



## Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 05:08 pm BST

PDB ID : 9I14 / pdb\_00009i14  
EMDB ID : EMD-52565  
Title : CRYO-EM STRUCTURE OF HCT15 POLYSOMES IN HYBRID-PRE STATE  
Authors : Rajan, K.S.; Yonath, A.  
Deposited on : 2025-01-15  
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

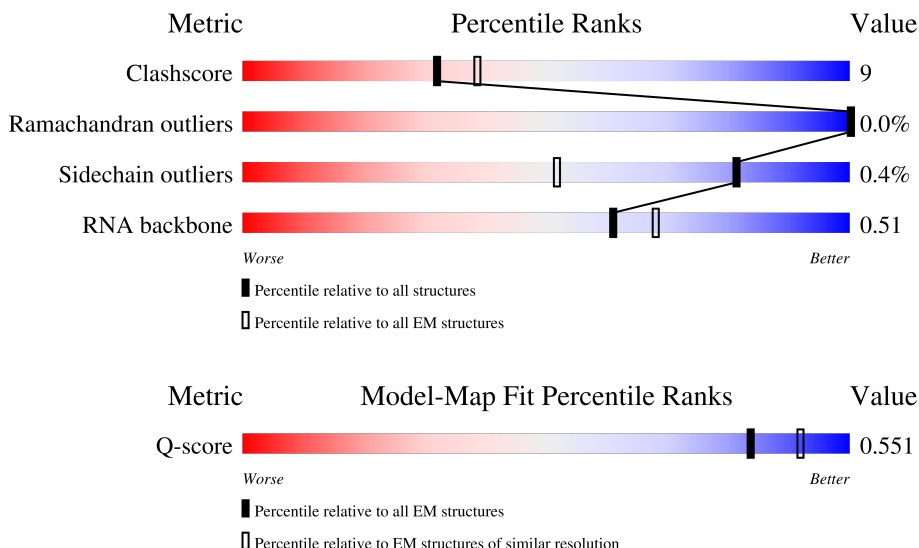
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.34 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                       | 14446 ( 2.84 - 3.84 )                                    |

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    | <br>77% 19%     |
| 2   | SA    | 295    | <br>57% 16% 26% |
| 3   | LB    | 403    | <br>76% 23%     |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | SB    | 264    |                  |
| 5   | A4    | 13     |                  |
| 6   | B4    | 75     |                  |
| 7   | D4    | 76     |                  |
| 8   | L5    | 5070   |                  |
| 9   | L7    | 120    |                  |
| 10  | L8    | 156    |                  |
| 11  | LC    | 427    |                  |
| 12  | LD    | 297    |                  |
| 13  | LE    | 288    |                  |
| 14  | LF    | 248    |                  |
| 15  | LG    | 266    |                  |
| 16  | LH    | 192    |                  |
| 17  | LJ    | 178    |                  |
| 18  | LL    | 211    |                  |
| 19  | LM    | 215    |                  |
| 20  | LN    | 204    |                  |
| 21  | LO    | 203    |                  |
| 22  | LP    | 184    |                  |
| 23  | LQ    | 188    |                  |
| 24  | LR    | 196    |                  |
| 25  | LS    | 176    |                  |
| 26  | LT    | 160    |                  |
| 27  | LU    | 128    |                  |
| 28  | LV    | 140    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | LW    | 157    |                  |
| 30  | LX    | 156    |                  |
| 31  | LY    | 145    |                  |
| 32  | LZ    | 136    |                  |
| 33  | La    | 148    |                  |
| 34  | Lb    | 159    |                  |
| 35  | Lc    | 115    |                  |
| 36  | Ld    | 125    |                  |
| 37  | Lf    | 110    |                  |
| 38  | Lg    | 117    |                  |
| 39  | Lh    | 123    |                  |
| 40  | Li    | 105    |                  |
| 41  | Lj    | 97     |                  |
| 42  | Lk    | 70     |                  |
| 43  | Ll    | 51     |                  |
| 44  | Lm    | 128    |                  |
| 45  | Ln    | 25     |                  |
| 46  | Lo    | 106    |                  |
| 47  | Lp    | 92     |                  |
| 48  | Lr    | 137    |                  |
| 49  | S2    | 1869   |                  |
| 50  | SC    | 293    |                  |
| 51  | SD    | 243    |                  |
| 52  | SE    | 263    |                  |
| 53  | SF    | 204    |                  |

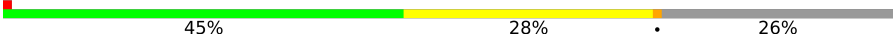
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | SG    | 249    |                  |
| 55  | SH    | 194    |                  |
| 56  | SI    | 208    |                  |
| 57  | SJ    | 194    |                  |
| 58  | SK    | 165    |                  |
| 59  | SL    | 158    |                  |
| 60  | SN    | 151    |                  |
| 61  | SO    | 151    |                  |
| 62  | SP    | 145    |                  |
| 63  | SQ    | 146    |                  |
| 64  | SR    | 135    |                  |
| 65  | SS    | 152    |                  |
| 66  | ST    | 145    |                  |
| 67  | SU    | 119    |                  |
| 68  | SV    | 83     |                  |
| 69  | SW    | 130    |                  |
| 70  | SX    | 143    |                  |
| 71  | SY    | 133    |                  |
| 72  | SZ    | 125    |                  |
| 73  | Sa    | 115    |                  |
| 74  | Sb    | 84     |                  |
| 75  | Sc    | 69     |                  |
| 76  | Sd    | 56     |                  |
| 77  | Se    | 59     |                  |
| 78  | Sf    | 156    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 79  | Sg    | 317    | <br>74% 23%     |
| 80  | SM    | 132    | <br>45% 28% 26% |
| 81  | Le    | 135    | <br>73% 21% 6%  |
| 82  | LI    | 214    | <br>74% 19% 5%  |

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 206575 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 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | LA    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1886  | 1183 | 386 | 311 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | SA    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1705  | 1084 | 300 | 313 | 8 |         |       |

- Molecule 3 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | LB    | 398      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3147  | 2008 | 591 | 534 | 14 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | SB    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1727  | 1096 | 309 | 308 | 14 |         |       |

- Molecule 5 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 5   | A4    | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 231   | 104 | 37 | 79 | 11 |         |       |

- Molecule 6 is a RNA chain called P/E tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | B4    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 7 is a RNA chain called A/P tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | D4    | 63       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1349  | 601 | 243 | 442 | 63 |         |       |

- Molecule 8 is a RNA chain called LSU 28S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 8   | L5    | 3465     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 74335 | 33126 | 13606 | 24139 | 3464 |         |       |

- Molecule 9 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 9   | L7    | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2538  | 1132 | 454 | 834 | 118 |         |       |

- Molecule 10 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 10  | L8    | 147      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3132  | 1399 | 557 | 1030 | 146 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | LC    | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2874  | 1808 | 574 | 477 | 15 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | LD    | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2391  | 1513 | 436 | 428 | 14 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | LE    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1648  | 1061 | 313 | 270 | 4 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | LF    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1846  | 1186 | 354 | 297 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | LG    | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1793  | 1143 | 343 | 303 | 4 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | LH    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1526  | 960 | 285 | 275 | 6 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | LJ    | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1330  | 841 | 249 | 234 | 6 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | LL    | 198      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1588  | 994 | 333 | 257 | 4 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LM    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 719 | 215 | 180 | 7 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | LN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | LO    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1646  | 1061 | 321 | 259 | 5 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | LP    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1267  | 794 | 243 | 221 | 9 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | LQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LR    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1458  | 902 | 317 | 230 | 9 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LS    | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 912 | 278 | 232 | 9 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LT    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 789 | 244 | 208 | 6 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LU    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 518 | 141 | 147 | 2 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LV    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | LW    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 420 | 129 | 112 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | LX    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 962   | 615 | 180 | 166 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | LY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1103  | 692 | 223 | 185 | 3 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | LZ    | 135      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1115  | 719 | 211 | 182 | 3 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1159  | 735 | 236 | 185 | 3 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Lb    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 747   | 465 | 163 | 117 | 2 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Lc    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 725   | 462 | 128 | 128 | 7 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Ld    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 871   | 552 | 170 | 147 | 2 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 867   | 550 | 173 | 141 | 3 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Lg    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 861   | 539 | 177 | 139 | 6 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 638 | 204 | 168 | 1 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | Li    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 512 | 174 | 127 | 5 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | Lj    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 440 | 158 | 112 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Lj    | 57      | THR      | ASN    | conflict | UNP P61927 |

- Molecule 42 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 553   | 356 | 100 | 96 | 1 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | Ll    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 435   | 275 | 97 | 62 | 1 |         |       |

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | Lm    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 411   | 255 | 87 | 63 | 6 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 45  | Ln    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 145 | 64 | 27 | 3 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | Lo    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 525 | 172 | 136 | 6 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 445 | 136 | 119 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Lr    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 992   | 615 | 207 | 166 | 4 |         |       |

- Molecule 49 is a RNA chain called SSU 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 49  | S2    | 1577     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33711 | 15068 | 6064 | 11003 | 1576 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | SC    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1102 | 293 | 300 | 9 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | SD    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1689  | 1077 | 304 | 301 | 7 |         |       |

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | SE    | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2050  | 1311 | 381 | 350 | 8 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | SF    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1486  | 929 | 282 | 268 | 7 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | SG    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1749  | 1097 | 349 | 296 | 7 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 55  | SH    | 177      | Total | C   | N   | O   |         |       |
|     |       |          | 1360  | 876 | 251 | 233 | 0       | 0     |

- Molecule 56 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | SI    | 197      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1582  | 991 | 311 | 275 | 5 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | SJ    | 178      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1482  | 944 | 296 | 240 | 2 | 0       | 0     |

- Molecule 58 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | SK    | 96       | Total | C   | N   | O   | S |         |       |
|     |       |          | 804   | 527 | 140 | 131 | 6 | 0       | 0     |

- Molecule 59 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | SL    | 140      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1147  | 731 | 216 | 194 | 6 | 0       | 0     |

- Molecule 60 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | SN    | 150      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1205  | 772 | 229 | 203 | 1 | 0       | 0     |

- Molecule 61 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SO    | 129      | Total | C   | N   | O   | S |         |       |
|     |       |          | 959   | 586 | 190 | 177 | 6 | 0       | 0     |

- Molecule 62 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | SP    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1060  | 672 | 202 | 179 | 7 |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | SQ    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1120  | 713 | 212 | 192 | 3 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | SR    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 663 | 197 | 189 | 4 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | SS    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1171  | 735 | 239 | 196 | 1 |         |       |

