-C4   | 3.56  | 120.15      | 111.75   |
| 78  | S2    | 1383 | A2M  | C2-N3-C4   | 3.55  | 120.14      | 111.75   |
| 79  | L5    | 4590 | A2M  | C2-N3-C4   | 3.55  | 120.14      | 111.75   |
| 78  | S2    | 590  | A2M  | C2-N3-C4   | 3.55  | 120.13      | 111.75   |
| 76  | Pt    | 47   | G7M  | O6-C6-C5   | -3.54 | 120.07      | 128.06   |
| 79  | L5    | 1871 | A2M  | C2-N3-C4   | 3.54  | 120.12      | 111.75   |
| 79  | L5    | 3867 | A2M  | C2-N3-C4   | 3.54  | 120.12      | 111.75   |
| 79  | L5    | 4220 | 6MZ  | N9-C8-N7   | -3.54 | 109.08      | 113.91   |
| 79  | L5    | 2401 | A2M  | C2-N3-C4   | 3.54  | 120.10      | 111.75   |
| 78  | S2    | 159  | A2M  | C2-N3-C4   | 3.52  | 120.08      | 111.75   |
| 78  | S2    | 1832 | 6MZ  | C2-N3-C4   | 3.51  | 120.05      | 111.75   |
| 78  | S2    | 468  | A2M  | C2-N3-C4   | 3.51  | 120.05      | 111.75   |
| 79  | L5    | 3718 | A2M  | N9-C8-N7   | -3.50 | 109.13      | 113.91   |
| 79  | L5    | 2815 | A2M  | O4'-C1'-N9 | 3.50  | 114.95      | 108.06   |
| 79  | L5    | 3825 | A2M  | C2-N3-C4   | 3.49  | 120.01      | 111.75   |
| 78  | S2    | 1804 | OMU  | C5-C4-N3   | 3.49  | 120.07      | 114.84   |
| 79  | L5    | 3830 | A2M  | C2-N3-C4   | 3.48  | 119.98      | 111.75   |
| 79  | L5    | 1326 | A2M  | O4'-C1'-N9 | 3.48  | 114.92      | 108.06   |
| 78  | S2    | 576  | A2M  | O4'-C1'-N9 | 3.47  | 114.90      | 108.06   |
| 78  | S2    | 1850 | MA6  | C2-N3-C4   | 3.46  | 119.92      | 111.75   |
| 79  | L5    | 400  | A2M  | O4'-C1'-N9 | 3.46  | 114.87      | 108.06   |
| 79  | L5    | 3718 | A2M  | C2-N3-C4   | 3.45  | 119.90      | 111.75   |
| 79  | L5    | 2415 | OMU  | C5-C4-N3   | 3.44  | 119.98      | 114.84   |
| 78  | S2    | 484  | A2M  | O4'-C1'-N9 | 3.43  | 114.82      | 108.06   |
| 79  | L5    | 1524 | A2M  | C2-N3-C4   | 3.43  | 119.86      | 111.75   |
| 78  | S2    | 668  | A2M  | C2-N3-C4   | 3.42  | 119.84      | 111.75   |
| 76  | Pt    | 8    | 4SU  | C5-C4-S4   | -3.41 | 120.07      | 124.47   |
| 78  | S2    | 576  | A2M  | C2-N3-C4   | 3.40  | 119.78      | 111.75   |
| 79  | L5    | 4220 | 6MZ  | C2-N3-C4   | 3.39  | 119.77      | 111.75   |
| 78  | S2    | 428  | OMU  | C5-C4-N3   | 3.36  | 119.87      | 114.84   |
| 79  | L5    | 4227 | OMU  | C5-C4-N3   | 3.36  | 119.87      | 114.84   |
| 79  | L5    | 3925 | OMU  | C5-C4-N3   | 3.35  | 119.86      | 114.84   |
| 78  | S2    | 354  | OMU  | C5-C4-N3   | 3.34  | 119.84      | 114.84   |
| 79  | L5    | 4306 | OMU  | C5-C4-N3   | 3.34  | 119.84      | 114.84   |
| 78  | S2    | 668  | A2M  | C2'-C1'-N9 | 3.33  | 119.14      | 113.53   |
| 79  | L5    | 2837 | OMU  | C5-C4-N3   | 3.33  | 119.83      | 114.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 78  | S2    | 1850 | MA6  | N3-C4-N9    | 3.31  | 132.53      | 127.08   |
| 78  | S2    | 627  | OMU  | C5-C4-N3    | 3.31  | 119.79      | 114.84   |
| 79  | L5    | 3867 | A2M  | O4'-C1'-N9  | 3.29  | 114.54      | 108.06   |
| 79  | L5    | 4620 | OMU  | C5-C4-N3    | 3.29  | 119.76      | 114.84   |
| 78  | S2    | 1288 | OMU  | C5-C4-N3    | 3.29  | 119.76      | 114.84   |
| 79  | L5    | 4498 | OMU  | C5-C4-N3    | 3.27  | 119.73      | 114.84   |
| 78  | S2    | 590  | A2M  | C5-N7-C8    | 3.26  | 108.14      | 103.51   |
| 78  | S2    | 116  | OMU  | C5-C4-N3    | 3.26  | 119.72      | 114.84   |
| 78  | S2    | 121  | OMU  | C5-C4-N3    | 3.25  | 119.70      | 114.84   |
| 78  | S2    | 1851 | MA6  | C5-N7-C8    | 3.25  | 108.13      | 103.51   |
| 78  | S2    | 1851 | MA6  | C4-C5-C6    | 3.24  | 119.50      | 115.88   |
| 78  | S2    | 172  | OMU  | C5-C4-N3    | 3.23  | 119.68      | 114.84   |
| 78  | S2    | 1678 | A2M  | C5-N7-C8    | 3.18  | 108.03      | 103.51   |
| 78  | S2    | 668  | A2M  | C4'-O4'-C1' | -3.18 | 102.46      | 109.47   |
| 79  | L5    | 4590 | A2M  | C4'-O4'-C1' | -3.17 | 102.49      | 109.47   |
| 79  | L5    | 1524 | A2M  | C5-N7-C8    | 3.16  | 108.00      | 103.51   |
| 76  | Pt    | 21   | H2U  | C5-C4-N3    | -3.16 | 113.10      | 116.65   |
| 79  | L5    | 3818 | UY1  | C6-C5-C4    | 3.15  | 120.40      | 118.20   |
| 79  | L5    | 1524 | A2M  | C4-N9-C8    | 3.14  | 109.13      | 105.73   |
| 78  | S2    | 166  | A2M  | C5-N7-C8    | 3.09  | 107.90      | 103.51   |
| 79  | L5    | 2363 | A2M  | C5-N7-C8    | 3.09  | 107.90      | 103.51   |
| 79  | L5    | 3785 | A2M  | O4'-C1'-C2' | -3.07 | 101.18      | 106.57   |
| 79  | L5    | 3867 | A2M  | N3-C4-N9    | 3.07  | 132.15      | 127.08   |
| 78  | S2    | 1639 | G7M  | C2-N1-C6    | -3.07 | 119.50      | 125.10   |
| 76  | Pt    | 33   | OMC  | C1'-N1-C2   | 3.06  | 125.25      | 118.42   |
| 78  | S2    | 1850 | MA6  | C5-N7-C8    | 3.06  | 107.85      | 103.51   |
| 79  | L5    | 3723 | A2M  | C5-N7-C8    | 3.06  | 107.85      | 103.51   |
| 79  | L5    | 4523 | A2M  | C4'-O4'-C1' | -3.05 | 102.73      | 109.47   |
| 79  | L5    | 4523 | A2M  | C5-N7-C8    | 3.05  | 107.85      | 103.51   |
| 79  | L5    | 2401 | A2M  | C5-N7-C8    | 3.04  | 107.83      | 103.51   |
| 79  | L5    | 1534 | A2M  | C5-N7-C8    | 3.03  | 107.82      | 103.51   |
| 79  | L5    | 4571 | A2M  | C5-N7-C8    | 3.03  | 107.82      | 103.51   |
| 78  | S2    | 99   | A2M  | C5-N7-C8    | 3.02  | 107.80      | 103.51   |
| 79  | L5    | 4590 | A2M  | C5-N7-C8    | 3.01  | 107.79      | 103.51   |
| 78  | S2    | 1678 | A2M  | N3-C4-N9    | 3.01  | 132.05      | 127.08   |
| 76  | Pt    | 47   | G7M  | C2-N1-C6    | -3.01 | 119.61      | 125.10   |
| 79  | L5    | 2815 | A2M  | C5-N7-C8    | 3.01  | 107.79      | 103.51   |
| 79  | L5    | 3785 | A2M  | C5-N7-C8    | 3.01  | 107.78      | 103.51   |
| 78  | S2    | 1031 | A2M  | C5-N7-C8    | 2.99  | 107.76      | 103.51   |
| 79  | L5    | 3825 | A2M  | C5-N7-C8    | 2.99  | 107.76      | 103.51   |
| 78  | S2    | 1639 | G7M  | N9-C4-N3    | 2.99  | 131.95      | 125.94   |
| 79  | L5    | 3785 | A2M  | N3-C4-N9    | 2.99  | 132.00      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 79  | L5    | 400  | A2M  | C5-N7-C8   | 2.98  | 107.75      | 103.51   |
| 78  | S2    | 1326 | UY1  | C6-C5-C4   | 2.98  | 120.28      | 118.20   |
| 78  | S2    | 590  | A2M  | C4-N9-C8   | 2.98  | 108.96      | 105.73   |
| 79  | L5    | 2415 | OMU  | O4-C4-C5   | -2.98 | 119.93      | 125.16   |
| 78  | S2    | 1804 | OMU  | O4-C4-C5   | -2.97 | 119.93      | 125.16   |
| 78  | S2    | 166  | A2M  | C2'-C1'-N9 | -2.97 | 108.53      | 113.53   |
| 78  | S2    | 27   | A2M  | C5-N7-C8   | 2.96  | 107.72      | 103.51   |
| 78  | S2    | 428  | OMU  | O4-C4-C5   | -2.96 | 119.95      | 125.16   |
| 79  | L5    | 1524 | A2M  | C2'-C1'-N9 | -2.95 | 108.57      | 113.53   |
| 78  | S2    | 576  | A2M  | C5-N7-C8   | 2.94  | 107.68      | 103.51   |
| 79  | L5    | 4552 | PSU  | O2-C2-N1   | -2.94 | 119.56      | 122.79   |
| 78  | S2    | 1832 | 6MZ  | C5-N7-C8   | 2.94  | 107.68      | 103.51   |
| 78  | S2    | 512  | A2M  | C5-N7-C8   | 2.93  | 107.67      | 103.51   |
| 78  | S2    | 668  | A2M  | C5-N7-C8   | 2.93  | 107.67      | 103.51   |
| 79  | L5    | 1536 | PSU  | O2-C2-N1   | -2.92 | 119.58      | 122.79   |
| 79  | L5    | 1326 | A2M  | C5-N7-C8   | 2.92  | 107.66      | 103.51   |
| 79  | L5    | 398  | A2M  | C5-N7-C8   | 2.91  | 107.65      | 103.51   |
| 79  | L5    | 3724 | A2M  | C5-N7-C8   | 2.91  | 107.64      | 103.51   |
| 78  | S2    | 468  | A2M  | C5-N7-C8   | 2.90  | 107.63      | 103.51   |
| 78  | S2    | 512  | A2M  | C2'-C1'-N9 | -2.90 | 108.65      | 113.53   |
| 78  | S2    | 159  | A2M  | C5-N7-C8   | 2.89  | 107.61      | 103.51   |
| 79  | L5    | 4620 | OMU  | O4-C4-C5   | -2.88 | 120.09      | 125.16   |
| 79  | L5    | 1871 | A2M  | C5-N7-C8   | 2.88  | 107.60      | 103.51   |
| 79  | L5    | 4628 | PSU  | O2-C2-N1   | -2.88 | 119.62      | 122.79   |
| 79  | L5    | 4306 | OMU  | O4-C4-C5   | -2.88 | 120.10      | 125.16   |
| 78  | S2    | 1383 | A2M  | C5-N7-C8   | 2.88  | 107.60      | 103.51   |
| 78  | S2    | 1248 | B8N  | N3-C2-N1   | 2.88  | 120.82      | 116.76   |
| 78  | S2    | 354  | OMU  | O4-C4-C5   | -2.88 | 120.10      | 125.16   |
| 79  | L5    | 3867 | A2M  | C5-N7-C8   | 2.87  | 107.59      | 103.51   |
| 79  | L5    | 3808 | OMC  | C1'-N1-C2  | 2.87  | 124.83      | 118.42   |
| 78  | S2    | 590  | A2M  | N3-C4-N9   | 2.87  | 131.81      | 127.08   |
| 78  | S2    | 172  | OMU  | O4-C4-C5   | -2.87 | 120.12      | 125.16   |
| 76  | Pt    | 47   | G7M  | N9-C4-N3   | 2.87  | 131.69      | 125.94   |
| 78  | S2    | 590  | A2M  | C2'-C1'-N9 | -2.86 | 108.71      | 113.53   |
| 79  | L5    | 3925 | OMU  | O4-C4-C5   | -2.86 | 120.13      | 125.16   |
| 78  | S2    | 484  | A2M  | N3-C4-N9   | 2.86  | 131.79      | 127.08   |
| 79  | L5    | 3830 | A2M  | C5-N7-C8   | 2.86  | 107.57      | 103.51   |
| 78  | S2    | 627  | OMU  | O4-C4-C5   | -2.85 | 120.15      | 125.16   |
| 79  | L5    | 1524 | A2M  | N3-C4-N9   | 2.84  | 131.77      | 127.08   |
| 78  | S2    | 121  | OMU  | O4-C4-C5   | -2.84 | 120.16      | 125.16   |
| 79  | L5    | 398  | A2M  | N3-C4-N9   | 2.84  | 131.77      | 127.08   |
| 79  | L5    | 3723 | A2M  | N3-C4-N9   | 2.84  | 131.77      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 2815 | A2M  | N3-C4-N9    | 2.84  | 131.76      | 127.08   |
| 78  | S2    | 1842 | 4AC  | C6-C5-C4    | 2.83  | 120.43      | 116.96   |
| 78  | S2    | 116  | OMU  | O4-C4-C5    | -2.83 | 120.18      | 125.16   |
| 79  | L5    | 4220 | 6MZ  | N3-C4-N9    | 2.83  | 131.74      | 127.08   |
| 79  | L5    | 4571 | A2M  | N3-C4-N9    | 2.83  | 131.74      | 127.08   |
| 79  | L5    | 1534 | A2M  | N3-C4-N9    | 2.82  | 131.74      | 127.08   |
| 79  | L5    | 4576 | PSU  | O2-C2-N1    | -2.82 | 119.69      | 122.79   |
| 78  | S2    | 1337 | 4AC  | C6-C5-C4    | 2.81  | 120.41      | 116.96   |
| 79  | L5    | 3718 | A2M  | N3-C4-N9    | 2.81  | 131.72      | 127.08   |
| 79  | L5    | 3724 | A2M  | N3-C4-N9    | 2.81  | 131.72      | 127.08   |
| 79  | L5    | 4531 | PSU  | O2-C2-N1    | -2.81 | 119.70      | 122.79   |
| 79  | L5    | 3762 | PSU  | O2-C2-N1    | -2.81 | 119.70      | 122.79   |
| 79  | L5    | 3851 | PSU  | O2-C2-N1    | -2.81 | 119.70      | 122.79   |
| 79  | L5    | 2837 | OMU  | O4-C4-C5    | -2.80 | 120.23      | 125.16   |
| 78  | S2    | 1288 | OMU  | O4-C4-C5    | -2.80 | 120.23      | 125.16   |
| 5   | L8    | 55   | PSU  | O2-C2-N1    | -2.78 | 119.72      | 122.79   |
| 78  | S2    | 484  | A2M  | C5-N7-C8    | 2.78  | 107.46      | 103.51   |
| 78  | S2    | 99   | A2M  | N3-C4-N9    | 2.78  | 131.67      | 127.08   |
| 79  | L5    | 2401 | A2M  | N3-C4-N9    | 2.78  | 131.66      | 127.08   |
| 78  | S2    | 1004 | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 79  | L5    | 2839 | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 78  | S2    | 36   | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 78  | S2    | 1031 | A2M  | N3-C4-N9    | 2.77  | 131.64      | 127.08   |
| 78  | S2    | 1678 | A2M  | C4'-O4'-C1' | -2.77 | 103.37      | 109.47   |
| 79  | L5    | 4227 | OMU  | O4-C4-C5    | -2.77 | 120.30      | 125.16   |
| 79  | L5    | 3844 | PSU  | O2-C2-N1    | -2.76 | 119.75      | 122.79   |
| 78  | S2    | 1383 | A2M  | C2'-C1'-N9  | -2.76 | 108.88      | 113.53   |
| 79  | L5    | 1326 | A2M  | N3-C4-N9    | 2.75  | 131.62      | 127.08   |
| 79  | L5    | 3785 | A2M  | O4'-C1'-N9  | 2.75  | 113.48      | 108.06   |
| 79  | L5    | 1779 | PSU  | O2-C2-N1    | -2.75 | 119.76      | 122.79   |
| 79  | L5    | 4523 | A2M  | N3-C4-N9    | 2.75  | 131.61      | 127.08   |
| 79  | L5    | 3818 | UY1  | C6-N1-C2    | -2.74 | 119.88      | 122.68   |
| 79  | L5    | 3785 | A2M  | C4'-O4'-C1' | -2.74 | 103.43      | 109.47   |
| 78  | S2    | 1832 | 6MZ  | N3-C4-N9    | 2.73  | 131.57      | 127.08   |
| 78  | S2    | 822  | PSU  | O2-C2-N1    | -2.72 | 119.79      | 122.79   |
| 79  | L5    | 3853 | PSU  | O2-C2-N1    | -2.72 | 119.79      | 122.79   |
| 79  | L5    | 400  | A2M  | N3-C4-N9    | 2.72  | 131.56      | 127.08   |
| 79  | L5    | 4403 | PSU  | O2-C2-N1    | -2.72 | 119.80      | 122.79   |
| 79  | L5    | 3867 | A2M  | C4'-O4'-C1' | -2.71 | 103.48      | 109.47   |
| 78  | S2    | 1232 | PSU  | O2-C2-N1    | -2.71 | 119.80      | 122.79   |
| 78  | S2    | 863  | PSU  | O2-C2-N1    | -2.71 | 119.81      | 122.79   |
| 79  | L5    | 1677 | PSU  | O2-C2-N1    | -2.71 | 119.81      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 3718 | A2M  | C5-N7-C8    | 2.71  | 107.36      | 103.51   |
| 78  | S2    | 1326 | UY1  | C6-N1-C2    | -2.71 | 119.91      | 122.68   |
| 78  | S2    | 159  | A2M  | N3-C4-N9    | 2.71  | 131.55      | 127.08   |
| 78  | S2    | 406  | PSU  | O2-C2-N1    | -2.70 | 119.81      | 122.79   |
| 78  | S2    | 1643 | PSU  | O2-C2-N1    | -2.70 | 119.82      | 122.79   |
| 79  | L5    | 4689 | PSU  | O2-C2-N1    | -2.70 | 119.82      | 122.79   |
| 78  | S2    | 1851 | MA6  | N3-C4-N9    | 2.69  | 131.52      | 127.08   |
| 78  | S2    | 1136 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 78  | S2    | 1243 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 78  | S2    | 512  | A2M  | N3-C4-N9    | 2.69  | 131.52      | 127.08   |