- Molecule 66 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | ST    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 689 | 210 | 196 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| ST    | 4       | PHE      | VAL    | conflict | UNP P39019 |

- Molecule 67 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | SU    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 790   | 495 | 152 | 139 | 4 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | SV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | SX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1082  | 685 | 213 | 181 | 3 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | SY    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 988   | 625 | 191 | 167 | 5 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | SZ    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 574   | 368 | 104 | 101 | 1 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | Sa    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 788   | 490 | 165 | 128 | 5 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | Sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 398 | 117 | 112 | 6 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 75  | Sc    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 489   | 299 | 97 | 91 | 2 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 76  | Sd    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 436   | 273 | 88 | 70 | 5 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 77  | Se    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 400   | 245 | 91 | 63 | 1 |         |       |

- Molecule 78 is a protein called Ubiquitin.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78  | Sf    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 489   | 308 | 91 | 83 | 7 |         |       |

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 79  | Sg    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2389  | 1507 | 417 | 453 | 12 |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | SM    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 722   | 451 | 134 | 130 | 7 |         |       |

- Molecule 81 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | Le    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1044  | 662 | 214 | 163 | 5 |         |       |

- Molecule 82 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 82  | LI    | 203      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1641  | 1042 | 316 | 270 | 13 |         |       |

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 83  | LA    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | B4    | 3        | Total | K  | 0       |
|     |       |          | 3     | 3  |         |
| 83  | L5    | 17       | Total | K  | 0       |
|     |       |          | 17    | 17 |         |
| 83  | L8    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | La    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | S2    | 15       | Total | K  | 0       |
|     |       |          | 15    | 15 |         |
| 83  | SN    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 83  | Le    | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 84  | A4    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 84  | B4    | 4        | Total | Mg  | 0       |
|     |       |          | 4     | 4   |         |
| 84  | D4    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 84  | L5    | 157      | Total | Mg  | 0       |
|     |       |          | 157   | 157 |         |
| 84  | L7    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 84  | L8    | 3        | Total | Mg  | 0       |
|     |       |          | 3     | 3   |         |
| 84  | LN    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 84  | LP    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

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| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 84  | LT    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 84  | Lp    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 84  | S2    | 93       | Total<br>93 | Mg<br>93 | 0       |
| 84  | LI    | 1        | Total<br>1  | Mg<br>1  | 0       |

- Molecule 85 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

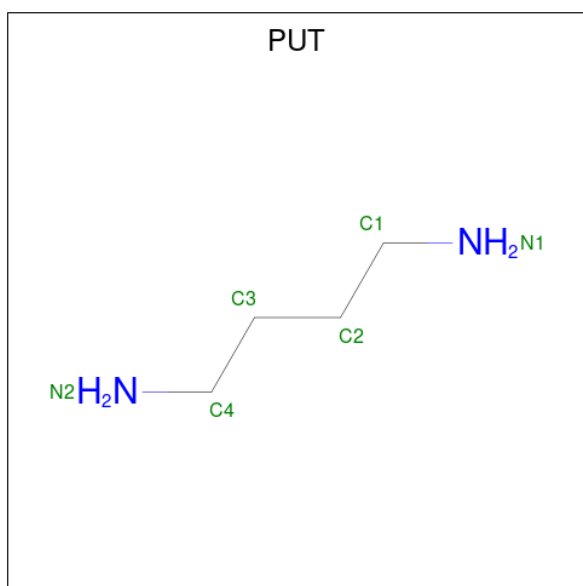
| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 85  | L5    | 12       | Total<br>12 | Na<br>12 | 0       |
| 85  | L7    | 1        | Total<br>1  | Na<br>1  | 0       |
| 85  | L8    | 1        | Total<br>1  | Na<br>1  | 0       |
| 85  | LP    | 1        | Total<br>1  | Na<br>1  | 0       |
| 85  | L1    | 1        | Total<br>1  | Na<br>1  | 0       |
| 85  | S2    | 7        | Total<br>7  | Na<br>7  | 0       |

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 86  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 87 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ) (labeled as "Ligand of Interest" by depositor).

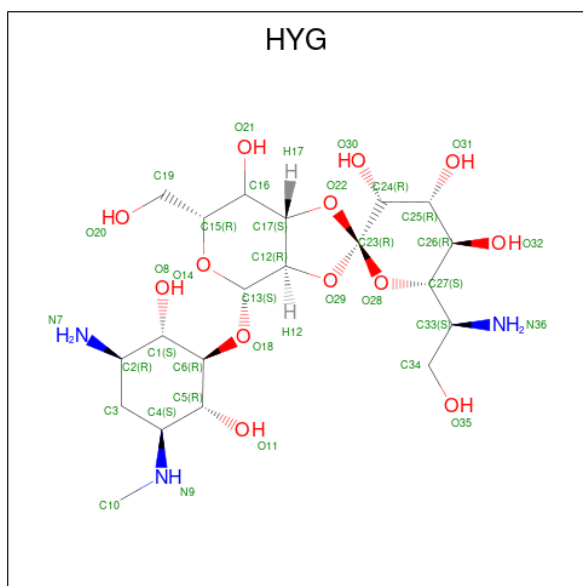


| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 87  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 88  | Lg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | Lj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | Lo    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | Lp    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | Sd    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | Sf    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | SM    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula:  $C_{20}H_{37}N_3O_{13}$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 90 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 90  | L5    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

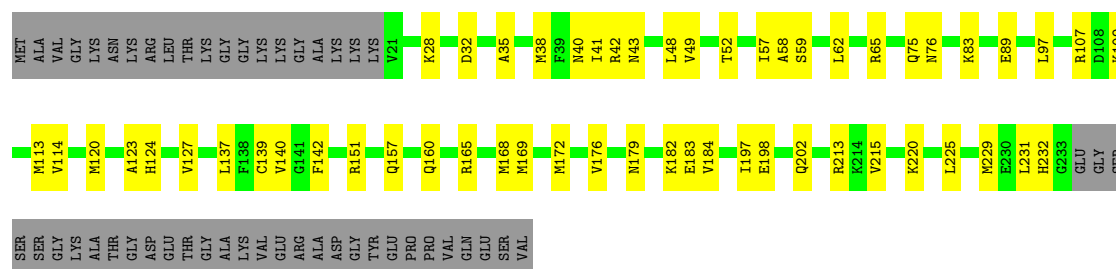
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| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 90  | L8    | 1        | Total<br>1 | O<br>1 | 0       |
| 90  | LH    | 1        | Total<br>1 | O<br>1 | 0       |
| 90  | LV    | 1        | Total<br>1 | O<br>1 | 0       |
| 90  | S2    | 1        | Total<br>1 | O<br>1 | 0       |
| 90  | SX    | 1        | Total<br>1 | O<br>1 | 0       |
| 90  | LI    | 1        | Total<br>1 | O<br>1 | 0       |



Chain SB:  60% 21% 19%

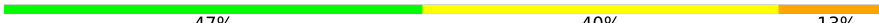


• Molecule 5: mRNA

Chain A4:  38% 46% 15%



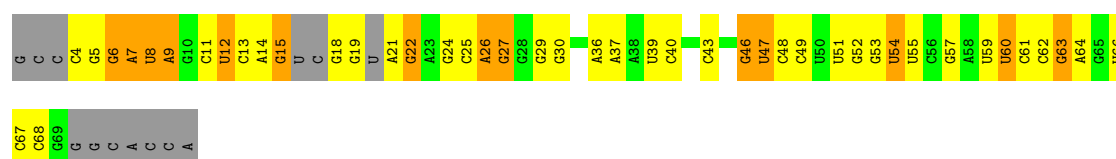
• Molecule 6: P/E tRNA

Chain B4:  47% 40% 13%

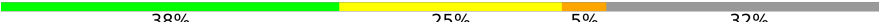


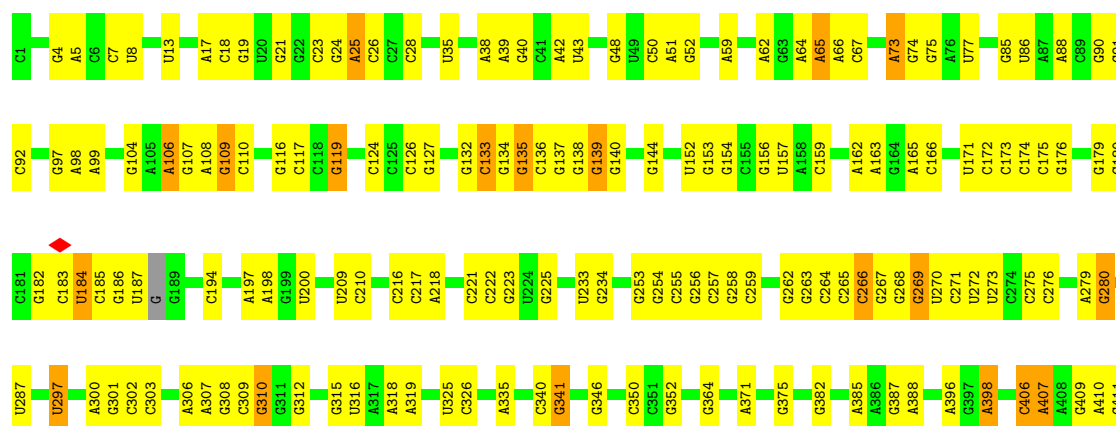
• Molecule 7: A/P tRNA

Chain D4:  24% 41% 18% 17%



• Molecule 8: LSU 28S rRNA

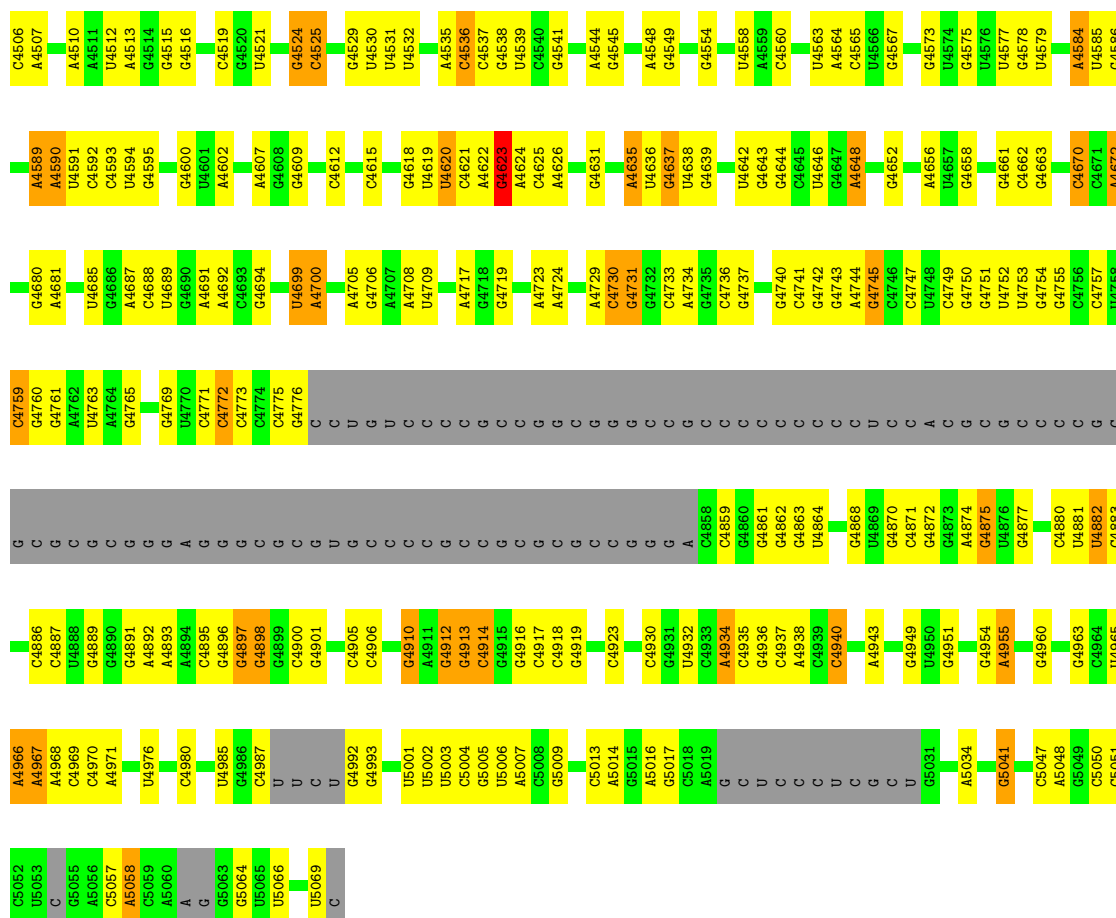
Chain L5:  38% 25% 5% 32%





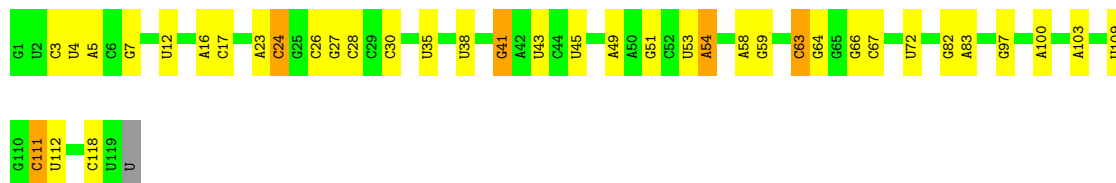






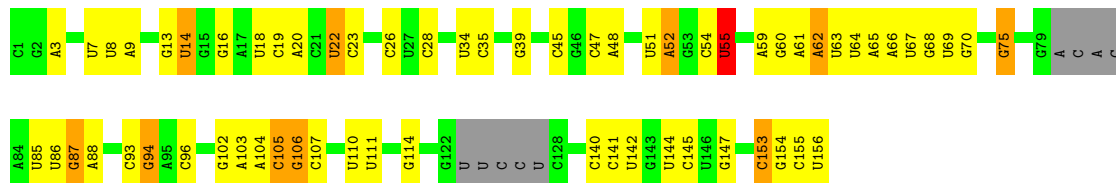
- Molecule 9: 5S rRNA

Chain L7:



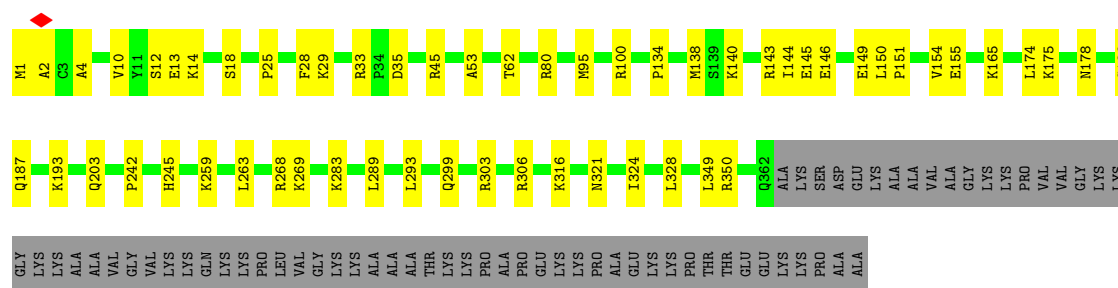
- Molecule 10: 5.8S rRNA

Chain L8:



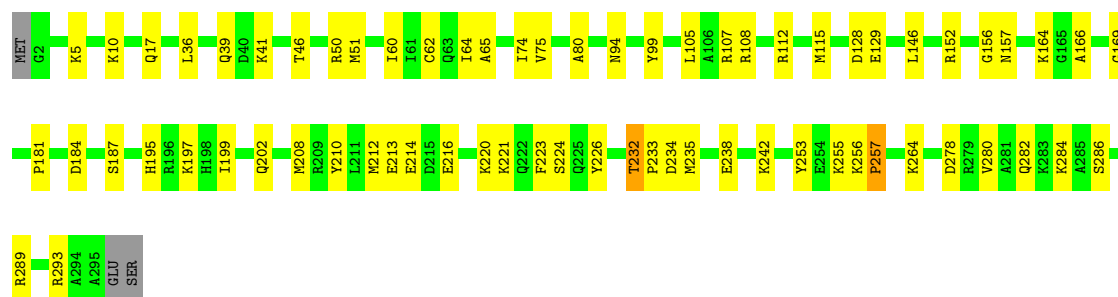
- Molecule 11: 60S ribosomal protein L4

Chain LC:



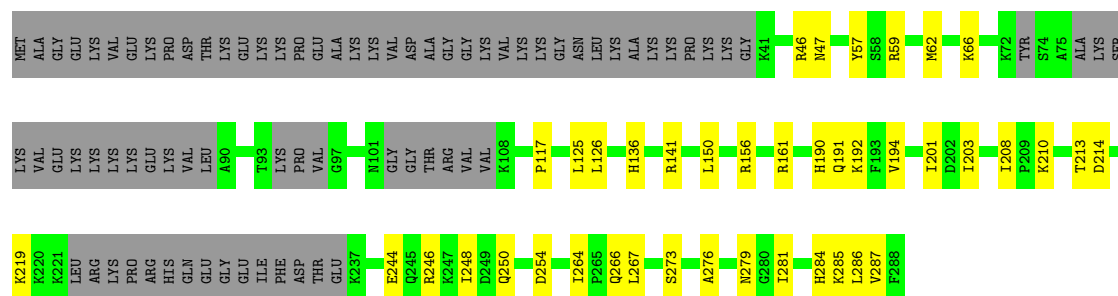
• Molecule 12: 60S ribosomal protein L5

Chain LD: 76% 22% ..



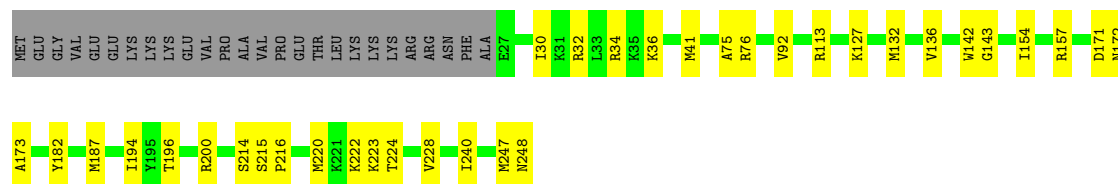
• Molecule 13: Large ribosomal subunit protein eL6

Chain LE: 58% 14% 27%



• Molecule 14: Large ribosomal subunit protein uL30

Chain LF: 75% 14% 10%

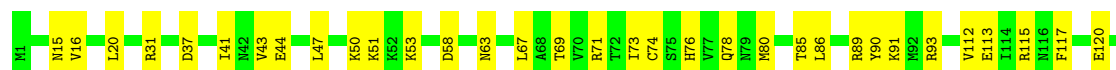


• Molecule 15: 60S ribosomal protein L7a

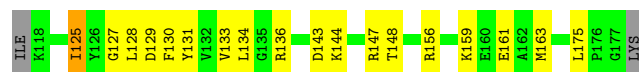
Chain LG: 70% 14% 16%



- Molecule 16: 60S ribosomal protein L9



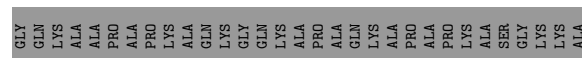
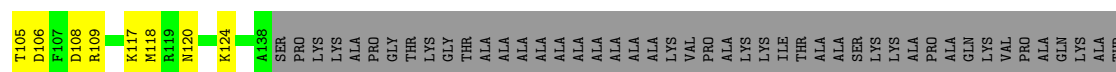
- Molecule 17: 60S ribosomal protein L11



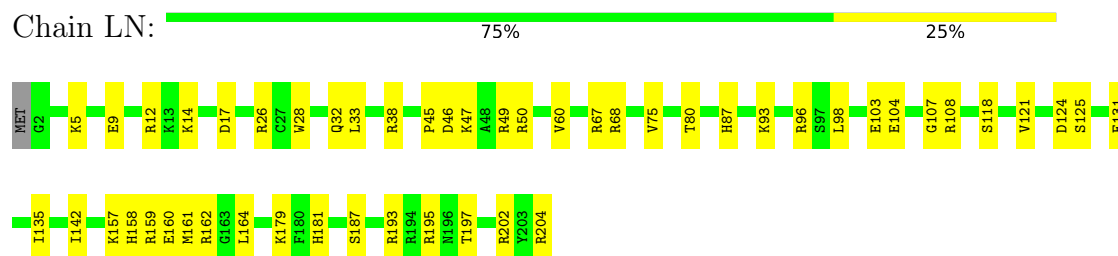
- Molecule 18: 60S ribosomal protein L13