| 78  | S2    | 649  | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 79  | L5    | 3729 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 79  | L5    | 1860 | PSU  | O2-C2-N1    | -2.68 | 119.84      | 122.79   |
| 78  | S2    | 1383 | A2M  | N3-C4-N9    | 2.68  | 131.50      | 127.08   |
| 78  | S2    | 609  | PSU  | O2-C2-N1    | -2.67 | 119.85      | 122.79   |
| 79  | L5    | 4353 | PSU  | O2-C2-N1    | -2.67 | 119.86      | 122.79   |
| 78  | S2    | 1174 | PSU  | O2-C2-N1    | -2.66 | 119.86      | 122.79   |
| 78  | S2    | 1238 | PSU  | O2-C2-N1    | -2.66 | 119.87      | 122.79   |
| 78  | S2    | 1367 | PSU  | O2-C2-N1    | -2.65 | 119.87      | 122.79   |
| 79  | L5    | 3724 | A2M  | C4'-O4'-C1' | -2.65 | 103.62      | 109.47   |
| 79  | L5    | 3764 | PSU  | O2-C2-N1    | -2.65 | 119.87      | 122.79   |
| 79  | L5    | 4628 | PSU  | C6-N1-C2    | -2.65 | 119.97      | 122.68   |
| 78  | S2    | 1692 | PSU  | O2-C2-N1    | -2.65 | 119.87      | 122.79   |
| 79  | L5    | 3770 | PSU  | O2-C2-N1    | -2.65 | 119.88      | 122.79   |
| 79  | L5    | 4498 | OMU  | O4-C4-C5    | -2.65 | 120.50      | 125.16   |
| 5   | L8    | 69   | PSU  | O2-C2-N1    | -2.65 | 119.88      | 122.79   |
| 79  | L5    | 4500 | PSU  | O2-C2-N1    | -2.64 | 119.88      | 122.79   |
| 78  | S2    | 468  | A2M  | N3-C4-N9    | 2.64  | 131.44      | 127.08   |
| 79  | L5    | 2363 | A2M  | N3-C4-N9    | 2.64  | 131.44      | 127.08   |
| 78  | S2    | 166  | A2M  | N3-C4-N9    | 2.64  | 131.43      | 127.08   |
| 79  | L5    | 3884 | PSU  | O2-C2-N1    | -2.64 | 119.88      | 122.79   |
| 78  | S2    | 27   | A2M  | N3-C4-N9    | 2.64  | 131.43      | 127.08   |
| 78  | S2    | 918  | PSU  | O2-C2-N1    | -2.64 | 119.89      | 122.79   |
| 78  | S2    | 801  | PSU  | O2-C2-N1    | -2.63 | 119.89      | 122.79   |
| 79  | L5    | 3639 | PSU  | O2-C2-N1    | -2.63 | 119.89      | 122.79   |
| 79  | L5    | 2351 | OMC  | C1'-N1-C6   | -2.62 | 115.13      | 120.84   |
| 79  | L5    | 1683 | PSU  | O2-C2-N1    | -2.61 | 119.91      | 122.79   |
| 79  | L5    | 4500 | PSU  | C6-C5-C4    | 2.61  | 120.03      | 118.20   |
| 79  | L5    | 1782 | PSU  | O2-C2-N1    | -2.61 | 119.91      | 122.79   |
| 78  | S2    | 686  | PSU  | O2-C2-N1    | -2.60 | 119.92      | 122.79   |
| 78  | S2    | 1248 | B8N  | O4-C4-N3    | -2.60 | 115.56      | 119.98   |
| 78  | S2    | 651  | PSU  | O2-C2-N1    | -2.60 | 119.93      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 4220 | 6MZ  | C5-N7-C8    | 2.59  | 107.19      | 103.51   |
| 79  | L5    | 1534 | A2M  | O4'-C1'-C2' | -2.59 | 102.03      | 106.57   |
| 79  | L5    | 4312 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 79  | L5    | 4636 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 79  | L5    | 4673 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 78  | S2    | 1244 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 78  | S2    | 1177 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 79  | L5    | 1871 | A2M  | C2'-C1'-N9  | -2.57 | 109.20      | 113.53   |
| 79  | L5    | 4590 | A2M  | N3-C4-N9    | 2.57  | 131.32      | 127.08   |
| 79  | L5    | 1534 | A2M  | C2'-C1'-N9  | 2.57  | 117.86      | 113.53   |
| 78  | S2    | 814  | PSU  | O2-C2-N1    | -2.57 | 119.96      | 122.79   |
| 79  | L5    | 3830 | A2M  | N3-C4-N9    | 2.57  | 131.31      | 127.08   |
| 78  | S2    | 1347 | PSU  | O2-C2-N1    | -2.57 | 119.97      | 122.79   |
| 78  | S2    | 34   | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 79  | L5    | 2861 | OMC  | C1'-N1-C2   | 2.56  | 124.14      | 118.42   |
| 79  | L5    | 1744 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 79  | L5    | 4296 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 79  | L5    | 4972 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 78  | S2    | 1056 | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 79  | L5    | 3825 | A2M  | N3-C4-N9    | 2.55  | 131.29      | 127.08   |
| 78  | S2    | 109  | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 78  | S2    | 1445 | PSU  | O2-C2-N1    | -2.54 | 119.99      | 122.79   |
| 78  | S2    | 296  | PSU  | O2-C2-N1    | -2.54 | 119.99      | 122.79   |
| 79  | L5    | 4521 | PSU  | O2-C2-N1    | -2.54 | 119.99      | 122.79   |
| 79  | L5    | 2401 | A2M  | C4'-O4'-C1' | -2.54 | 103.86      | 109.47   |
| 79  | L5    | 4442 | PSU  | O2-C2-N1    | -2.54 | 119.99      | 122.79   |
| 79  | L5    | 4531 | PSU  | C6-C5-C4    | 2.53  | 119.97      | 118.20   |
| 79  | L5    | 3758 | PSU  | O2-C2-N1    | -2.53 | 120.00      | 122.79   |
| 79  | L5    | 1871 | A2M  | N3-C4-N9    | 2.53  | 131.25      | 127.08   |
| 79  | L5    | 1536 | PSU  | C6-N1-C2    | -2.52 | 120.11      | 122.68   |
| 78  | S2    | 572  | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 79  | L5    | 1792 | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 79  | L5    | 2401 | A2M  | C2'-C1'-N9  | -2.52 | 109.29      | 113.53   |
| 78  | S2    | 576  | A2M  | N3-C4-N9    | 2.52  | 131.23      | 127.08   |
| 78  | S2    | 966  | PSU  | O2-C2-N1    | -2.51 | 120.02      | 122.79   |
| 79  | L5    | 4471 | PSU  | O2-C2-N1    | -2.51 | 120.03      | 122.79   |
| 79  | L5    | 4431 | PSU  | O2-C2-N1    | -2.51 | 120.03      | 122.79   |
| 78  | S2    | 573  | PSU  | O2-C2-N1    | -2.51 | 120.03      | 122.79   |
| 78  | S2    | 918  | PSU  | O4'-C1'-C2' | 2.51  | 108.68      | 105.14   |
| 79  | L5    | 2508 | PSU  | O2-C2-N1    | -2.50 | 120.03      | 122.79   |
| 79  | L5    | 3637 | PSU  | C6-N1-C2    | -2.50 | 120.13      | 122.68   |
| 79  | L5    | 4361 | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 4493 | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |
| 79  | L5    | 2632 | PSU  | O2-C2-N1    | -2.50 | 120.04      | 122.79   |
| 78  | S2    | 1851 | MA6  | C4-N9-C8    | 2.50  | 108.43      | 105.73   |
| 79  | L5    | 4530 | UR3  | C6-N1-C2    | -2.49 | 119.56      | 121.79   |
| 78  | S2    | 1625 | PSU  | O2-C2-N1    | -2.49 | 120.05      | 122.79   |
| 78  | S2    | 863  | PSU  | C6-N1-C2    | -2.49 | 120.14      | 122.68   |
| 76  | Pt    | 56   | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 78  | S2    | 668  | A2M  | N3-C4-N9    | 2.48  | 131.18      | 127.08   |
| 79  | L5    | 3734 | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 79  | L5    | 3768 | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 79  | L5    | 4532 | PSU  | O2-C2-N1    | -2.48 | 120.06      | 122.79   |
| 79  | L5    | 3715 | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 78  | S2    | 93   | PSU  | O2-C2-N1    | -2.47 | 120.07      | 122.79   |
| 78  | S2    | 36   | PSU  | C6-N1-C2    | -2.46 | 120.17      | 122.68   |
| 79  | L5    | 3844 | PSU  | C6-N1-C2    | -2.46 | 120.17      | 122.68   |
| 79  | L5    | 1524 | A2M  | C4'-O4'-C1' | -2.45 | 104.06      | 109.47   |
| 78  | S2    | 119  | PSU  | C6-N1-C2    | -2.45 | 120.18      | 122.68   |
| 78  | S2    | 918  | PSU  | C6-N1-C2    | -2.45 | 120.18      | 122.68   |
| 79  | L5    | 3695 | PSU  | O2-C2-N1    | -2.45 | 120.09      | 122.79   |
| 78  | S2    | 1004 | PSU  | C6-N1-C2    | -2.44 | 120.19      | 122.68   |
| 79  | L5    | 3884 | PSU  | C6-N1-C2    | -2.44 | 120.19      | 122.68   |
| 78  | S2    | 166  | A2M  | C4'-O4'-C1' | -2.44 | 104.10      | 109.47   |
| 79  | L5    | 4636 | PSU  | C6-N1-C2    | -2.43 | 120.19      | 122.68   |
| 79  | L5    | 4299 | PSU  | O2-C2-N1    | -2.43 | 120.11      | 122.79   |
| 79  | L5    | 5001 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 78  | S2    | 609  | PSU  | C6-N1-C2    | -2.43 | 120.20      | 122.68   |
| 79  | L5    | 2876 | OMG  | CM2-O2'-C2' | 2.43  | 120.89      | 114.52   |
| 79  | L5    | 3718 | A2M  | C5-C4-N9    | 2.43  | 108.61      | 105.78   |
| 78  | S2    | 815  | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 79  | L5    | 4420 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 79  | L5    | 4579 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 79  | L5    | 4590 | A2M  | C2'-C1'-N9  | -2.42 | 109.45      | 113.53   |
| 78  | S2    | 681  | PSU  | O2-C2-N1    | -2.42 | 120.13      | 122.79   |
| 79  | L5    | 2839 | PSU  | C6-N1-C2    | -2.41 | 120.22      | 122.68   |
| 78  | S2    | 1337 | 4AC  | C5-C4-N3    | -2.41 | 118.72      | 122.59   |
| 79  | L5    | 4423 | PSU  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 78  | S2    | 1842 | 4AC  | C5-C4-N3    | -2.41 | 118.72      | 122.59   |
| 78  | S2    | 1326 | UY1  | O2-C2-N1    | -2.41 | 120.14      | 122.79   |
| 78  | S2    | 866  | PSU  | O2-C2-N1    | -2.40 | 120.15      | 122.79   |
| 79  | L5    | 1781 | PSU  | O2-C2-N1    | -2.40 | 120.15      | 122.79   |
| 79  | L5    | 4293 | PSU  | C6-N1-C2    | -2.40 | 120.23      | 122.68   |
| 79  | L5    | 5001 | PSU  | C6-N1-C2    | -2.40 | 120.23      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 3920 | PSU  | O2-C2-N1    | -2.40 | 120.15      | 122.79   |
| 78  | S2    | 1232 | PSU  | C6-N1-C2    | -2.40 | 120.23      | 122.68   |
| 79  | L5    | 4500 | PSU  | C6-N1-C2    | -2.39 | 120.24      | 122.68   |
| 78  | S2    | 1383 | A2M  | C4'-O4'-C1' | -2.39 | 104.20      | 109.47   |
| 79  | L5    | 3639 | PSU  | C6-N1-C2    | -2.39 | 120.24      | 122.68   |
| 79  | L5    | 3729 | PSU  | C6-N1-C2    | -2.39 | 120.24      | 122.68   |
| 79  | L5    | 1326 | A2M  | C4'-O4'-C1' | -2.39 | 104.21      | 109.47   |
| 78  | S2    | 119  | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 79  | L5    | 1683 | PSU  | C6-N1-C2    | -2.38 | 120.25      | 122.68   |
| 79  | L5    | 4457 | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 79  | L5    | 4471 | PSU  | C6-N1-C2    | -2.38 | 120.25      | 122.68   |
| 79  | L5    | 5010 | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 79  | L5    | 2632 | PSU  | C6-N1-C2    | -2.37 | 120.26      | 122.68   |
| 78  | S2    | 296  | PSU  | C6-N1-C2    | -2.37 | 120.26      | 122.68   |
| 79  | L5    | 4569 | PSU  | O2-C2-N1    | -2.37 | 120.18      | 122.79   |
| 79  | L5    | 3825 | A2M  | C5-C4-N9    | 2.37  | 108.54      | 105.78   |
| 79  | L5    | 3734 | PSU  | C6-N1-C2    | -2.37 | 120.26      | 122.68   |
| 78  | S2    | 1174 | PSU  | C6-N1-C2    | -2.36 | 120.27      | 122.68   |
| 79  | L5    | 1582 | PSU  | O2-C2-N1    | -2.36 | 120.19      | 122.79   |
| 79  | L5    | 2363 | A2M  | C4-C5-N7    | -2.35 | 107.76      | 110.62   |
| 78  | S2    | 105  | PSU  | O2-C2-N1    | -2.34 | 120.21      | 122.79   |
| 79  | L5    | 1862 | PSU  | O2-C2-N1    | -2.34 | 120.21      | 122.79   |
| 5   | L8    | 69   | PSU  | C6-N1-C2    | -2.34 | 120.29      | 122.68   |
| 79  | L5    | 4579 | PSU  | C6-N1-C2    | -2.34 | 120.29      | 122.68   |
| 79  | L5    | 4689 | PSU  | C6-N1-C2    | -2.34 | 120.29      | 122.68   |
| 78  | S2    | 406  | PSU  | C6-N1-C2    | -2.33 | 120.30      | 122.68   |
| 79  | L5    | 4293 | PSU  | O2-C2-N1    | -2.33 | 120.22      | 122.79   |
| 79  | L5    | 4673 | PSU  | C6-N1-C2    | -2.33 | 120.30      | 122.68   |
| 76  | Pt    | 33   | OMC  | C1'-N1-C6   | -2.33 | 115.77      | 120.84   |
| 78  | S2    | 1851 | MA6  | C4-C5-N7    | -2.33 | 107.78      | 110.62   |
| 79  | L5    | 3764 | PSU  | C6-N1-C2    | -2.33 | 120.31      | 122.68   |
| 79  | L5    | 3825 | A2M  | C4-C5-N7    | -2.33 | 107.79      | 110.62   |
| 79  | L5    | 3770 | PSU  | C6-N1-C2    | -2.32 | 120.31      | 122.68   |
| 79  | L5    | 3830 | A2M  | C2'-C1'-N9  | -2.32 | 109.62      | 113.53   |
| 78  | S2    | 649  | PSU  | C6-N1-C2    | -2.32 | 120.31      | 122.68   |
| 79  | L5    | 4312 | PSU  | C6-N1-C2    | -2.32 | 120.31      | 122.68   |
| 78  | S2    | 99   | A2M  | C4'-O4'-C1' | -2.31 | 104.36      | 109.47   |
| 78  | S2    | 1239 | PSU  | O2-C2-N1    | -2.31 | 120.24      | 122.79   |
| 78  | S2    | 1248 | B8N  | O4'-C1'-C2' | 2.31  | 108.40      | 105.14   |
| 5   | L8    | 55   | PSU  | C6-N1-C2    | -2.31 | 120.32      | 122.68   |
| 79  | L5    | 4403 | PSU  | O4'-C1'-C2' | 2.31  | 108.40      | 105.14   |
| 78  | S2    | 590  | A2M  | C4-C5-N7    | -2.30 | 107.81      | 110.62   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 79  | L5    | 3768 | PSU  | C6-N1-C2  | -2.30 | 120.33      | 122.68   |
| 78  | S2    | 166  | A2M  | C4-C5-N7  | -2.30 | 107.82      | 110.62   |
| 79  | L5    | 3920 | PSU  | C6-N1-C2  | -2.30 | 120.33      | 122.68   |
| 79  | L5    | 4552 | PSU  | C6-N1-C2  | -2.29 | 120.34      | 122.68   |
| 78  | S2    | 1244 | PSU  | C6-N1-C2  | -2.29 | 120.34      | 122.68   |
| 78  | S2    | 1643 | PSU  | C6-N1-C2  | -2.29 | 120.34      | 122.68   |
| 79  | L5    | 1779 | PSU  | C6-N1-C2  | -2.29 | 120.34      | 122.68   |
| 79  | L5    | 4423 | PSU  | C6-N1-C2  | -2.29 | 120.34      | 122.68   |
| 79  | L5    | 4442 | PSU  | C6-N1-C2  | -2.29 | 120.34      | 122.68   |
| 78  | S2    | 572  | PSU  | C6-N1-C2  | -2.29 | 120.35      | 122.68   |
| 78  | S2    | 681  | PSU  | C6-N1-C2  | -2.29 | 120.35      | 122.68   |
| 78  | S2    | 814  | PSU  | C6-N1-C2  | -2.28 | 120.35      | 122.68   |
| 78  | S2    | 1625 | PSU  | C6-N1-C2  | -2.28 | 120.35      | 122.68   |
| 79  | L5    | 2843 | PSU  | O2-C2-N1  | -2.28 | 120.28      | 122.79   |
| 79  | L5    | 4590 | A2M  | C4-N9-C8  | 2.28  | 108.20      | 105.73   |
| 78  | S2    | 1367 | PSU  | C6-N1-C2  | -2.28 | 120.35      | 122.68   |
| 79  | L5    | 1860 | PSU  | C6-N1-C2  | -2.28 | 120.35      | 122.68   |
| 78  | S2    | 218  | PSU  | O2-C2-N1  | -2.28 | 120.28      | 122.79   |
| 79  | L5    | 4456 | OMC  | C1'-N1-C2 | 2.28  | 123.50      | 118.42   |
| 79  | L5    | 3695 | PSU  | C6-N1-C2  | -2.27 | 120.36      | 122.68   |
| 79  | L5    | 4299 | PSU  | C6-N1-C2  | -2.27 | 120.36      | 122.68   |
| 79  | L5    | 1781 | PSU  | C6-N1-C2  | -2.27 | 120.36      | 122.68   |
| 78  | S2    | 1081 | PSU  | O2-C2-N1  | -2.27 | 120.29      | 122.79   |
| 79  | L5    | 3762 | PSU  | C6-N1-C2  | -2.27 | 120.36      | 122.68   |
| 79  | L5    | 1744 | PSU  | C6-N1-C2  | -2.27 | 120.36      | 122.68   |
| 78  | S2    | 1692 | PSU  | C6-N1-C2  | -2.26 | 120.37      | 122.68   |
| 79  | L5    | 4571 | A2M  | C4-C5-N7  | -2.26 | 107.87      | 110.62   |
| 79  | L5    | 4403 | PSU  | C6-C5-C4  | 2.26  | 119.78      | 118.20   |
| 79  | L5    | 1677 | PSU  | C6-N1-C2  | -2.26 | 120.38      | 122.68   |
| 79  | L5    | 4353 | PSU  | C6-N1-C2  | -2.26 | 120.38      | 122.68   |
| 78  | S2    | 1678 | A2M  | C4-C5-N7  | -2.25 | 107.87      | 110.62   |
| 79  | L5    | 4531 | PSU  | C6-N1-C2  | -2.25 | 120.38      | 122.68   |
| 79  | L5    | 3718 | A2M  | C6-C5-C4  | 2.25  | 120.21      | 117.18   |
| 78  | S2    | 573  | PSU  | C6-N1-C2  | -2.25 | 120.38      | 122.68   |
| 79  | L5    | 4361 | PSU  | C6-N1-C2  | -2.25 | 120.38      | 122.68   |
| 78  | S2    | 484  | A2M  | C5-C4-N9  | 2.25  | 108.40      | 105.78   |
| 78  | S2    | 109  | PSU  | C6-N1-C2  | -2.25 | 120.39      | 122.68   |
| 79  | L5    | 4576 | PSU  | C6-N1-C2  | -2.25 | 120.39      | 122.68   |
| 79  | L5    | 4590 | A2M  | C4-C5-N7  | -2.25 | 107.88      | 110.62   |
| 79  | L5    | 4420 | PSU  | C6-N1-C2  | -2.24 | 120.39      | 122.68   |
| 79  | L5    | 2422 | OMC  | C1'-N1-C2 | 2.24  | 123.42      | 118.42   |
| 79  | L5    | 4569 | PSU  | C6-N1-C2  | -2.24 | 120.39      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 78  | S2    | 172  | OMU  | O2-C2-N1    | -2.24 | 119.81      | 122.79   |
| 78  | S2    | 822  | PSU  | C6-N1-C2    | -2.24 | 120.39      | 122.68   |
| 78  | S2    | 1804 | OMU  | O2-C2-N1    | -2.23 | 119.82      | 122.79   |
| 79  | L5    | 2815 | A2M  | C4-C5-N7    | -2.23 | 107.90      | 110.62   |
| 79  | L5    | 4532 | PSU  | C6-N1-C2    | -2.23 | 120.40      | 122.68   |
| 78  | S2    | 93   | PSU  | C6-N1-C2    | -2.23 | 120.40      | 122.68   |
| 79  | L5    | 3723 | A2M  | C4-C5-N7    | -2.23 | 107.90      | 110.62   |
| 78  | S2    | 34   | PSU  | C6-N1-C2    | -2.23 | 120.41      | 122.68   |
| 78  | S2    | 1136 | PSU  | C6-N1-C2    | -2.23 | 120.41      | 122.68   |
| 79  | L5    | 1782 | PSU  | C6-N1-C2    | -2.23 | 120.41      | 122.68   |
| 78  | S2    | 1678 | A2M  | C4-N9-C8    | 2.23  | 108.14      | 105.73   |
| 78  | S2    | 1850 | MA6  | C4-N9-C8    | 2.23  | 108.14      | 105.73   |
| 78  | S2    | 1177 | PSU  | C6-N1-C2    | -2.23 | 120.41      | 122.68   |
| 78  | S2    | 668  | A2M  | C5-C4-N9    | 2.22  | 108.37      | 105.78   |
| 78  | S2    | 1238 | PSU  | C6-N1-C2    | -2.22 | 120.41      | 122.68   |
| 79  | L5    | 3715 | PSU  | C6-N1-C2    | -2.22 | 120.42      | 122.68   |
| 78  | S2    | 1031 | A2M  | C2'-C1'-N9  | -2.22 | 109.80      | 113.53   |
| 78  | S2    | 576  | A2M  | C4-C5-N7    | -2.21 | 107.92      | 110.62   |
| 79  | L5    | 1534 | A2M  | C4-C5-N7    | -2.21 | 107.93      | 110.62   |
| 78  | S2    | 686  | PSU  | C6-N1-C2    | -2.21 | 120.42      | 122.68   |
| 79  | L5    | 2363 | A2M  | C5-C4-N9    | 2.21  | 108.35      | 105.78   |
| 78  | S2    | 512  | A2M  | C5-C4-N9    | 2.21  | 108.35      | 105.78   |
| 79  | L5    | 2401 | A2M  | C4-C5-N7    | -2.20 | 107.93      | 110.62   |
| 78  | S2    | 1056 | PSU  | C6-N1-C2    | -2.20 | 120.43      | 122.68   |
| 78  | S2    | 1832 | 6MZ  | C5-C4-N9    | 2.20  | 108.34      | 105.78   |
| 78  | S2    | 668  | A2M  | C4-C5-N7    | -2.20 | 107.94      | 110.62   |
| 79  | L5    | 400  | A2M  | C4-C5-N7    | -2.20 | 107.94      | 110.62   |
| 79  | L5    | 5010 | PSU  | C6-N1-C2    | -2.20 | 120.44      | 122.68   |
| 78  | S2    | 966  | PSU  | C6-N1-C2    | -2.20 | 120.44      | 122.68   |
| 79  | L5    | 3785 | A2M  | C4-N9-C8    | 2.20  | 108.11      | 105.73   |
| 78  | S2    | 801  | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 79  | L5    | 4431 | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 78  | S2    | 159  | A2M  | C5-C4-N9    | 2.19  | 108.33      | 105.78   |
| 79  | L5    | 400  | A2M  | C4'-O4'-C1' | -2.19 | 104.64      | 109.47   |
| 79  | L5    | 2815 | A2M  | C4'-O4'-C1' | -2.19 | 104.64      | 109.47   |
| 78  | S2    | 166  | A2M  | C5-C4-N9    | 2.19  | 108.33      | 105.78   |
| 78  | S2    | 468  | A2M  | C5-C4-N9    | 2.19  | 108.33      | 105.78   |
| 79  | L5    | 4523 | A2M  | C4-C5-N7    | -2.19 | 107.96      | 110.62   |
| 78  | S2    | 1347 | PSU  | C6-N1-C2    | -2.19 | 120.45      | 122.68   |
| 79  | L5    | 3853 | PSU  | C6-N1-C2    | -2.18 | 120.45      | 122.68   |
| 78  | S2    | 27   | A2M  | C5-C4-N9    | 2.18  | 108.32      | 105.78   |
| 79  | L5    | 2837 | OMU  | O2-C2-N1    | -2.18 | 119.88      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 4523 | A2M  | O4'-C4'-C3' | -2.18 | 100.80      | 105.11   |
| 79  | L5    | 4628 | PSU  | C6-C5-C4    | 2.18  | 119.72      | 118.20   |
| 78  | S2    | 27   | A2M  | C4-C5-N7    | -2.18 | 107.96      | 110.62   |
| 78  | S2    | 1842 | 4AC  | N4-C4-N3    | 2.18  | 117.51      | 113.85   |
| 78  | S2    | 512  | A2M  | O4'-C1'-C2' | -2.18 | 102.75      | 106.57   |
| 78  | S2    | 815  | PSU  | C6-N1-C2    | -2.18 | 120.46      | 122.68   |
| 78  | S2    | 354  | OMU  | O2-C2-N1    | -2.17 | 119.89      | 122.79   |
| 79  | L5    | 3818 | UY1  | O2-C2-N1    | -2.17 | 120.40      | 122.79   |
| 79  | L5    | 4521 | PSU  | C6-N1-C2    | -2.17 | 120.46      | 122.68   |
| 79  | L5    | 4420 | PSU  | O4'-C1'-C2' | 2.17  | 108.21      | 105.14   |
| 78  | S2    | 116  | OMU  | O2-C2-N1    | -2.17 | 119.90      | 122.79   |
| 79  | L5    | 3830 | A2M  | C5-C4-N9    | 2.17  | 108.31      | 105.78   |
| 78  | S2    | 1136 | PSU  | C6-C5-C4    | 2.17  | 119.72      | 118.20   |
| 78  | S2    | 1031 | A2M  | C4-C5-N7    | -2.17 | 107.98      | 110.62   |
| 79  | L5    | 3925 | OMU  | O2-C2-N1    | -2.17 | 119.90      | 122.79   |
| 79  | L5    | 1534 | A2M  | C4-N9-C8    | 2.17  | 108.08      | 105.73   |
| 78  | S2    | 99   | A2M  | C4-C5-N7    | -2.17 | 107.98      | 110.62   |
| 78  | S2    | 1243 | PSU  | C6-N1-C2    | -2.16 | 120.47      | 122.68   |
| 78  | S2    | 1445 | PSU  | C6-N1-C2    | -2.16 | 120.47      | 122.68   |
| 78  | S2    | 651  | PSU  | C6-N1-C2    | -2.16 | 120.47      | 122.68   |
| 79  | L5    | 2843 | PSU  | C6-N1-C2    | -2.16 | 120.47      | 122.68   |
| 78  | S2    | 105  | PSU  | C6-N1-C2    | -2.16 | 120.47      | 122.68   |
| 78  | S2    | 468  | A2M  | C4'-O4'-C1' | -2.16 | 104.71      | 109.47   |
| 79  | L5    | 3718 | A2M  | C4-C5-N7    | -2.16 | 107.99      | 110.62   |
| 78  | S2    | 1383 | A2M  | C5-C4-N9    | 2.16  | 108.29      | 105.78   |
| 79  | L5    | 4442 | PSU  | O4'-C1'-C2' | 2.16  | 108.19      | 105.14   |
| 78  | S2    | 468  | A2M  | C2'-C1'-N9  | -2.16 | 109.90      | 113.53   |
| 79  | L5    | 3723 | A2M  | C4'-O4'-C1' | -2.16 | 104.72      | 109.47   |
| 79  | L5    | 1524 | A2M  | C4-C5-N7    | -2.15 | 107.99      | 110.62   |
| 79  | L5    | 3758 | PSU  | C6-N1-C2    | -2.15 | 120.48      | 122.68   |
| 78  | S2    | 159  | A2M  | C4-C5-N7    | -2.15 | 108.00      | 110.62   |
| 78  | S2    | 512  | A2M  | C4-C5-N7    | -2.15 | 108.00      | 110.62   |
| 79  | L5    | 1322 | 1MA  | N1-C6-N6    | 2.15  | 125.23      | 119.77   |
| 79  | L5    | 3851 | PSU  | C6-N1-C2    | -2.15 | 120.49      | 122.68   |
| 78  | S2    | 468  | A2M  | C4-C5-N7    | -2.14 | 108.01      | 110.62   |
| 78  | S2    | 576  | A2M  | C5-C4-N9    | 2.14  | 108.28      | 105.78   |
| 79  | L5    | 3808 | OMC  | C1'-N1-C6   | -2.14 | 116.17      | 120.84   |
| 79  | L5    | 4571 | A2M  | C5-C4-N9    | 2.14  | 108.27      | 105.78   |
| 79  | L5    | 4296 | PSU  | C6-N1-C2    | -2.14 | 120.50      | 122.68   |
| 79  | L5    | 3764 | PSU  | O4'-C1'-C2' | 2.13  | 108.15      | 105.14   |
| 79  | L5    | 2508 | PSU  | C6-N1-C2    | -2.13 | 120.50      | 122.68   |
| 79  | L5    | 4306 | OMU  | O2-C2-N1    | -2.13 | 119.95      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 398  | A2M  | C5-C4-N9    | 2.13  | 108.26      | 105.78   |
| 79  | L5    | 400  | A2M  | C5-C4-N9    | 2.13  | 108.26      | 105.78   |
| 79  | L5    | 1792 | PSU  | C6-N1-C2    | -2.13 | 120.51      | 122.68   |
| 79  | L5    | 2815 | A2M  | C5-C4-N9    | 2.13  | 108.26      | 105.78   |
| 79  | L5    | 1871 | A2M  | C5-C4-N9    | 2.13  | 108.25      | 105.78   |
| 79  | L5    | 2824 | OMC  | C1'-N1-C2   | 2.13  | 123.16      | 118.42   |
| 79  | L5    | 1326 | A2M  | C4-C5-N7    | -2.13 | 108.03      | 110.62   |
| 79  | L5    | 3637 | PSU  | O2-C2-N1    | -2.12 | 120.45      | 122.79   |
| 79  | L5    | 1871 | A2M  | C4'-O4'-C1' | -2.12 | 104.80      | 109.47   |
| 78  | S2    | 1239 | PSU  | C6-N1-C2    | -2.11 | 120.52      | 122.68   |
| 79  | L5    | 3825 | A2M  | C4'-O4'-C1' | -2.11 | 104.81      | 109.47   |
| 79  | L5    | 4620 | OMU  | O2-C2-N1    | -2.11 | 119.98      | 122.79   |
| 79  | L5    | 398  | A2M  | C4-C5-N7    | -2.11 | 108.05      | 110.62   |
| 5   | L8    | 69   | PSU  | O4'-C1'-C2' | 2.11  | 108.12      | 105.14   |
| 79  | L5    | 2363 | A2M  | C4'-O4'-C1' | -2.11 | 104.82      | 109.47   |
| 79  | L5    | 1326 | A2M  | C5-C4-N9    | 2.11  | 108.23      | 105.78   |
| 78  | S2    | 822  | PSU  | O4'-C1'-C2' | 2.11  | 108.11      | 105.14   |
| 79  | L5    | 4636 | PSU  | O4'-C1'-C2' | 2.10  | 108.11      | 105.14   |
| 79  | L5    | 4493 | PSU  | C6-N1-C2    | -2.10 | 120.54      | 122.68   |
| 78  | S2    | 218  | PSU  | C6-N1-C2    | -2.10 | 120.54      | 122.68   |
| 79  | L5    | 3830 | A2M  | C4-C5-N7    | -2.10 | 108.06      | 110.62   |
| 78  | S2    | 99   | A2M  | C2'-C1'-N9  | -2.09 | 110.00      | 113.53   |
| 78  | S2    | 99   | A2M  | C5-C4-N9    | 2.09  | 108.22      | 105.78   |
| 78  | S2    | 1031 | A2M  | C5-C4-N9    | 2.09  | 108.22      | 105.78   |
| 79  | L5    | 1871 | A2M  | C4-C5-N7    | -2.09 | 108.07      | 110.62   |
| 79  | L5    | 3867 | A2M  | C6-C5-C4    | 2.09  | 119.99      | 117.18   |
| 79  | L5    | 4590 | A2M  | C5-C4-N9    | 2.09  | 108.21      | 105.78   |
| 79  | L5    | 3723 | A2M  | C5-C4-N9    | 2.09  | 108.21      | 105.78   |
| 79  | L5    | 4523 | A2M  | C5-C4-N9    | 2.08  | 108.20      | 105.78   |
| 79  | L5    | 2401 | A2M  | C5-C4-N9    | 2.07  | 108.19      | 105.78   |
| 79  | L5    | 3724 | A2M  | C4-C5-N7    | -2.07 | 108.09      | 110.62   |
| 78  | S2    | 166  | A2M  | C4-N9-C8    | 2.07  | 107.97      | 105.73   |
| 78  | S2    | 484  | A2M  | C4-C5-N7    | -2.07 | 108.09      | 110.62   |
| 78  | S2    | 1832 | 6MZ  | C4-C5-N7    | -2.07 | 108.10      | 110.62   |
| 78  | S2    | 1081 | PSU  | C6-N1-C2    | -2.07 | 120.57      | 122.68   |
| 78  | S2    | 121  | OMU  | O2-C2-N1    | -2.07 | 120.04      | 122.79   |
| 79  | L5    | 4457 | PSU  | C6-N1-C2    | -2.06 | 120.58      | 122.68   |
| 79  | L5    | 4972 | PSU  | C6-N1-C2    | -2.06 | 120.58      | 122.68   |
| 79  | L5    | 1862 | PSU  | C6-N1-C2    | -2.06 | 120.58      | 122.68   |
| 78  | S2    | 1445 | PSU  | C6-C5-C4    | 2.06  | 119.64      | 118.20   |
| 79  | L5    | 1582 | PSU  | C6-N1-C2    | -2.06 | 120.58      | 122.68   |
| 78  | S2    | 1031 | A2M  | C4'-O4'-C1' | -2.06 | 104.93      | 109.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | L5    | 4457 | PSU  | O4'-C1'-C2' | 2.06  | 108.04      | 105.14   |
| 78  | S2    | 1383 | A2M  | C4-C5-N7    | -2.05 | 108.12      | 110.62   |
| 79  | L5    | 4227 | OMU  | O2-C2-N1    | -2.05 | 120.06      | 122.79   |
| 78  | S2    | 218  | PSU  | O4'-C1'-C2' | 2.04  | 108.02      | 105.14   |
| 79  | L5    | 1534 | A2M  | C5-C4-N9    | 2.04  | 108.15      | 105.78   |
| 79  | L5    | 3724 | A2M  | C5-C4-N9    | 2.04  | 108.15      | 105.78   |
| 79  | L5    | 3715 | PSU  | O4'-C1'-C2' | 2.03  | 108.01      | 105.14   |
| 78  | S2    | 576  | A2M  | C4-N9-C8    | 2.03  | 107.92      | 105.73   |
| 79  | L5    | 4571 | A2M  | C6-C5-C4    | 2.03  | 119.91      | 117.18   |
| 78  | S2    | 866  | PSU  | C6-N1-C2    | -2.03 | 120.61      | 122.68   |
| 79  | L5    | 1677 | PSU  | C6-C5-C4    | 2.02  | 119.61      | 118.20   |
| 79  | L5    | 2401 | A2M  | C4-N9-C8    | 2.02  | 107.92      | 105.73   |
| 46  | La    | 39   | V5N  | O-C-CA      | -2.02 | 119.48      | 124.78   |
| 78  | S2    | 1337 | 4AC  | N4-C4-N3    | 2.02  | 117.24      | 113.85   |
| 79  | L5    | 3867 | A2M  | C4-C5-N7    | -2.02 | 108.16      | 110.62   |
| 76  | Pt    | 56   | PSU  | C6-N1-C2    | -2.01 | 120.62      | 122.68   |
| 1   | LA    | 216  | V5N  | O-C-CA      | -2.01 | 119.50      | 124.78   |
| 78  | S2    | 1081 | PSU  | O4'-C1'-C2' | 2.01  | 107.98      | 105.14   |
| 78  | S2    | 1643 | PSU  | C6-C5-C4    | 2.01  | 119.60      | 118.20   |
| 79  | L5    | 4498 | OMU  | O2-C2-N1    | -2.00 | 120.12      | 122.79   |
| 78  | S2    | 1643 | PSU  | O4'-C1'-C2' | 2.00  | 107.97      | 105.14   |
| 78  | S2    | 1842 | 4AC  | CM7-C7-N4   | 2.00  | 118.75      | 115.29   |