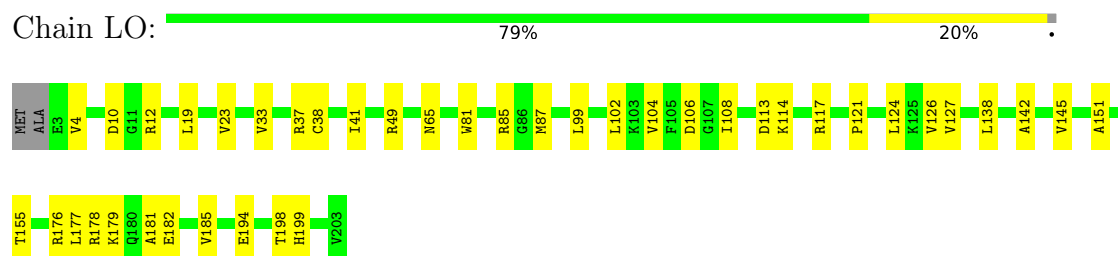
- Molecule 19: 60S ribosomal protein L14



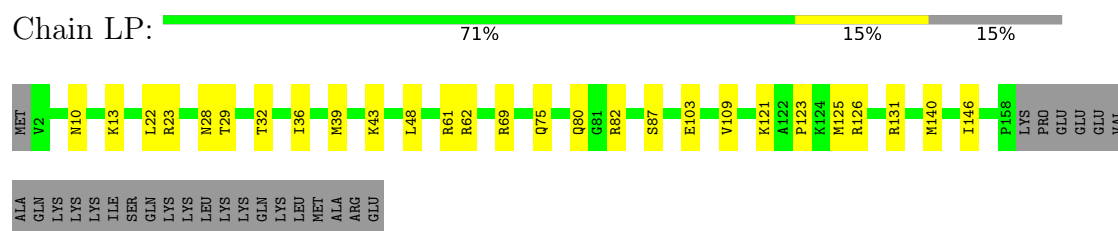
- Molecule 20: 60S ribosomal protein L15



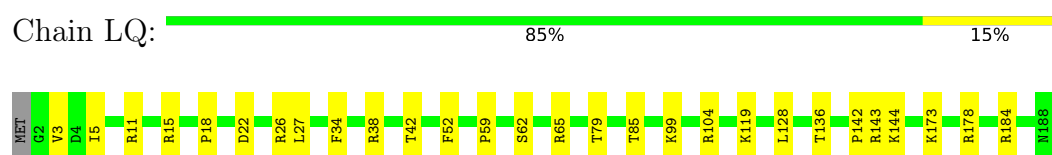
- Molecule 21: 60S ribosomal protein L13a



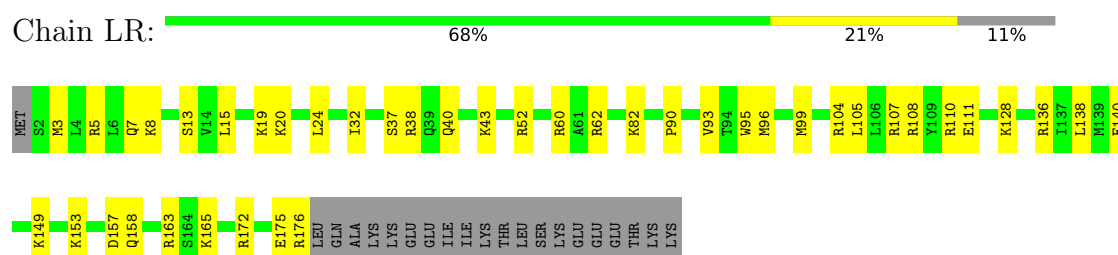
- Molecule 22: 60S ribosomal protein L17



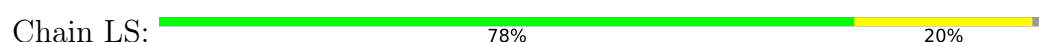
- Molecule 23: 60S ribosomal protein L18

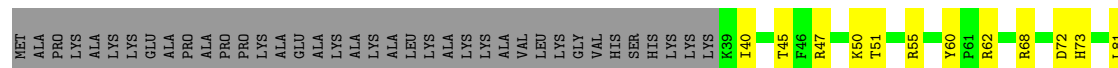


- Molecule 24: 60S ribosomal protein L19



- Molecule 25: 60S ribosomal protein L18a

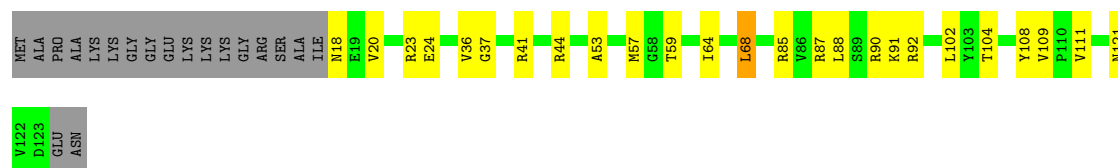






- Molecule 36: 60S ribosomal protein L31

Chain Ld:  65% 19% 15%



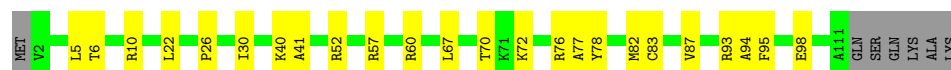
- Molecule 37: 60S ribosomal protein L35a

Chain Lf:  75% 24%



- Molecule 38: 60S ribosomal protein L34

Chain Lg:  74% 21% 6%



- Molecule 39: 60S ribosomal protein L35

Chain Lh:  89% 10%



- Molecule 40: 60S ribosomal protein L36

Chain Li:  84% 10% 5%



- Molecule 41: Large ribosomal subunit protein eL37

Chain Lj:  74% 14% 10%



- Molecule 42: 60S ribosomal protein L38

Chain Lk:  70% 29%



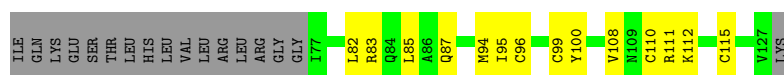
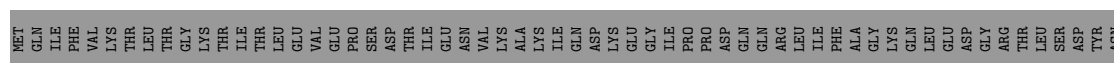
- Molecule 43: 60S ribosomal protein L39

Chain Ll: 71% 25% .



- Molecule 44: Ubiquitin-60S ribosomal protein L40

Chain Lm: 29% 11% 60%



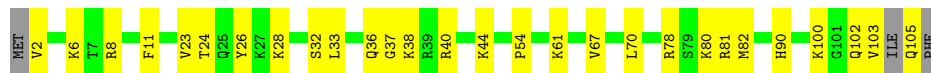
- Molecule 45: 60S ribosomal protein L41

Chain Ln: 88% 12%



- Molecule 46: 60S ribosomal protein L36a

Chain Lo: 71% 26% .



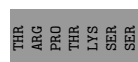
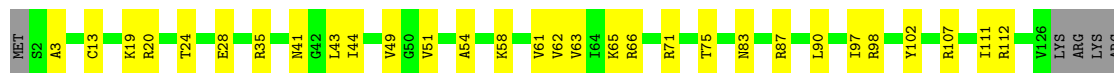
- Molecule 47: 60S ribosomal protein L37a

Chain Lp: 84% 15% .



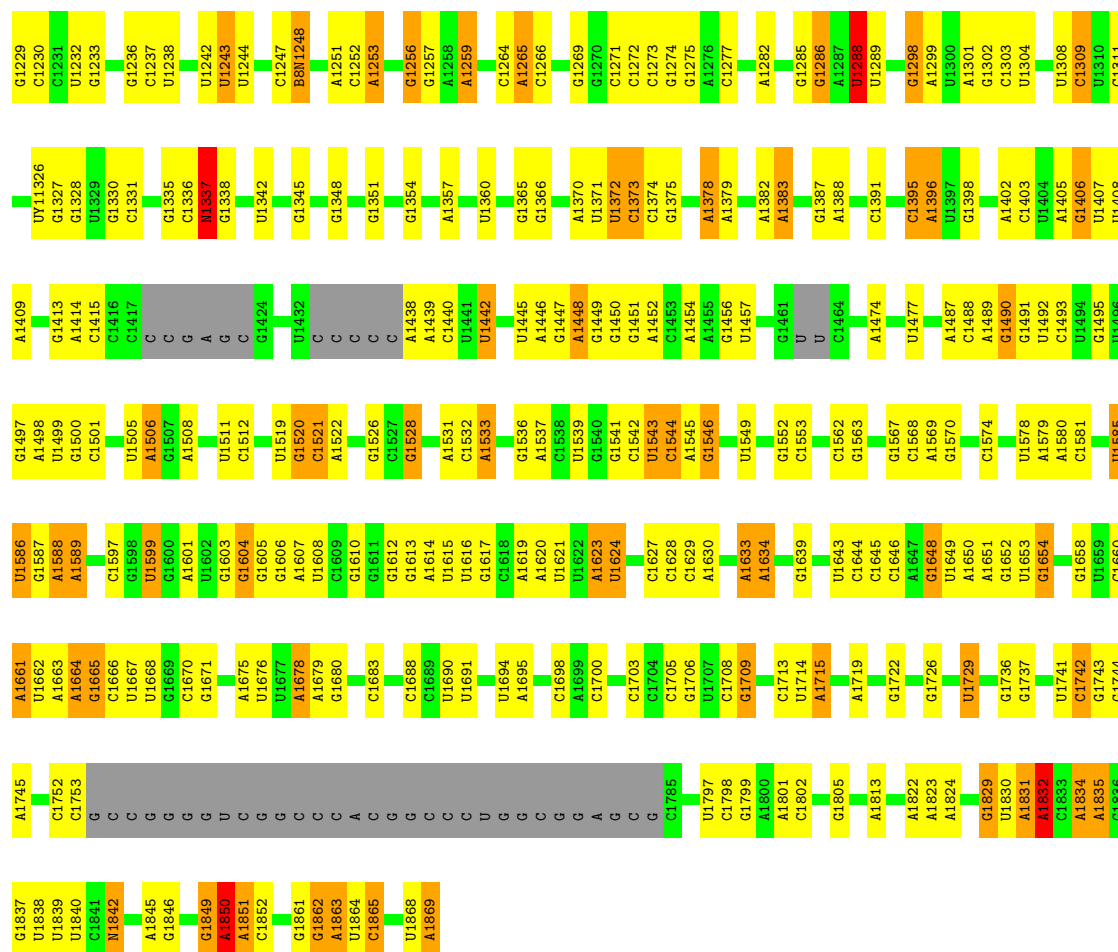
- Molecule 48: 60S ribosomal protein L28