There are no chirality outliers.

All (173) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | LA    | 216 | V5N  | O-C-CA-CB       |
| 46  | La    | 39  | V5N  | O2-CB-CG-CD2    |
| 61  | Lb    | 5   | MLZ  | N-CA-CB-CG      |
| 61  | Lb    | 5   | MLZ  | C-CA-CB-CG      |
| 74  | Lo    | 53  | MLZ  | O-C-CA-CB       |
| 76  | Pt    | 21  | H2U  | O4'-C1'-N1-C6   |
| 78  | S2    | 27  | A2M  | C1'-C2'-O2'-CM' |
| 78  | S2    | 99  | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 99  | A2M  | C1'-C2'-O2'-CM' |
| 78  | S2    | 354 | OMU  | C1'-C2'-O2'-CM2 |
| 78  | S2    | 468 | A2M  | C1'-C2'-O2'-CM' |
| 78  | S2    | 484 | A2M  | C1'-C2'-O2'-CM' |
| 78  | S2    | 512 | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 512 | A2M  | C1'-C2'-O2'-CM' |
| 78  | S2    | 576 | A2M  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 78  | S2    | 601  | OMG  | C1'-C2'-O2'-CM2 |
| 78  | S2    | 644  | OMG  | O4'-C4'-C5'-O5' |
| 78  | S2    | 668  | A2M  | C3'-C4'-C5'-O5' |
| 78  | S2    | 683  | OMG  | O4'-C4'-C5'-O5' |
| 78  | S2    | 683  | OMG  | C3'-C4'-C5'-O5' |
| 78  | S2    | 822  | PSU  | C3'-C4'-C5'-O5' |
| 78  | S2    | 822  | PSU  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1248 | B8N  | N34-C33-C34-O35 |
| 78  | S2    | 1248 | B8N  | C31-C32-C33-N34 |
| 78  | S2    | 1326 | UY1  | C2'-C1'-C5-C6   |
| 78  | S2    | 1326 | UY1  | O4'-C1'-C5-C6   |
| 78  | S2    | 1328 | OMG  | C1'-C2'-O2'-CM2 |
| 78  | S2    | 1383 | A2M  | C1'-C2'-O2'-CM' |
| 78  | S2    | 1678 | A2M  | C1'-C2'-O2'-CM' |
| 78  | S2    | 1804 | OMU  | C1'-C2'-O2'-CM2 |
| 78  | S2    | 1851 | MA6  | O4'-C4'-C5'-O5' |
| 79  | L5    | 398  | A2M  | O4'-C4'-C5'-O5' |
| 79  | L5    | 398  | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 2351 | OMC  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 2415 | OMU  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 2815 | A2M  | C3'-C4'-C5'-O5' |
| 79  | L5    | 2824 | OMC  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 2876 | OMG  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 3701 | OMC  | C2'-C1'-N1-C6   |
| 79  | L5    | 3723 | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 3724 | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 3825 | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 3867 | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 3925 | OMU  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 4220 | 6MZ  | C5-C6-N6-C9     |
| 79  | L5    | 4220 | 6MZ  | N1-C6-N6-C9     |
| 79  | L5    | 4420 | PSU  | C2'-C1'-C5-C4   |
| 79  | L5    | 4420 | PSU  | C2'-C1'-C5-C6   |
| 79  | L5    | 4523 | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 4571 | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 4620 | OMU  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 4636 | PSU  | C3'-C4'-C5'-O5' |
| 79  | L5    | 4637 | OMG  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4637 | OMG  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 3701 | OMC  | C2'-C1'-N1-C2   |
| 79  | L5    | 4590 | A2M  | C4'-C5'-O5'-P   |
| 78  | S2    | 99   | A2M  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 78  | S2    | 590  | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 590  | A2M  | C3'-C4'-C5'-O5' |
| 78  | S2    | 644  | OMG  | C3'-C4'-C5'-O5' |
| 78  | S2    | 668  | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 918  | PSU  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1243 | PSU  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 79  | L5    | 2876 | OMG  | C3'-C4'-C5'-O5' |
| 79  | L5    | 3785 | A2M  | O4'-C4'-C5'-O5' |
| 79  | L5    | 3785 | A2M  | C3'-C4'-C5'-O5' |
| 79  | L5    | 4636 | PSU  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4637 | OMG  | C3'-C4'-C5'-O5' |
| 61  | Lb    | 5    | MLZ  | CG-CD-CE-NZ     |
| 78  | S2    | 159  | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 468  | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 512  | A2M  | C3'-C4'-C5'-O5' |
| 78  | S2    | 576  | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 918  | PSU  | C3'-C4'-C5'-O5' |
| 78  | S2    | 1243 | PSU  | C3'-C4'-C5'-O5' |
| 79  | L5    | 398  | A2M  | C3'-C4'-C5'-O5' |
| 79  | L5    | 2815 | A2M  | O4'-C4'-C5'-O5' |
| 79  | L5    | 2876 | OMG  | O4'-C4'-C5'-O5' |
| 79  | L5    | 3729 | PSU  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4228 | OMG  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4228 | OMG  | C3'-C4'-C5'-O5' |
| 79  | L5    | 4420 | PSU  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4532 | PSU  | C3'-C4'-C5'-O5' |
| 76  | Pt    | 21   | H2U  | C2'-C1'-N1-C6   |
| 78  | S2    | 428  | OMU  | C2'-C1'-N1-C6   |
| 78  | S2    | 1639 | G7M  | C3'-C4'-C5'-O5' |
| 78  | S2    | 1248 | B8N  | N34-C33-C34-O36 |
| 76  | Pt    | 21   | H2U  | C2'-C1'-N1-C2   |
| 78  | S2    | 1447 | OMG  | C3'-C4'-C5'-O5' |
| 79  | L5    | 4532 | PSU  | O4'-C4'-C5'-O5' |
| 61  | Lb    | 5    | MLZ  | CE-CD-CG-CB     |
| 78  | S2    | 428  | OMU  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1639 | G7M  | O4'-C4'-C5'-O5' |
| 79  | L5    | 2364 | OMG  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4447 | 5MC  | C2'-C1'-N1-C6   |
| 79  | L5    | 3729 | PSU  | C3'-C4'-C5'-O5' |
| 79  | L5    | 4420 | PSU  | C3'-C4'-C5'-O5' |
| 79  | L5    | 1792 | PSU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 79  | L5    | 3867 | A2M  | C3'-C4'-C5'-O5' |
| 78  | S2    | 428  | OMU  | C2'-C1'-N1-C2   |
| 76  | Pt    | 47   | G7M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 27   | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 428  | OMU  | O4'-C1'-N1-C6   |
| 78  | S2    | 428  | OMU  | C3'-C4'-C5'-O5' |
| 78  | S2    | 166  | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 1316 | OMG  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 3785 | A2M  | C1'-C2'-O2'-CM' |
| 74  | Lo    | 53   | MLZ  | CG-CD-CE-NZ     |
| 79  | L5    | 4447 | 5MC  | O4'-C1'-N1-C6   |
| 76  | Pt    | 21   | H2U  | O4'-C1'-N1-C2   |
| 79  | L5    | 1326 | A2M  | C4'-C5'-O5'-P   |
| 79  | L5    | 3844 | PSU  | C4'-C5'-O5'-P   |
| 78  | S2    | 436  | OMG  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1447 | OMG  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1490 | OMG  | O4'-C4'-C5'-O5' |
| 79  | L5    | 1625 | OMG  | C3'-C4'-C5'-O5' |
| 79  | L5    | 3867 | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1248 | B8N  | C31-C32-C33-C34 |
| 79  | L5    | 1524 | A2M  | C3'-C2'-O2'-CM' |
| 79  | L5    | 3785 | A2M  | C3'-C2'-O2'-CM' |
| 79  | L5    | 4494 | OMG  | C3'-C2'-O2'-CM2 |
| 79  | L5    | 2815 | A2M  | C4'-C5'-O5'-P   |
| 79  | L5    | 3818 | UY1  | C4'-C5'-O5'-P   |
| 79  | L5    | 4500 | PSU  | C4'-C5'-O5'-P   |
| 79  | L5    | 3701 | OMC  | O4'-C1'-N1-C6   |
| 79  | L5    | 1534 | A2M  | C4'-C5'-O5'-P   |
| 79  | L5    | 4447 | 5MC  | O4'-C1'-N1-C2   |
| 78  | S2    | 509  | OMG  | O4'-C4'-C5'-O5' |
| 78  | S2    | 1248 | B8N  | C32-C33-C34-O35 |
| 78  | S2    | 428  | OMU  | O4'-C1'-N1-C2   |
| 79  | L5    | 3701 | OMC  | O4'-C1'-N1-C2   |
| 76  | Pt    | 21   | H2U  | C4'-C5'-O5'-P   |
| 78  | S2    | 1490 | OMG  | C4'-C5'-O5'-P   |
| 79  | L5    | 3887 | OMC  | C4'-C5'-O5'-P   |
| 78  | S2    | 1248 | B8N  | C32-C33-C34-O36 |
| 78  | S2    | 644  | OMG  | C4'-C5'-O5'-P   |
| 76  | Pt    | 21   | H2U  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4447 | 5MC  | C2'-C1'-N1-C2   |
| 78  | S2    | 576  | A2M  | C4'-C5'-O5'-P   |
| 78  | S2    | 590  | A2M  | C3'-C2'-O2'-CM' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 79  | L5    | 3818 | UY1  | C3'-C2'-O2'-CM2 |
| 79  | L5    | 2351 | OMC  | C2'-C1'-N1-C6   |
| 79  | L5    | 1322 | 1MA  | C2'-C1'-N9-C8   |
| 79  | L5    | 1322 | 1MA  | C2'-C1'-N9-C4   |
| 78  | S2    | 119  | PSU  | O4'-C4'-C5'-O5' |
| 79  | L5    | 3782 | 5MC  | O4'-C4'-C5'-O5' |
| 79  | L5    | 2351 | OMC  | C2'-C1'-N1-C2   |
| 78  | S2    | 590  | A2M  | C2'-C1'-N9-C8   |
| 78  | S2    | 159  | A2M  | C3'-C4'-C5'-O5' |
| 79  | L5    | 1792 | PSU  | C3'-C4'-C5'-O5' |
| 79  | L5    | 2364 | OMG  | C3'-C4'-C5'-O5' |
| 78  | S2    | 116  | OMU  | C1'-C2'-O2'-CM2 |
| 78  | S2    | 159  | A2M  | C1'-C2'-O2'-CM' |
| 79  | L5    | 4370 | OMG  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 3818 | UY1  | C1'-C2'-O2'-CM2 |
| 79  | L5    | 4370 | OMG  | C3'-C2'-O2'-CM2 |
| 76  | Pt    | 33   | OMC  | C2'-C1'-N1-C2   |
| 78  | S2    | 590  | A2M  | O4'-C1'-N9-C8   |
| 79  | L5    | 1524 | A2M  | O4'-C1'-N9-C8   |
| 79  | L5    | 2422 | OMC  | C3'-C4'-C5'-O5' |
| 79  | L5    | 1677 | PSU  | O4'-C1'-C5-C6   |
| 76  | Pt    | 47   | G7M  | C3'-C4'-C5'-O5' |
| 79  | L5    | 1534 | A2M  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4523 | A2M  | O4'-C4'-C5'-O5' |
| 78  | S2    | 590  | A2M  | C2'-C1'-N9-C4   |
| 78  | S2    | 1851 | MA6  | C4'-C5'-O5'-P   |
| 78  | S2    | 436  | OMG  | C3'-C4'-C5'-O5' |
| 78  | S2    | 509  | OMG  | C3'-C4'-C5'-O5' |
| 79  | L5    | 2351 | OMC  | O4'-C4'-C5'-O5' |
| 79  | L5    | 2422 | OMC  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4361 | PSU  | O4'-C4'-C5'-O5' |
| 79  | L5    | 4196 | OMG  | C4'-C5'-O5'-P   |