Chain Lr: 69% 22% 9%



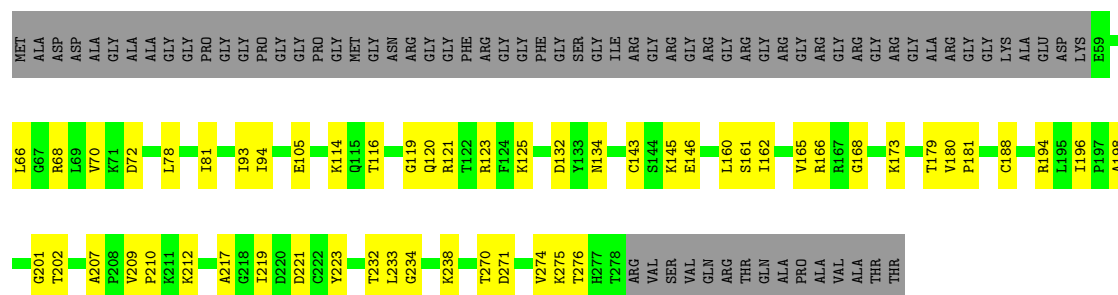
Chain S2: 





• Molecule 50: 40S ribosomal protein S2

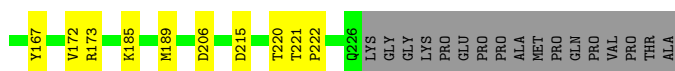
Chain SC: 57% 18% 25%



• Molecule 51: 40S ribosomal protein S3

Chain SD: 75% 17% 8%





- Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE: 68% 30%



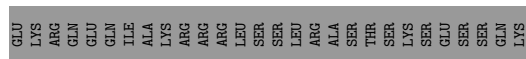
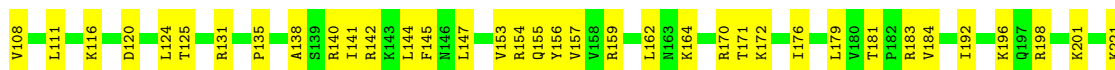
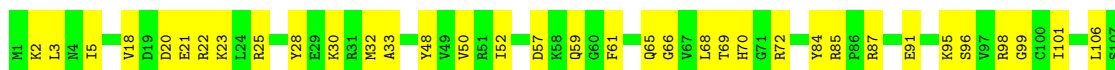
- Molecule 53: 40S ribosomal protein S5

Chain SF: 82% 9% 8%



- Molecule 54: 40S ribosomal protein S6

Chain SG: 60% 29% 11%



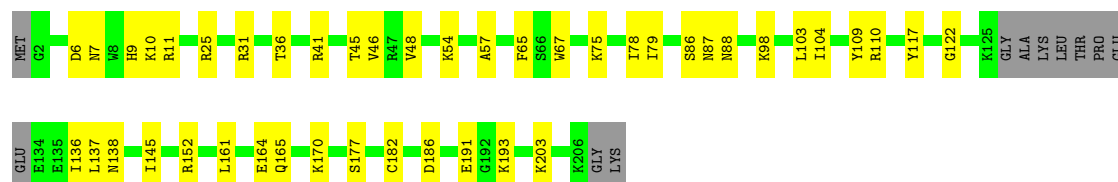
- Molecule 55: 40S ribosomal protein S7

Chain SH: 69% 22% 9%



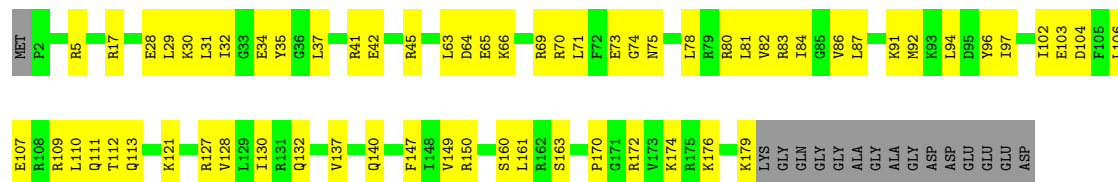
- Molecule 56: 40S ribosomal protein S8

Chain SI: 74% 21% 5%



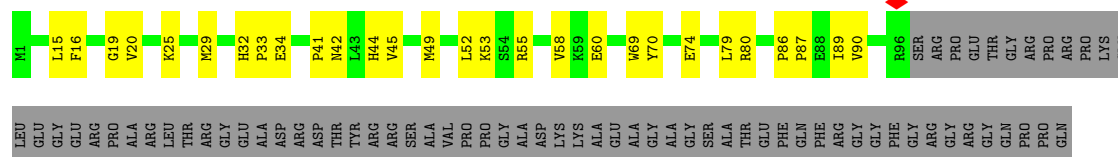
- Molecule 57: 40S ribosomal protein S9

Chain SJ: 59% 33% 8%



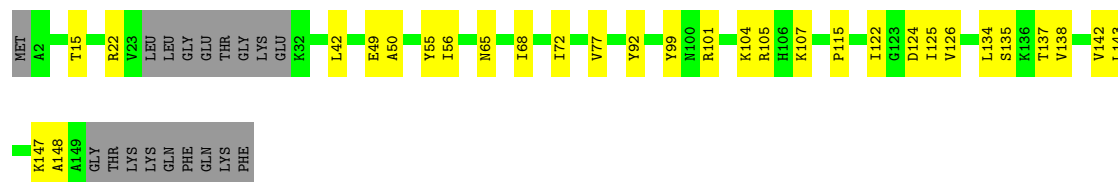
- Molecule 58: 40S ribosomal protein S10

Chain SK: 41% 17% 42%



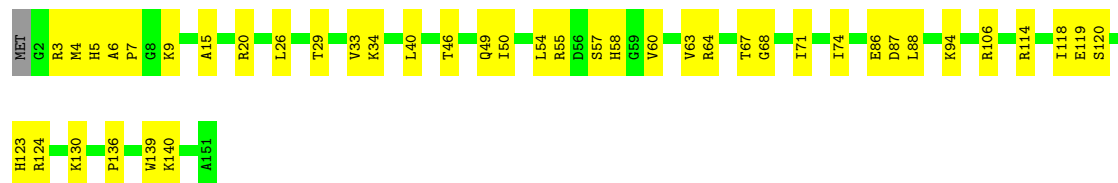
- Molecule 59: 40S ribosomal protein S11

Chain SL: 70% 19% 11%



- Molecule 60: 40S ribosomal protein S13

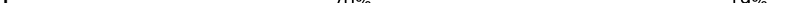
Chain SN: 72% 28%

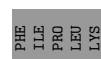


- Molecule 61: 40S ribosomal protein S14

Chain SO: 58% 28% 15%

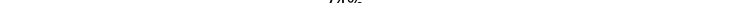


- Chain SP:  70% 19% 11%

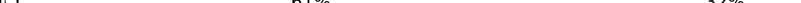


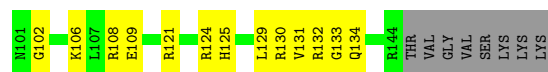
- Chain SQ:  75% 21% .

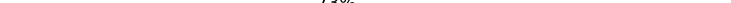


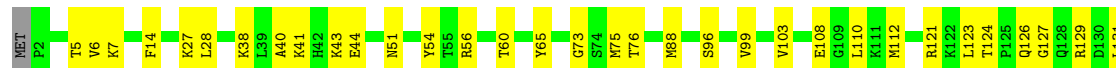
- Chain SR:  74% 22%



- Chain SS: 



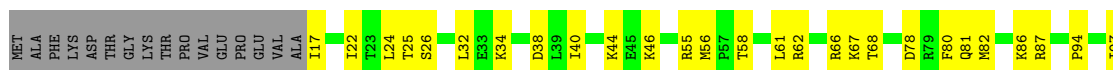
- Chain ST:  73% 24%





- Molecule 67: 40S ribosomal protein S20

Chain SU: 58% 27% 15%



- Molecule 68: 40S ribosomal protein S21

Chain SV: 83% 17%



- Molecule 69: 40S ribosomal protein S15a

Chain SW: 75% 23% ..



- Molecule 70: 40S ribosomal protein S23

Chain SX: 85% 13% .



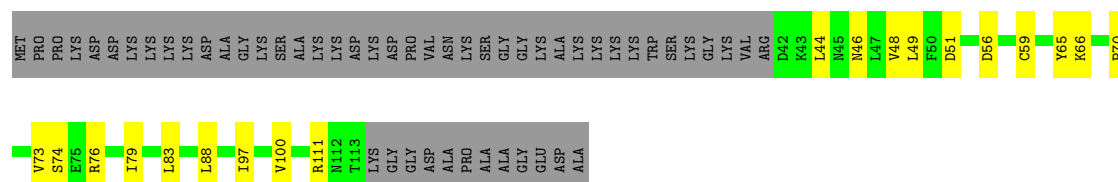
- Molecule 71: 40S ribosomal protein S24

Chain SY: 62% 30% 8%



- Molecule 72: 40S ribosomal protein S25

Chain SZ: 42% 15% 42%



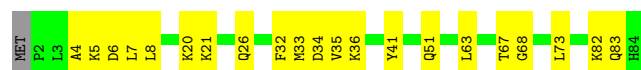
- Molecule 73: 40S ribosomal protein S26

Chain Sa: 70% 17% 14%



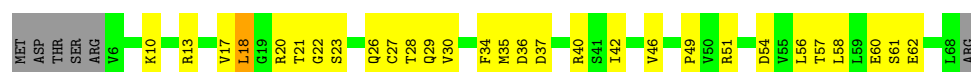
- Molecule 74: 40S ribosomal protein S27

Chain Sb: 74% 25% .