There are no ring outliers.

76 monomers are involved in 96 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 78  | S2    | 99   | A2M  | 1       | 0            |
| 78  | S2    | 1391 | OMC  | 1       | 0            |
| 78  | S2    | 354  | OMU  | 2       | 0            |
| 79  | L5    | 3723 | A2M  | 2       | 0            |
| 79  | L5    | 4536 | OMC  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 78  | S2    | 1804 | OMU  | 1       | 0            |
| 79  | L5    | 3884 | PSU  | 1       | 0            |
| 79  | L5    | 4299 | PSU  | 1       | 0            |
| 79  | L5    | 4571 | A2M  | 1       | 0            |
| 78  | S2    | 436  | OMG  | 1       | 0            |
| 78  | S2    | 484  | A2M  | 1       | 0            |
| 61  | Lb    | 5    | MLZ  | 1       | 0            |
| 79  | L5    | 4196 | OMG  | 2       | 0            |
| 78  | S2    | 509  | OMG  | 2       | 0            |
| 78  | S2    | 572  | PSU  | 1       | 0            |
| 79  | L5    | 2363 | A2M  | 1       | 0            |
| 78  | S2    | 1678 | A2M  | 1       | 0            |
| 79  | L5    | 4442 | PSU  | 2       | 0            |
| 78  | S2    | 1842 | 4AC  | 3       | 0            |
| 78  | S2    | 601  | OMG  | 1       | 0            |
| 78  | S2    | 649  | PSU  | 1       | 0            |
| 78  | S2    | 863  | PSU  | 1       | 0            |
| 79  | L5    | 4499 | OMG  | 1       | 0            |
| 78  | S2    | 1643 | PSU  | 1       | 0            |
| 79  | L5    | 4579 | PSU  | 2       | 0            |
| 78  | S2    | 1288 | OMU  | 1       | 0            |
| 78  | S2    | 512  | A2M  | 1       | 0            |
| 78  | S2    | 1031 | A2M  | 1       | 0            |
| 79  | L5    | 3724 | A2M  | 1       | 0            |
| 79  | L5    | 1781 | PSU  | 1       | 0            |
| 78  | S2    | 576  | A2M  | 1       | 0            |
| 79  | L5    | 4457 | PSU  | 1       | 0            |
| 79  | L5    | 3867 | A2M  | 1       | 0            |
| 79  | L5    | 5001 | PSU  | 1       | 0            |
| 79  | L5    | 3764 | PSU  | 1       | 0            |
| 79  | L5    | 1326 | A2M  | 1       | 0            |
| 79  | L5    | 4620 | OMU  | 4       | 0            |
| 78  | S2    | 1447 | OMG  | 2       | 0            |
| 79  | L5    | 2415 | OMU  | 2       | 0            |
| 79  | L5    | 2508 | PSU  | 2       | 0            |
| 78  | S2    | 1639 | G7M  | 1       | 0            |
| 78  | S2    | 1232 | PSU  | 2       | 0            |
| 78  | S2    | 801  | PSU  | 1       | 0            |
| 79  | L5    | 1683 | PSU  | 2       | 0            |
| 79  | L5    | 3785 | A2M  | 1       | 0            |
| 78  | S2    | 159  | A2M  | 1       | 0            |
| 78  | S2    | 1383 | A2M  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 79  | L5    | 3627 | OMG  | 1       | 0            |
| 76  | Pt    | 47   | G7M  | 2       | 0            |
| 78  | S2    | 116  | OMU  | 3       | 0            |
| 78  | S2    | 1243 | PSU  | 1       | 0            |
| 76  | Pt    | 56   | PSU  | 1       | 0            |
| 78  | S2    | 644  | OMG  | 1       | 0            |
| 79  | L5    | 2876 | OMG  | 1       | 0            |
| 79  | L5    | 4228 | OMG  | 1       | 0            |
| 79  | L5    | 4353 | PSU  | 1       | 0            |
| 78  | S2    | 121  | OMU  | 1       | 0            |
| 78  | S2    | 609  | PSU  | 1       | 0            |
| 3   | LB    | 245  | HIC  | 1       | 0            |
| 5   | L8    | 75   | OMG  | 1       | 0            |
| 79  | L5    | 3770 | PSU  | 1       | 0            |
| 79  | L5    | 4523 | A2M  | 1       | 0            |
| 79  | L5    | 3715 | PSU  | 1       | 0            |
| 79  | L5    | 1316 | OMG  | 1       | 0            |
| 79  | L5    | 3925 | OMU  | 1       | 0            |
| 78  | S2    | 1850 | MA6  | 1       | 0            |
| 78  | S2    | 1851 | MA6  | 1       | 0            |
| 79  | L5    | 4637 | OMG  | 1       | 0            |
| 79  | L5    | 4500 | PSU  | 1       | 0            |
| 79  | L5    | 1582 | PSU  | 1       | 0            |
| 79  | L5    | 4456 | OMC  | 2       | 0            |
| 78  | S2    | 1328 | OMG  | 1       | 0            |
| 79  | L5    | 3718 | A2M  | 3       | 0            |
| 79  | L5    | 1871 | A2M  | 1       | 0            |
| 76  | Pt    | 33   | OMC  | 1       | 0            |
| 79  | L5    | 2424 | OMG  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 140 ligands modelled in this entry, 134 are monoatomic - leaving 6 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 |
| 84  | SAC  | SA    | 2    | -    | 7,8,9        | 0.41 | 0        | 8,9,11      | 1.66 | 1 (12%)  |
| 84  | SAC  | Lr    | 2    | -    | 7,8,9        | 0.36 | 0        | 8,9,11      | 1.14 | 1 (12%)  |
| 88  | MET  | Pt    | 78   | -    | 6,7,8        | 0.46 | 0        | 2,7,9       | 0.21 | 0        |
| 87  | AME  | SV    | 1    | -    | 9,10,11      | 1.44 | 1 (11%)  | 9,11,13     | 1.53 | 2 (22%)  |
| 90  | ANM  | L5    | 5101 | -    | 20,20,20     | 4.06 | 10 (50%) | 22,27,27    | 1.53 | 4 (18%)  |
| 89  | HYG  | S2    | 1901 | -    | 35,39,39     | 3.09 | 11 (31%) | 43,60,60    | 1.51 | 7 (16%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 84  | SAC  | SA    | 2    | -    | -       | 3/7/8/10   | -       |
| 84  | SAC  | Lr    | 2    | -    | -       | 2/7/8/10   | -       |
| 88  | MET  | Pt    | 78   | -    | -       | 1/5/6/8    | -       |
| 87  | AME  | SV    | 1    | -    | -       | 3/9/10/12  | -       |
| 90  | ANM  | L5    | 5101 | -    | -       | 4/10/23/23 | 0/2/2/2 |
| 89  | HYG  | S2    | 1901 | -    | -       | 4/12/87/87 | 0/4/4/4 |