- Molecule 75: 40S ribosomal protein S28

Chain Sc: 49% 41% . 9%



- Molecule 76: 40S ribosomal protein S29

Chain Sd: 62% 29% . 7%



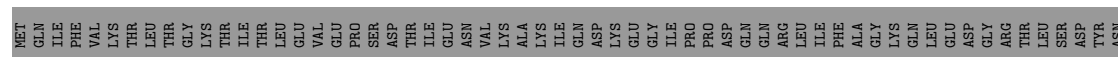
- Molecule 77: 40S ribosomal protein S30

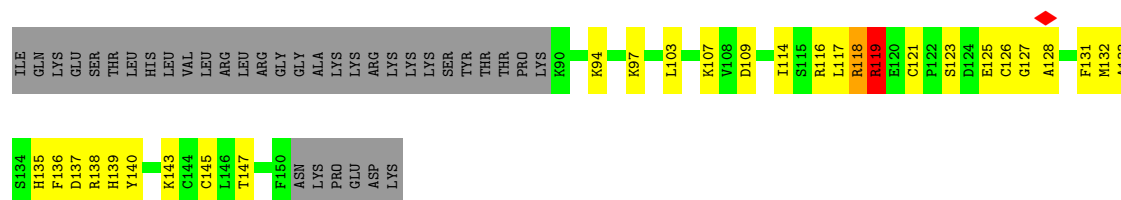
Chain Se: 68% 17% 15%



- Molecule 78: Ubiquitin

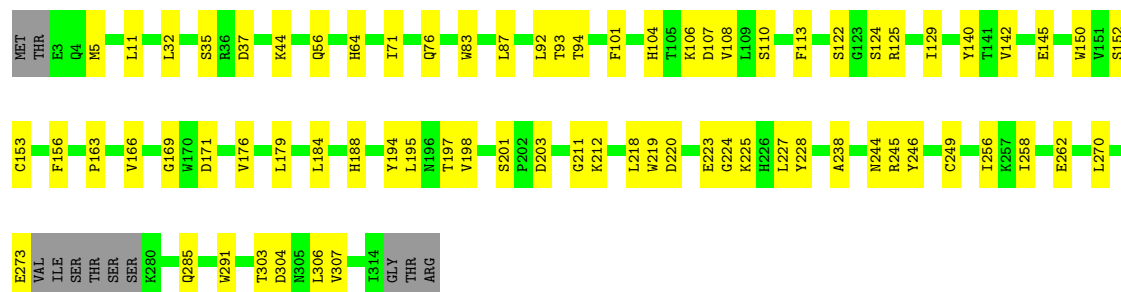
Chain Sf: 21% 17% . 61%





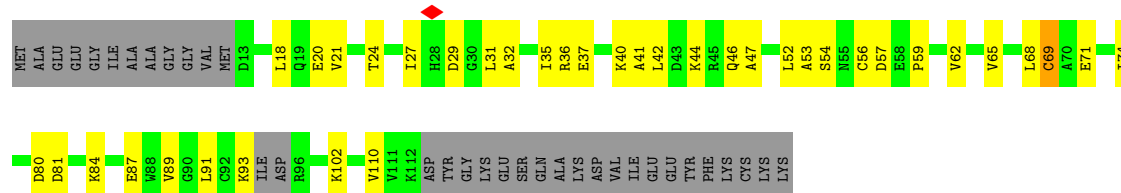
• Molecule 79: Receptor of activated protein C kinase 1

Chain Sg: 74% 23% .



• Molecule 80: 40S ribosomal protein S12

Chain SM: 45% 28% 26% .



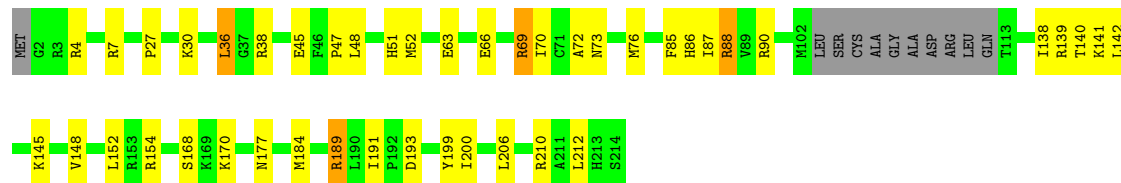
• Molecule 81: 60S ribosomal protein L32

Chain Le: 73% 21% 6% .



• Molecule 82: 60S ribosomal protein L10

Chain LI: 74% 19% 5% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 15395                                   | 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 ( $e^-/\text{\AA}^2$ ) | 1.022                                   | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 1700                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.113                                   | Depositor |
| Minimum map value                    | -0.078                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.004                                   | Depositor |
| Recommended contour level            | 0.005                                   | Depositor |
| Map size (Å)                         | 395.76, 395.76, 395.76                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.8245, 0.8245, 0.8245                  | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, G7M, 4AC, SPD, OMG, A2M, K, 6MZ, MA6, B8N, PSU, UY1, OMU, PUT, ZN, HYG, NA, MG

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    | 0.23         | 0/1924        | 0.35        | 0/2581        |
| 2   | SA    | 0.22         | 0/1742        | 0.46        | 4/2368 (0.2%) |
| 3   | LB    | 0.20         | 0/3215        | 0.31        | 0/4314        |
| 4   | SB    | 0.22         | 0/1754        | 0.31        | 0/2347        |
| 5   | A4    | 0.32         | 0/257         | 0.36        | 0/397         |
| 6   | B4    | 0.22         | 0/1795        | 0.30        | 0/2798        |
| 7   | D4    | 0.20         | 0/1506        | 0.35        | 0/2342        |
| 8   | L5    | 0.24         | 0/81933       | 0.28        | 0/127773      |
| 9   | L7    | 0.23         | 0/2836        | 0.24        | 0/4421        |
| 10  | L8    | 0.23         | 0/3425        | 0.28        | 0/5333        |
| 11  | LC    | 0.20         | 0/2928        | 0.29        | 0/3933        |
| 12  | LD    | 0.72         | 7/2437 (0.3%) | 0.93        | 8/3263 (0.2%) |
| 13  | LE    | 0.17         | 0/1677        | 0.30        | 0/2250        |
| 14  | LF    | 0.22         | 0/1880        | 0.30        | 0/2505        |
| 15  | LG    | 0.18         | 0/1824        | 0.29        | 0/2462        |
| 16  | LH    | 0.18         | 0/1545        | 0.31        | 0/2077        |
| 17  | LJ    | 0.31         | 1/1352 (0.1%) | 0.36        | 0/1809        |
| 18  | LL    | 0.19         | 0/1616        | 0.31        | 0/2163        |
| 19  | LM    | 0.20         | 0/1143        | 0.35        | 0/1530        |
| 20  | LN    | 0.23         | 0/1746        | 0.30        | 0/2338        |
| 21  | LO    | 0.20         | 0/1678        | 0.30        | 0/2245        |
| 22  | LP    | 0.20         | 0/1294        | 0.29        | 0/1739        |
| 23  | LQ    | 0.20         | 0/1537        | 0.28        | 0/2052        |
| 24  | LR    | 0.19         | 0/1474        | 0.28        | 0/1949        |
| 25  | LS    | 0.19         | 0/1469        | 0.31        | 0/1970        |
| 26  | LT    | 0.20         | 0/1272        | 0.28        | 0/1698        |
| 27  | LU    | 0.14         | 0/822         | 0.37        | 0/1103        |
| 28  | LV    | 0.23         | 0/993         | 0.35        | 0/1332        |
| 29  | LW    | 0.18         | 0/676         | 0.26        | 0/906         |
| 30  | LX    | 0.19         | 0/979         | 0.30        | 0/1319        |
| 31  | LY    | 0.18         | 0/1120        | 0.28        | 0/1491        |