All (22) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 90  | L5    | 5101 | ANM  | C2-C16  | -11.68 | 1.30        | 1.53     |
| 89  | S2    | 1901 | HYG  | O29-C12 | 10.88  | 1.61        | 1.43     |
| 90  | L5    | 5101 | ANM  | C16-N1  | 8.95   | 1.67        | 1.48     |
| 89  | S2    | 1901 | HYG  | O22-C17 | 6.61   | 1.53        | 1.43     |
| 89  | S2    | 1901 | HYG  | O14-C13 | 6.55   | 1.58        | 1.41     |
| 89  | S2    | 1901 | HYG  | O28-C23 | 6.01   | 1.47        | 1.40     |
| 90  | L5    | 5101 | ANM  | O4-C3   | -5.11  | 1.32        | 1.43     |
| 89  | S2    | 1901 | HYG  | C16-C15 | 4.33   | 1.62        | 1.53     |
| 90  | L5    | 5101 | ANM  | O2-C5   | 4.25   | 1.44        | 1.35     |
| 89  | S2    | 1901 | HYG  | C17-C12 | -4.16  | 1.44        | 1.53     |
| 90  | L5    | 5101 | ANM  | C4-N1   | -3.85  | 1.33        | 1.47     |
| 90  | L5    | 5101 | ANM  | O2-C2   | 3.71   | 1.50        | 1.44     |
| 87  | SV    | 1    | AME  | CT1-N   | 3.21   | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 89  | S2    | 1901 | HYG  | O28-C27 | 3.15  | 1.48        | 1.44     |
| 90  | L5    | 5101 | ANM  | C15-C12 | 2.93  | 1.58        | 1.51     |
| 90  | L5    | 5101 | ANM  | C3-C2   | 2.91  | 1.59        | 1.53     |
| 89  | S2    | 1901 | HYG  | C25-C24 | -2.63 | 1.48        | 1.53     |
| 89  | S2    | 1901 | HYG  | O18-C13 | -2.62 | 1.34        | 1.41     |
| 89  | S2    | 1901 | HYG  | O30-C24 | 2.43  | 1.47        | 1.42     |
| 90  | L5    | 5101 | ANM  | C4-C3   | 2.29  | 1.56        | 1.53     |
| 90  | L5    | 5101 | ANM  | C15-C16 | 2.23  | 1.58        | 1.53     |
| 89  | S2    | 1901 | HYG  | O31-C25 | 2.19  | 1.48        | 1.43     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 90  | L5    | 5101 | ANM  | O2-C5-C6    | 5.02  | 120.32      | 111.09   |
| 89  | S2    | 1901 | HYG  | O29-C12-C13 | 4.74  | 123.29      | 110.86   |
| 89  | S2    | 1901 | HYG  | O22-C17-C16 | 4.15  | 121.33      | 111.22   |
| 84  | SA    | 2    | SAC  | CA-N-C1A    | 4.08  | 130.68      | 123.15   |
| 89  | S2    | 1901 | HYG  | O28-C27-C26 | 3.12  | 112.95      | 108.52   |
| 89  | S2    | 1901 | HYG  | C13-O18-C6  | -2.67 | 111.35      | 117.96   |
| 89  | S2    | 1901 | HYG  | O14-C15-C16 | 2.56  | 114.33      | 109.69   |
| 87  | SV    | 1    | AME  | CE-SD-CG    | 2.54  | 109.13      | 100.40   |
| 89  | S2    | 1901 | HYG  | O22-C17-C12 | 2.44  | 107.49      | 103.58   |
| 84  | Lr    | 2    | SAC  | CA-N-C1A    | 2.37  | 127.52      | 123.15   |
| 87  | SV    | 1    | AME  | CT2-CT1-N   | 2.25  | 119.91      | 116.10   |
| 90  | L5    | 5101 | ANM  | C2-O2-C5    | -2.18 | 114.35      | 117.72   |
| 90  | L5    | 5101 | ANM  | C12-C15-C16 | -2.11 | 109.67      | 113.33   |
| 89  | S2    | 1901 | HYG  | C19-C15-C16 | -2.09 | 108.12      | 113.00   |
| 90  | L5    | 5101 | ANM  | C3-C2-C16   | -2.08 | 101.29      | 104.29   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 84  | SA    | 2    | SAC  | CB-CA-N-C1A     |
| 84  | SA    | 2    | SAC  | C-CA-CB-OG      |
| 87  | SV    | 1    | AME  | O-C-CA-CB       |
| 88  | Pt    | 78   | MET  | N-CA-CB-CG      |
| 89  | S2    | 1901 | HYG  | C27-C33-C34-O35 |
| 89  | S2    | 1901 | HYG  | O14-C13-O18-C6  |
| 90  | L5    | 5101 | ANM  | C1-C9-O1-C14    |
| 90  | L5    | 5101 | ANM  | C10-C9-O1-C14   |
| 84  | Lr    | 2    | SAC  | C2A-C1A-N-CA    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 84  | Lr    | 2    | SAC  | OAC-C1A-N-CA    |
| 87  | SV    | 1    | AME  | CB-CG-SD-CE     |
| 87  | SV    | 1    | AME  | N-CA-CB-CG      |
| 89  | S2    | 1901 | HYG  | O28-C27-C33-C34 |
| 84  | SA    | 2    | SAC  | N-CA-CB-OG      |
| 89  | S2    | 1901 | HYG  | N36-C33-C34-O35 |
| 90  | L5    | 5101 | ANM  | C13-C12-C15-C16 |
| 90  | L5    | 5101 | ANM  | C11-C12-C15-C16 |

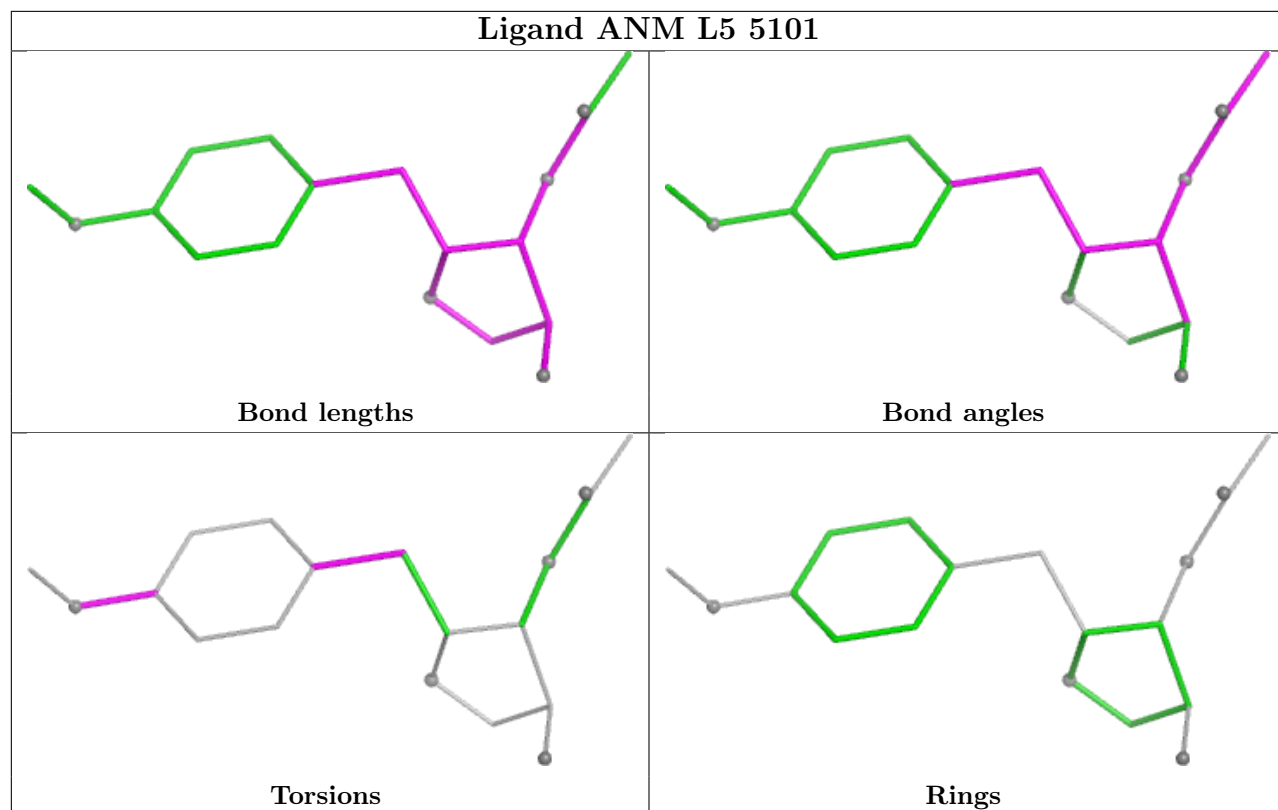
There are no ring outliers.

1 monomer is involved in 1 short contact:

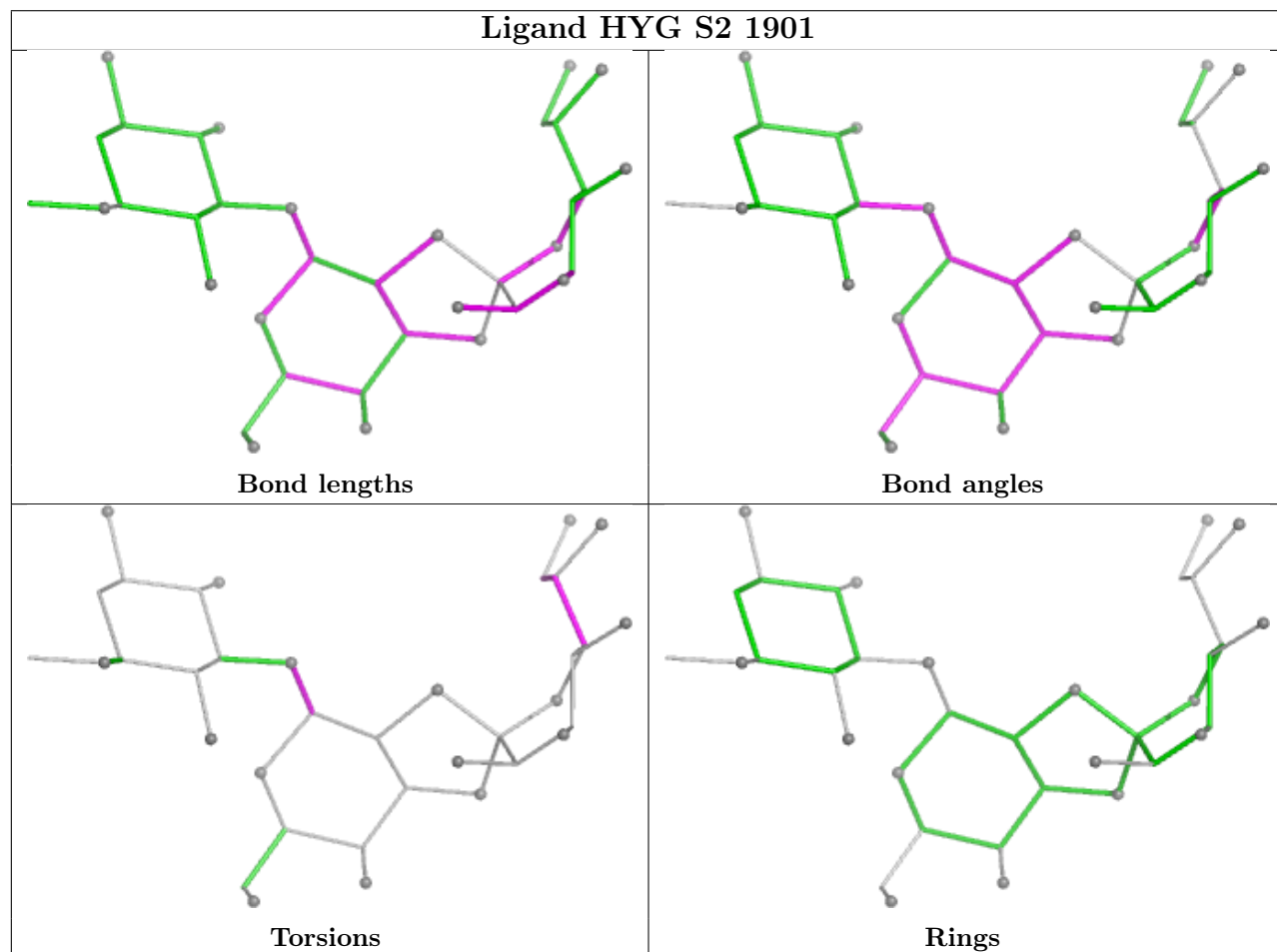
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 90  | L5    | 5101 | ANM  | 1       | 0            |

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

## Ligand ANM L5 5101



## Ligand HYG S2 1901



## 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 |
|-----|-------|------------------|
| 20  | SM    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | SM    | 72:HIS    | C      | 105:GLY   | N      | 25.35        |

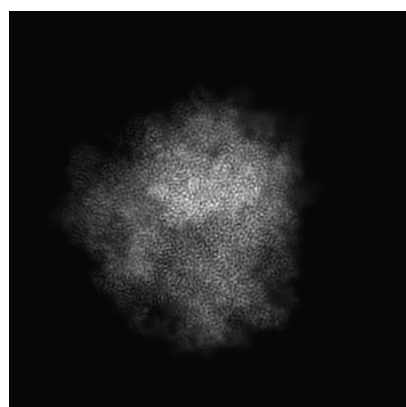
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54267. These allow visual inspection of the internal detail of the map and identification of artifacts.

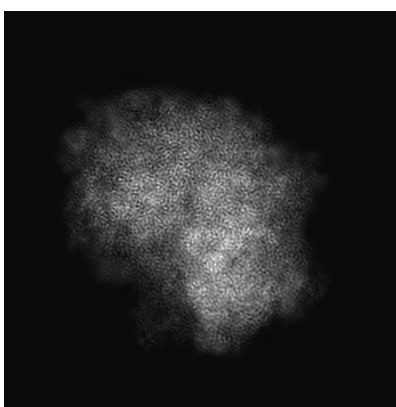
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

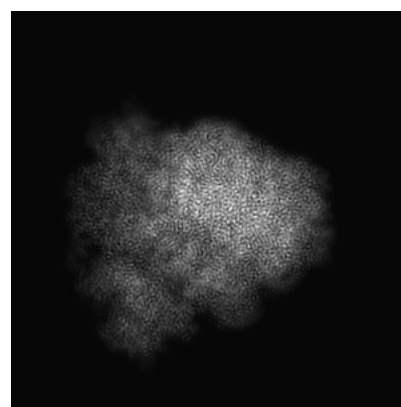
#### 6.1.1 Primary map



X



Y

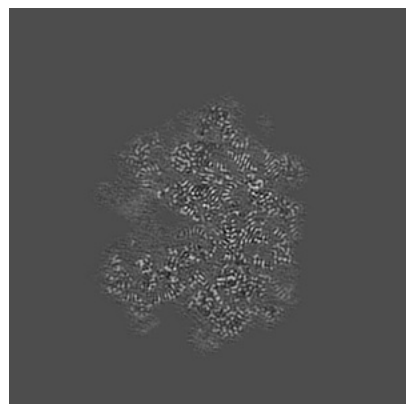


Z

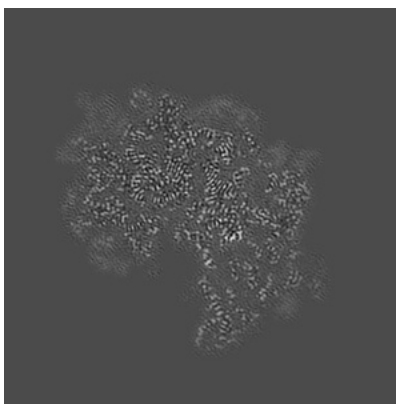
The images above show the map projected in three orthogonal directions.