| Mol | Chain | Bond lengths |                | Bond angles |               |
|-----|-------|--------------|----------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5       |
| 32  | LZ    | 0.19         | 0/1141         | 0.33        | 0/1521        |
| 33  | La    | 0.21         | 0/1188         | 0.28        | 0/1587        |
| 34  | Lb    | 0.20         | 0/759          | 0.29        | 0/1003        |
| 35  | Lc    | 0.33         | 0/736          | 0.52        | 0/988         |
| 36  | Ld    | 0.19         | 0/886          | 0.31        | 0/1194        |
| 37  | Lf    | 0.24         | 0/886          | 0.38        | 0/1189        |
| 38  | Lg    | 0.22         | 0/871          | 0.29        | 0/1164        |
| 39  | Lh    | 0.17         | 0/1019         | 0.31        | 0/1347        |
| 40  | Li    | 0.15         | 0/829          | 0.28        | 0/1097        |
| 41  | Lj    | 0.29         | 0/730          | 0.40        | 0/965         |
| 42  | Lk    | 0.22         | 0/559          | 0.51        | 1/745 (0.1%)  |
| 43  | Ll    | 0.19         | 0/445          | 0.25        | 0/588         |
| 44  | Lm    | 0.28         | 0/417          | 0.53        | 0/555         |
| 45  | Ln    | 0.26         | 0/240          | 0.26        | 0/305         |
| 46  | Lo    | 0.20         | 0/851          | 0.31        | 0/1121        |
| 47  | Lp    | 0.22         | 0/717          | 0.28        | 0/953         |
| 48  | Lr    | 0.20         | 0/1007         | 0.28        | 0/1351        |
| 49  | S2    | 0.27         | 1/37049 (0.0%) | 0.30        | 0/57713       |
| 50  | SC    | 0.21         | 0/1741         | 0.36        | 0/2354        |
| 51  | SD    | 0.21         | 0/1715         | 0.29        | 0/2313        |
| 52  | SE    | 0.22         | 0/2092         | 0.34        | 0/2816        |
| 53  | SF    | 0.21         | 0/1507         | 0.29        | 0/2024        |
| 54  | SG    | 0.18         | 0/1772         | 0.32        | 0/2366        |
| 55  | SH    | 0.16         | 0/1380         | 0.34        | 0/1856        |
| 56  | SI    | 0.21         | 0/1609         | 0.33        | 0/2155        |
| 57  | SJ    | 0.17         | 0/1507         | 0.32        | 0/2015        |
| 58  | SK    | 0.59         | 2/828 (0.2%)   | 1.12        | 5/1118 (0.4%) |
| 59  | SL    | 0.20         | 0/1167         | 0.32        | 0/1563        |
| 60  | SN    | 0.35         | 1/1229 (0.1%)  | 0.33        | 1/1652 (0.1%) |
| 61  | SO    | 0.23         | 0/971          | 0.32        | 0/1302        |
| 62  | SP    | 0.25         | 0/1081         | 0.36        | 0/1445        |
| 63  | SQ    | 0.20         | 0/1138         | 0.29        | 0/1523        |
| 64  | SR    | 0.21         | 0/1067         | 0.31        | 0/1433        |
| 65  | SS    | 0.22         | 0/1189         | 0.32        | 0/1592        |
| 66  | ST    | 0.20         | 0/1118         | 0.27        | 0/1499        |
| 67  | SU    | 0.22         | 0/800          | 0.39        | 0/1075        |
| 68  | SV    | 0.17         | 0/643          | 0.28        | 0/860         |
| 69  | SW    | 0.21         | 0/1051         | 0.30        | 0/1406        |
| 70  | SX    | 0.21         | 0/1100         | 0.35        | 0/1471        |
| 71  | SY    | 0.15         | 0/1005         | 0.28        | 0/1340        |
| 72  | SZ    | 0.20         | 0/580          | 0.36        | 0/780         |
| 73  | Sa    | 0.50         | 2/801 (0.2%)   | 0.94        | 3/1074 (0.3%) |
| 74  | Sb    | 0.19         | 0/647          | 0.37        | 0/870         |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 75  | Sc    | 0.27         | 0/491            | 0.39        | 0/658            |
| 76  | Sd    | 0.21         | 0/446            | 0.29        | 0/591            |
| 77  | Se    | 0.16         | 0/403            | 0.26        | 0/527            |
| 78  | Sf    | 0.34         | 0/498            | 0.61        | 1/661 (0.2%)     |
| 79  | Sg    | 0.17         | 0/2445           | 0.33        | 0/3326           |
| 80  | SM    | 0.29         | 0/727            | 0.51        | 0/981            |
| 81  | Le    | 0.22         | 0/1062           | 0.31        | 0/1417           |
| 82  | LI    | 0.25         | 0/1679           | 0.41        | 1/2243 (0.0%)    |
| All | All   | 0.25         | 14/219668 (0.0%) | 0.33        | 24/322500 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 35  | Lc    | 0                   | 1                   |
| 41  | Lj    | 0                   | 2                   |
| 78  | Sf    | 0                   | 3                   |
| 82  | LI    | 0                   | 3                   |
| All | All   | 0                   | 9                   |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 12  | LD    | 257 | PRO  | CB-CG   | 21.12  | 2.55        | 1.49     |
| 12  | LD    | 257 | PRO  | CG-CD   | -17.03 | 0.92        | 1.50     |
| 12  | LD    | 233 | PRO  | CG-CD   | -15.34 | 0.98        | 1.50     |
| 58  | SK    | 87  | PRO  | CB-CG   | -11.60 | 0.91        | 1.49     |
| 60  | SN    | 136 | PRO  | CA-C    | -9.20  | 1.46        | 1.51     |
| 12  | LD    | 233 | PRO  | N-CD    | 7.75   | 1.58        | 1.47     |
| 73  | Sa    | 97  | PRO  | CB-CG   | -7.62  | 1.11        | 1.49     |
| 73  | Sa    | 97  | PRO  | CG-CD   | -7.10  | 1.26        | 1.50     |
| 17  | LJ    | 17  | ILE  | CG1-CD1 | -7.03  | 1.24        | 1.51     |
| 12  | LD    | 232 | THR  | C-O     | -6.39  | 1.15        | 1.23     |
| 58  | SK    | 87  | PRO  | CG-CD   | -6.17  | 1.29        | 1.50     |
| 12  | LD    | 257 | PRO  | N-CA    | -5.83  | 1.39        | 1.47     |
| 12  | LD    | 257 | PRO  | N-CD    | 5.66   | 1.55        | 1.47     |
| 49  | S2    | 428 | OMU  | O3'-P   | 5.52   | 1.61        | 1.56     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 12  | LD    | 257 | PRO  | CB-CG-CD  | -32.49 | 2.13        | 106.10   |
| 12  | LD    | 233 | PRO  | N-CD-CG   | -24.19 | 66.91       | 103.20   |
| 58  | SK    | 87  | PRO  | CB-CG-CD  | 23.08  | 179.95      | 106.10   |
| 73  | Sa    | 97  | PRO  | N-CD-CG   | -18.80 | 75.00       | 103.20   |
| 58  | SK    | 87  | PRO  | CA-CB-CG  | -17.06 | 72.08       | 104.50   |
| 73  | Sa    | 97  | PRO  | CA-CB-CG  | -16.64 | 72.88       | 104.50   |
| 58  | SK    | 87  | PRO  | N-CD-CG   | -16.29 | 78.76       | 103.20   |
| 12  | LD    | 233 | PRO  | CA-CB-CG  | -15.56 | 74.93       | 104.50   |
| 12  | LD    | 257 | PRO  | CA-N-CD   | -13.74 | 92.77       | 112.00   |
| 12  | LD    | 257 | PRO  | N-CA-CB   | -12.28 | 92.67       | 103.35   |
| 2   | SA    | 199 | PRO  | N-CD-CG   | -10.30 | 87.75       | 103.20   |
| 58  | SK    | 87  | PRO  | CA-N-CD   | -10.17 | 97.77       | 112.00   |
| 12  | LD    | 257 | PRO  | CA-CB-CG  | -9.50  | 86.46       | 104.50   |
| 73  | Sa    | 97  | PRO  | CA-N-CD   | -8.70  | 99.82       | 112.00   |
| 58  | SK    | 86  | PRO  | O-C-N     | -8.69  | 117.31      | 121.31   |
| 2   | SA    | 199 | PRO  | CA-CB-CG  | -8.35  | 88.64       | 104.50   |
| 12  | LD    | 233 | PRO  | CA-N-CD   | -7.96  | 100.86      | 112.00   |
| 60  | SN    | 136 | PRO  | O-C-N     | -6.79  | 118.19      | 121.31   |
| 82  | LI    | 36  | LEU  | CB-CG-CD1 | -6.74  | 90.49       | 110.70   |
| 42  | Lk    | 62  | PRO  | CA-N-CD   | -6.01  | 103.58      | 112.00   |
| 2   | SA    | 199 | PRO  | CA-N-CD   | -5.58  | 104.19      | 112.00   |
| 2   | SA    | 199 | PRO  | N-CA-CB   | -5.40  | 98.08       | 103.48   |
| 78  | Sf    | 119 | ARG  | N-CA-C    | 5.35   | 118.60      | 111.75   |
| 12  | LD    | 232 | THR  | O-C-N     | -5.07  | 115.86      | 121.53   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 82  | LI    | 189 | ARG  | Sidechain |
| 82  | LI    | 69  | ARG  | Sidechain |
| 82  | LI    | 88  | ARG  | Sidechain |
| 35  | Lc    | 17  | ARG  | Sidechain |
| 41  | Lj    | 43  | ARG  | Sidechain |
| 41  | Lj    | 55  | ARG  | Sidechain |
| 78  | Sf    | 116 | ARG  | Sidechain |
| 78  | Sf    | 118 | ARG  | Sidechain |
| 78  | Sf    | 119 | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | LA    | 1886  | 0        | 1973     | 40      | 0            |
| 2   | SA    | 1705  | 0        | 1704     | 35      | 0            |
| 3   | LB    | 3147  | 0        | 3237     | 75      | 0            |
| 4   | SB    | 1727  | 0        | 1796     | 41      | 0            |
| 5   | A4    | 231   | 0        | 116      | 9       | 0            |
| 6   | B4    | 1604  | 0        | 816      | 27      | 0            |
| 7   | D4    | 1349  | 0        | 682      | 34      | 0            |
| 8   | L5    | 74335 | 0        | 37632    | 923     | 0            |
| 9   | L7    | 2538  | 0        | 1286     | 25      | 0            |
| 10  | L8    | 3132  | 0        | 1593     | 48      | 0            |
| 11  | LC    | 2874  | 0        | 3043     | 50      | 0            |
| 12  | LD    | 2391  | 0        | 2426     | 60      | 0            |
| 13  | LE    | 1648  | 0        | 1750     | 31      | 0            |
| 14  | LF    | 1846  | 0        | 1976     | 30      | 0            |
| 15  | LG    | 1793  | 0        | 1898     | 34      | 0            |
| 16  | LH    | 1526  | 0        | 1605     | 37      | 0            |
| 17  | LJ    | 1330  | 0        | 1354     | 38      | 0            |
| 18  | LL    | 1588  | 0        | 1682     | 33      | 0            |
| 19  | LM    | 1121  | 0        | 1181     | 35      | 0            |
| 20  | LN    | 1701  | 0        | 1749     | 40      | 0            |
| 21  | LO    | 1646  | 0        | 1790     | 29      | 0            |
| 22  | LP    | 1267  | 0        | 1293     | 20      | 0            |
| 23  | LQ    | 1513  | 0        | 1628     | 22      | 0            |
| 24  | LR    | 1458  | 0        | 1599     | 38      | 0            |
| 25  | LS    | 1431  | 0        | 1461     | 28      | 0            |
| 26  | LT    | 1247  | 0        | 1302     | 27      | 0            |
| 27  | LU    | 808   | 0        | 831      | 25      | 0            |
| 28  | LV    | 979   | 0        | 1039     | 27      | 0            |
| 29  | LW    | 663   | 0        | 612      | 10      | 0            |
| 30  | LX    | 962   | 0        | 1029     | 25      | 0            |
| 31  | LY    | 1103  | 0        | 1177     | 29      | 0            |
| 32  | LZ    | 1115  | 0        | 1195     | 32      | 0            |
| 33  | La    | 1159  | 0        | 1209     | 26      | 0            |
| 34  | Lb    | 747   | 0        | 798      | 21      | 0            |
| 35  | Lc    | 725   | 0        | 763      | 36      | 0            |
| 36  | Ld    | 871   | 0        | 915      | 16      | 0            |
| 37  | Lf    | 867   | 0        | 897      | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38  | Lg    | 861   | 0        | 937      | 23      | 0            |
| 39  | Lh    | 1011  | 0        | 1137     | 9       | 0            |
| 40  | Li    | 818   | 0        | 899      | 9       | 0            |
| 41  | Lj    | 715   | 0        | 751      | 15      | 0            |
| 42  | Lk    | 553   | 0        | 602      | 13      | 0            |
| 43  | Ll    | 435   | 0        | 472      | 13      | 0            |
| 44  | Lm    | 411   | 0        | 438      | 14      | 0            |
| 45  | Ln    | 239   | 0        | 289      | 2       | 0            |
| 46  | Lo    | 839   | 0        | 902      | 22      | 0            |
| 47  | Lp    | 707   | 0        | 756      | 12      | 0            |
| 48  | Lr    | 992   | 0        | 1045     | 23      | 0            |
| 49  | S2    | 33711 | 0        | 17041    | 450     | 0            |
| 50  | SC    | 1704  | 0        | 1784     | 37      | 0            |
| 51  | SD    | 1689  | 0        | 1734     | 31      | 0            |
| 52  | SE    | 2050  | 0        | 2156     | 64      | 0            |
| 53  | SF    | 1486  | 0        | 1538     | 13      | 0            |
| 54  | SG    | 1749  | 0        | 1875     | 56      | 0            |
| 55  | SH    | 1360  | 0        | 1390     | 33      | 0            |
| 56  | SI    | 1582  | 0        | 1607     | 32      | 0            |
| 57  | SJ    | 1482  | 0        | 1591     | 49      | 0            |
| 58  | SK    | 804   | 0        | 825      | 21      | 0            |
| 59  | SL    | 1147  | 0        | 1207     | 22      | 0            |
| 60  | SN    | 1205  | 0        | 1292     | 30      | 0            |
| 61  | SO    | 959   | 0        | 974      | 27      | 0            |
| 62  | SP    | 1060  | 0        | 1104     | 20      | 0            |
| 63  | SQ    | 1120  | 0        | 1189     | 24      | 0            |
| 64  | SR    | 1053  | 0        | 1109     | 27      | 0            |
| 65  | SS    | 1171  | 0        | 1226     | 33      | 0            |
| 66  | ST    | 1098  | 0        | 1120     | 31      | 0            |
| 67  | SU    | 790   | 0        | 847      | 30      | 0            |
| 68  | SV    | 636   | 0        | 637      | 9       | 0            |
| 69  | SW    | 1034  | 0        | 1080     | 32      | 0            |
| 70  | SX    | 1082  | 0        | 1141     | 17      | 0            |
| 71  | SY    | 988   | 0        | 1034     | 35      | 0            |
| 72  | SZ    | 574   | 0        | 627      | 13      | 0            |
| 73  | Sa    | 788   | 0        | 837      | 13      | 0            |
| 74  | Sb    | 633   | 0        | 631      | 19      | 0            |
| 75  | Sc    | 489   | 0        | 512      | 17      | 0            |
| 76  | Sd    | 436   | 0        | 430      | 15      | 0            |
| 77  | Se    | 400   | 0        | 440      | 8       | 0            |
| 78  | Sf    | 489   | 0        | 486      | 32      | 0            |
| 79  | Sg    | 2389  | 0        | 2343     | 54      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 80  | SM    | 722   | 0        | 730      | 32      | 0            |
| 81  | Le    | 1044  | 0        | 1136     | 21      | 0            |
| 82  | LI    | 1641  | 0        | 1683     | 33      | 0            |
| 83  | B4    | 3     | 0        | 0        | 0       | 0            |
| 83  | L5    | 17    | 0        | 0        | 0       | 0            |
| 83  | L8    | 1     | 0        | 0        | 0       | 0            |
| 83  | LA    | 1     | 0        | 0        | 0       | 0            |
| 83  | La    | 1     | 0        | 0        | 0       | 0            |
| 83  | Le    | 1     | 0        | 0        | 0       | 0            |
| 83  | S2    | 15    | 0        | 0        | 0       | 0            |
| 83  | SN    | 1     | 0        | 0        | 0       | 0            |
| 84  | A4    | 2     | 0        | 0        | 0       | 0            |
| 84  | B4    | 4     | 0        | 0        | 0       | 0            |
| 84  | D4    | 1     | 0        | 0        | 0       | 0            |
| 84  | L5    | 157   | 0        | 0        | 0       | 0            |
| 84  | L7    | 2     | 0        | 0        | 0       | 0            |
| 84  | L8    | 3     | 0        | 0        | 0       | 0            |
| 84  | LI    | 1     | 0        | 0        | 0       | 0            |
| 84  | LN    | 1     | 0        | 0        | 0       | 0            |
| 84  | LP    | 1     | 0        | 0        | 0       | 0            |
| 84  | LT    | 1     | 0        | 0        | 0       | 0            |
| 84  | Lp    | 1     | 0        | 0        | 0       | 0            |
| 84  | S2    | 93    | 0        | 0        | 0       | 0            |
| 85  | L5    | 12    | 0        | 0        | 0       | 0            |
| 85  | L7    | 1     | 0        | 0        | 0       | 0            |
| 85  | L8    | 1     | 0        | 0        | 0       | 0            |
| 85  | LP    | 1     | 0        | 0        | 0       | 0            |
| 85  | Ll    | 1     | 0        | 0        | 0       | 0            |
| 85  | S2    | 7     | 0        | 0        | 0       | 0            |
| 86  | L5    | 10    | 0        | 19       | 2       | 0            |
| 87  | L5    | 6     | 0        | 12       | 1       | 0            |
| 88  | Lg    | 1     | 0        | 0        | 0       | 0            |
| 88  | Lj    | 1     | 0        | 0        | 0       | 0            |
| 88  | Lo    | 1     | 0        | 0        | 0       | 0            |
| 88  | Lp    | 1     | 0        | 0        | 0       | 0            |
| 88  | SM    | 1     | 0        | 0        | 0       | 0            |
| 88  | Sd    | 1     | 0        | 0        | 0       | 0            |
| 88  | Sf    | 1     | 0        | 0        | 0       | 0            |
| 89  | S2    | 36    | 0        | 37       | 0       | 0            |
| 90  | L5    | 1     | 0        | 0        | 0       | 0            |
| 90  | L8    | 1     | 0        | 0        | 0       | 0            |
| 90  | LH    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 90  | LI    | 1      | 0        | 0        | 0       | 0            |
| 90  | LV    | 1      | 0        | 0        | 1       | 0            |
| 90  | S2    | 1      | 0        | 0        | 0       | 0            |
| 90  | SX    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 206575 | 0        | 152689   | 3039    | 0            |