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

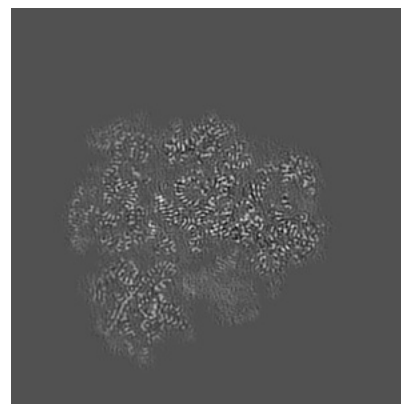
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

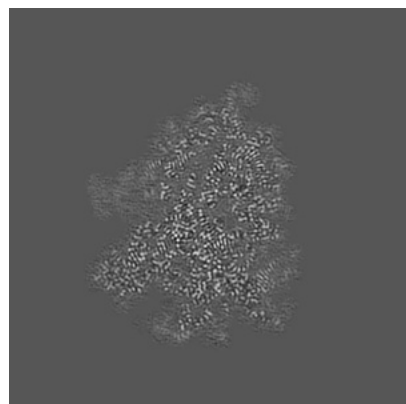


Z Index: 240

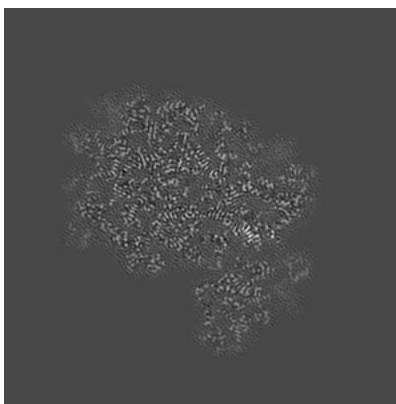
The images above show central slices of the map in three orthogonal directions.

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

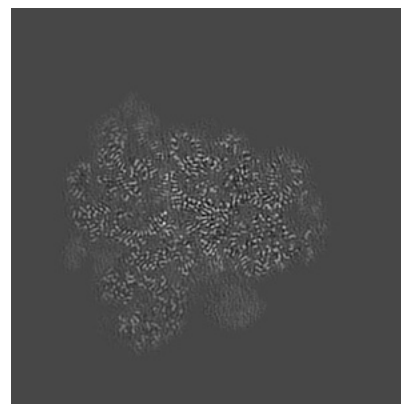
### 6.3.1 Primary map



X Index: 272



Y Index: 258

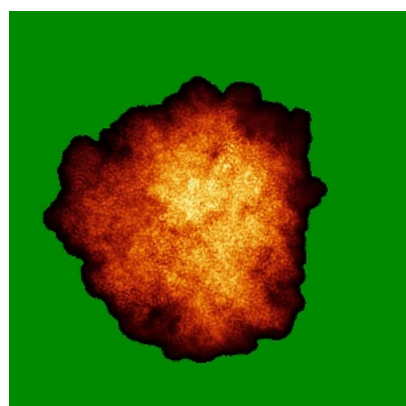


Z Index: 261

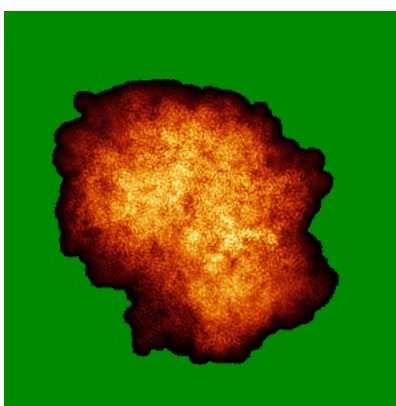
The images above show the largest variance slices of the map in three orthogonal directions.

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

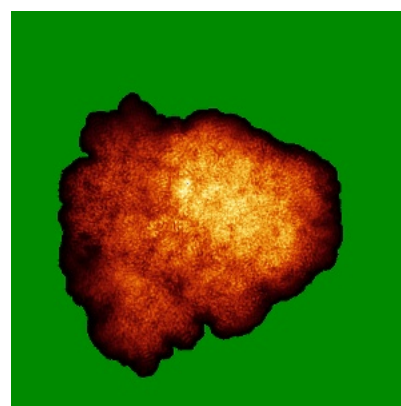
### 6.4.1 Primary map



X



Y

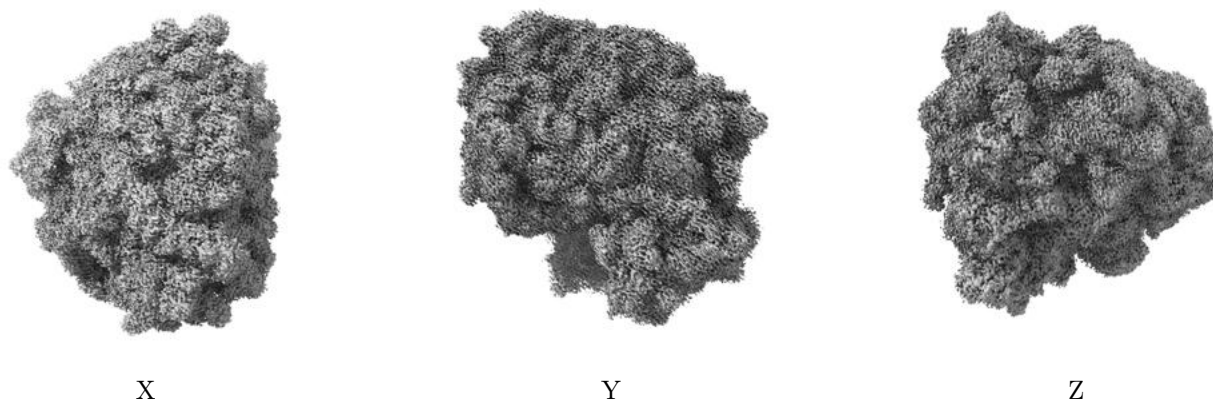


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

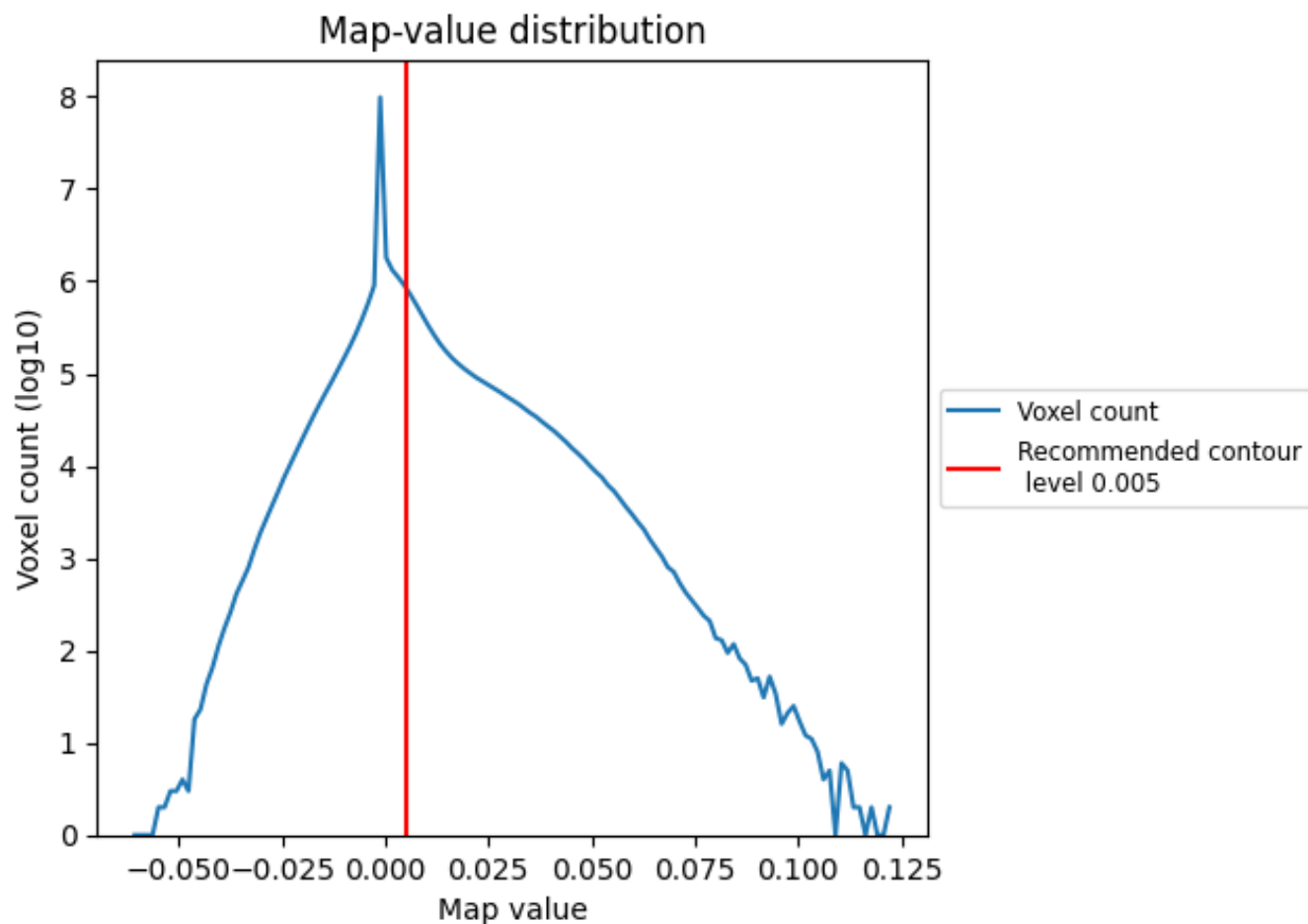
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

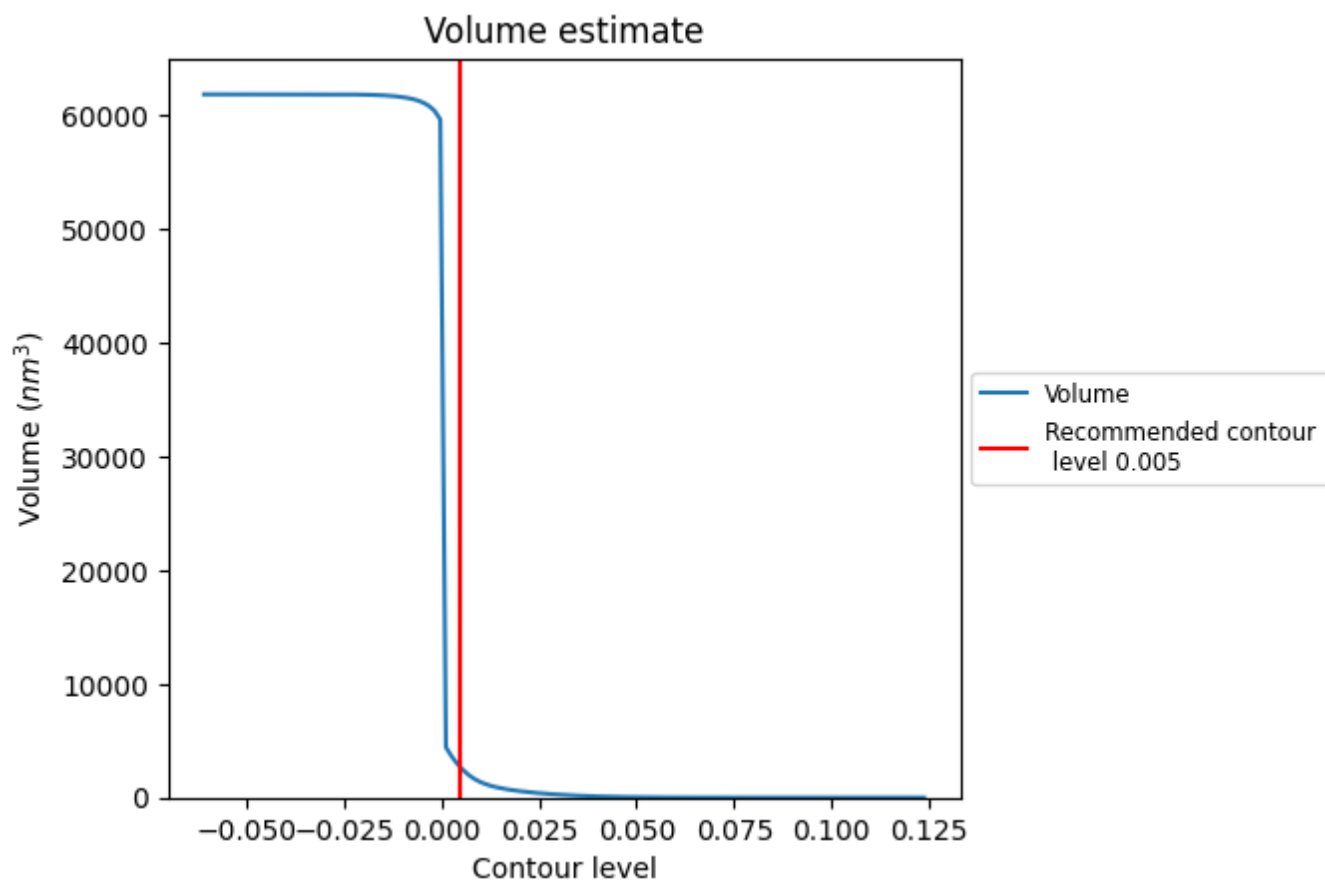
This section contains the results of statistical analysis of the map.

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



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

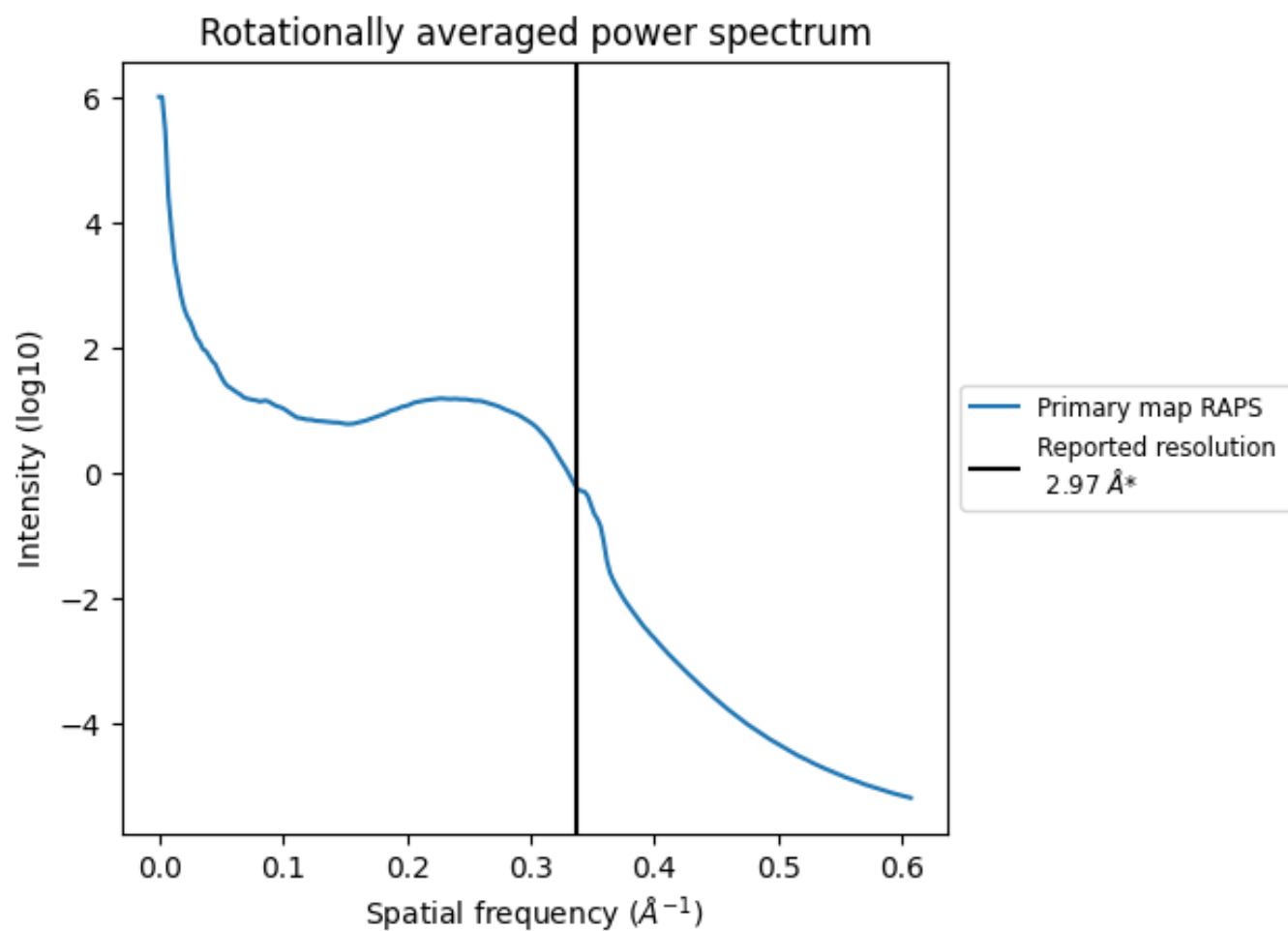
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2631  $\text{nm}^3$ ; this corresponds to an approximate mass of 2376 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 0.337 Å<sup>-1</sup>

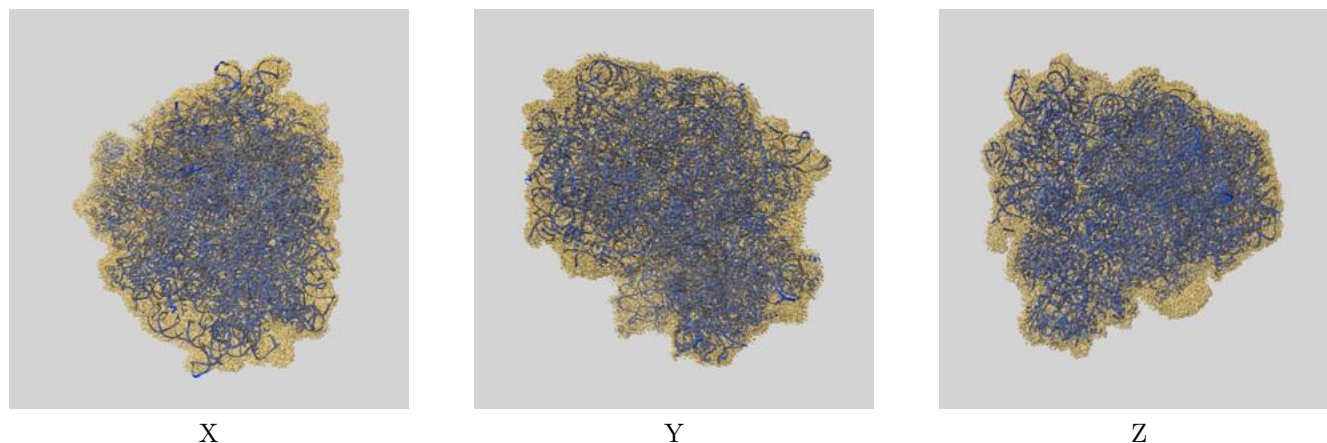
## 8 Fourier-Shell correlation ⓘ

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

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

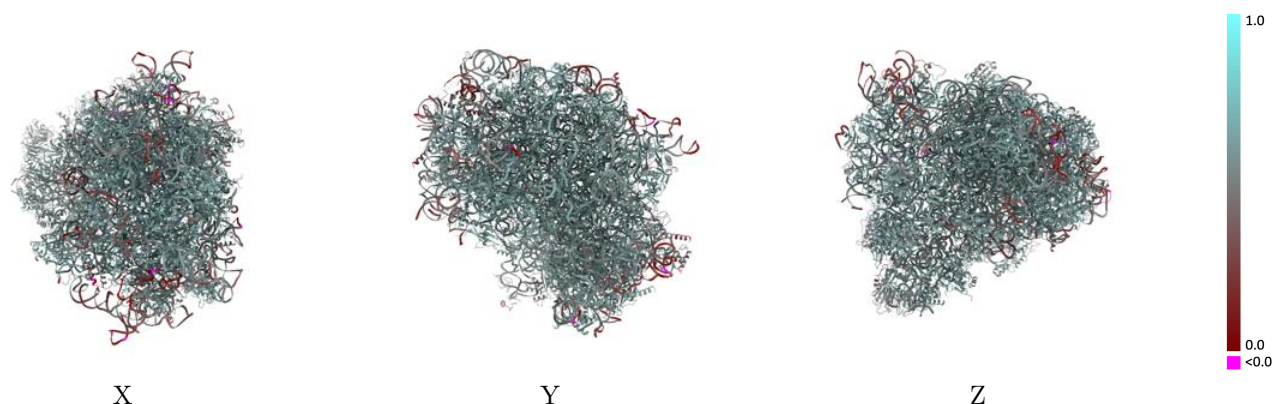
This section contains information regarding the fit between EMDB map EMD-54267 and PDB model 9RU9. Per-residue inclusion information can be found in section [3](#) on page [28](#).

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



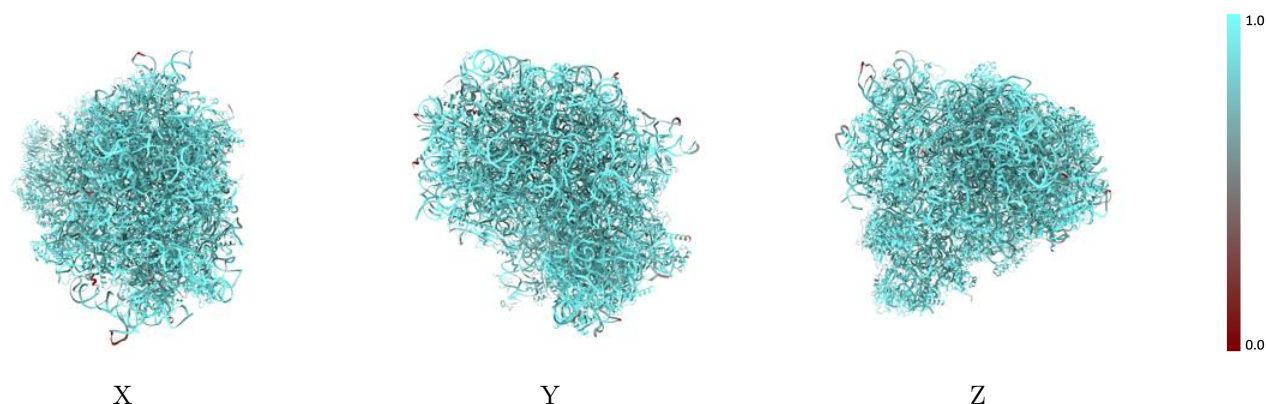
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



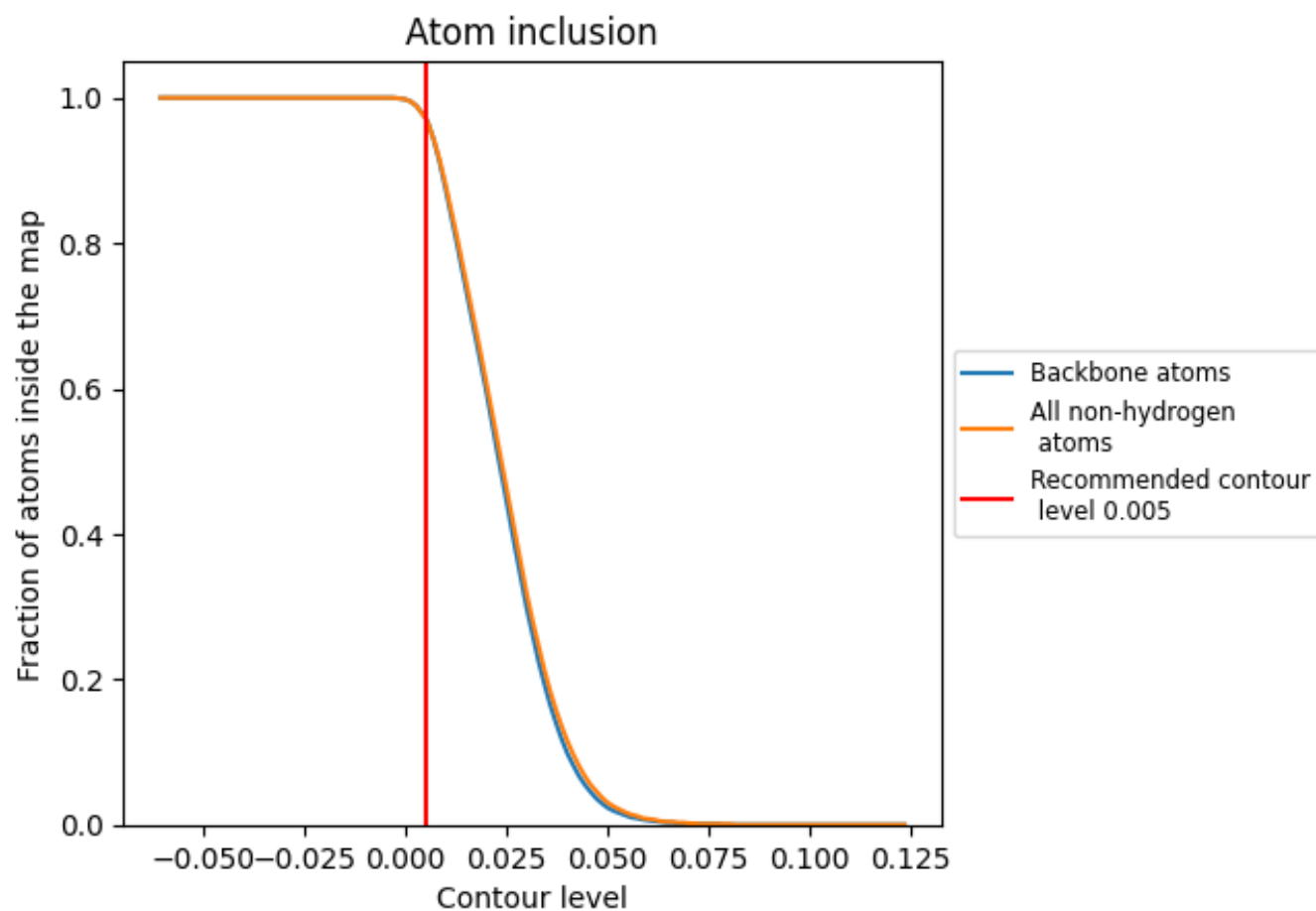
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9710   |  0.5650   |
| A     |  1.0000   |  0.7620   |
| C     |  1.0000   |  0.7760   |
| D     |  1.0000   |  0.7260   |
| Et    |  0.8770   |  0.2960   |
| L5    |  0.9710   |  0.5520   |
| L7    |  0.9930   |  0.5930   |
| L8    |  0.9860   |  0.5690   |
| LA    |  0.9960   |  0.6190   |
| LB    |  0.9900   |  0.6130   |
| LC    |  0.9720   |  0.6010   |
| LD    |  0.9710   |  0.5870   |
| LE    |  0.9720   |  0.5740   |
| LF    |  0.9890   |  0.6070   |
| LG    |  0.9380  |  0.5550  |
| LH    |  0.9830 |  0.6030 |
| LI    |  0.9830 |  0.6100 |
| LJ    |  0.9750 |  0.5830 |
| LL    |  0.9750 |  0.5850 |
| LM    |  0.9800 |  0.5940 |
| LN    |  0.9960 |  0.6230 |
| LO    |  0.9880 |  0.6100 |
| LP    |  0.9880 |  0.6080 |
| LQ    |  0.9910 |  0.6150 |
| LR    |  0.9650 |  0.5760 |
| LS    |  0.9940 |  0.6160 |
| LT    |  0.9870 |  0.5970 |
| LU    |  0.9710 |  0.5460 |
| LV    |  0.9960 |  0.6130 |
| LW    |  0.9960 |  0.6150 |
| LX    |  0.9900 |  0.5990 |
| LY    |  0.9890 |  0.6130 |
| LZ    |  0.9830 |  0.5910 |
| La    |  0.9940 |  0.6180 |
| Lb    |  0.9070 |  0.5270 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Lc    |  0.9920   |  0.5940   |
| Ld    |  0.9920   |  0.5840   |
| Le    |  0.9940   |  0.6150   |
| Lf    |  0.9940   |  0.6240   |
| Lg    |  0.9920   |  0.6000   |
| Lh    |  0.9790   |  0.6020   |
| Li    |  0.9710   |  0.5820   |
| Lj    |  0.9970   |  0.6150   |
| Lk    |  0.9780   |  0.5700   |
| Ll    |  0.9950   |  0.6080   |
| Lm    |  0.9860   |  0.5940   |
| Ln    |  0.9950   |  0.5800   |
| Lo    |  0.9860   |  0.6070   |
| Lp    |  0.9930   |  0.6040   |
| Lr    |  0.9850   |  0.6100   |
| Pt    |  0.9200   |  0.4720   |
| S2    |  0.9700   |  0.5510   |
| SA    |  0.9720  |  0.5860  |
| SB    |  0.9830 |  0.5870 |
| SC    |  0.9770 |  0.5950 |
| SD    |  0.9400 |  0.5480 |
| SE    |  0.9780 |  0.5930 |
| SF    |  0.9740 |  0.5790 |
| SG    |  0.9640 |  0.5490 |
| SH    |  0.9310 |  0.5370 |
| SI    |  0.9660 |  0.5680 |
| SJ    |  0.9660 |  0.5880 |
| SK    |  0.9430 |  0.5400 |
| SL    |  0.9830 |  0.5990 |
| SM    |  0.7800 |  0.3940 |
| SN    |  0.9860 |  0.5910 |
| SO    |  0.9810 |  0.5920 |
| SP    |  0.9500 |  0.5460 |
| SQ    |  0.9710 |  0.5830 |
| SR    |  0.9200 |  0.5470 |
| SS    |  0.9680 |  0.5670 |
| ST    |  0.9780 |  0.5800 |
| SU    |  0.9440 |  0.5380 |
| SV    |  0.9660 |  0.5820 |
| SW    |  0.9800 |  0.6030 |
| SX    |  0.9900 |  0.5990 |
| SY    |  0.9750 |  0.5790 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| SZ    |  0.9520 |  0.5560 |
| Sa    |  0.9770 |  0.5840 |
| Sb    |  0.9590 |  0.5620 |
| Sc    |  0.9660 |  0.5780 |
| Sd    |  0.9860 |  0.5980 |
| Se    |  0.9750 |  0.5780 |
| Sf    |  0.8510 |  0.4260 |
| Sg    |  0.9150 |  0.5300 |
| mR    |  0.8790 |  0.4760 |