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

All (3039) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:LD:257:PRO:CG  | 12:LD:257:PRO:N    | 1.89                     | 1.33              |
| 12:LD:257:PRO:CD  | 12:LD:257:PRO:HG3  | 1.69                     | 1.17              |
| 78:Sf:119:ARG:HG2 | 78:Sf:132:MET:HE2  | 1.18                     | 1.09              |
| 12:LD:257:PRO:CD  | 12:LD:257:PRO:HG2  | 1.69                     | 1.08              |
| 12:LD:257:PRO:CG  | 12:LD:257:PRO:HD3  | 1.58                     | 1.07              |
| 12:LD:257:PRO:CG  | 12:LD:257:PRO:HD2  | 1.58                     | 1.06              |
| 49:S2:1091:C:HO2' | 69:SW:2:VAL:N      | 1.52                     | 1.05              |
| 80:SM:54:SER:OG   | 80:SM:80:ASP:HA    | 1.60                     | 1.01              |
| 58:SK:53:LYS:NZ   | 58:SK:60:GLU:OE1   | 1.96                     | 0.99              |
| 12:LD:257:PRO:CG  | 12:LD:257:PRO:CD   | 0.92                     | 0.92              |
| 78:Sf:119:ARG:HG2 | 78:Sf:132:MET:CE   | 1.99                     | 0.92              |
| 8:L5:364:G:O6     | 41:Lj:52:LYS:HE3   | 1.70                     | 0.91              |
| 8:L5:496:G:N2     | 8:L5:658:C:O2      | 2.06                     | 0.89              |
| 8:L5:184:U:O2     | 8:L5:254:G:N1      | 2.06                     | 0.89              |
| 82:LI:30:LYS:HG2  | 82:LI:66:GLU:HG3   | 1.56                     | 0.88              |
| 66:ST:126:GLN:HA  | 66:ST:126:GLN:HE21 | 1.39                     | 0.86              |
| 8:L5:2520:C:O2    | 8:L5:2640:G:N2     | 2.09                     | 0.86              |
| 16:LH:128:MET:HE2 | 16:LH:134:CYS:HB2  | 1.57                     | 0.85              |
| 44:Lm:110:CYS:SG  | 44:Lm:111:ARG:N    | 2.47                     | 0.84              |
| 10:L8:55:PSU:HN3  | 10:L8:62:A:H2      | 1.26                     | 0.82              |
| 35:Lc:17:ARG:HD2  | 35:Lc:108:MET:HE1  | 1.62                     | 0.82              |
| 8:L5:222:C:OP2    | 11:LC:165:LYS:NZ   | 2.14                     | 0.81              |
| 8:L5:1524:A2M:H61 | 8:L5:1651:G:H1     | 1.29                     | 0.81              |
| 37:Lf:104:MET:O   | 37:Lf:105:LEU:HD12 | 1.80                     | 0.80              |
| 49:S2:1849:G:O2'  | 49:S2:1850:MA6:H8  | 1.80                     | 0.80              |
| 66:ST:126:GLN:HA  | 66:ST:126:GLN:NE2  | 1.97                     | 0.80              |
| 37:Lf:78:HIS:HB3  | 37:Lf:83:MET:O     | 1.81                     | 0.80              |
| 62:SP:34:MET:HE1  | 62:SP:46:ASN:OD1   | 1.80                     | 0.80              |
| 49:S2:190:G:O2'   | 49:S2:209:A:N6     | 2.15                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:D4:8:U:H3        | 7:D4:13:C:H3'      | 1.48                     | 0.79              |
| 41:Lj:56:ARG:O     | 41:Lj:57:THR:HG22  | 1.82                     | 0.79              |
| 8:L5:308:G:H2'     | 40:Li:41:ARG:HH22  | 1.46                     | 0.78              |
| 6:B4:32:C:OP2      | 63:SQ:146:ARG:NH2  | 2.16                     | 0.78              |
| 49:S2:1488:C:O2'   | 49:S2:1490:G:OP2   | 1.99                     | 0.78              |
| 7:D4:13:C:O2'      | 7:D4:22:G:N2       | 2.14                     | 0.78              |
| 1:LA:248:GLY:HA3   | 49:S2:1069:U:H4'   | 1.66                     | 0.78              |
| 49:S2:952:G:H21    | 61:SO:52:THR:HG21  | 1.50                     | 0.77              |
| 49:S2:1613:G:OP1   | 62:SP:42:ARG:NH2   | 2.16                     | 0.77              |
| 8:L5:3722:G:H2'    | 8:L5:3723:A2M:H8   | 1.67                     | 0.76              |
| 74:Sb:33:MET:HE1   | 74:Sb:73:LEU:HD11  | 1.66                     | 0.76              |
| 49:S2:1115:U:N3    | 49:S2:1118:C:N4    | 2.34                     | 0.76              |
| 8:L5:1353:G:N7     | 23:LQ:104:ARG:NH2  | 2.34                     | 0.76              |
| 49:S2:809:A:O4'    | 52:SE:221:ARG:NH2  | 2.18                     | 0.76              |
| 49:S2:927:C:O2     | 74:Sb:51:GLN:NE2   | 2.17                     | 0.76              |
| 8:L5:1468:C:OP1    | 33:La:132:ARG:NH2  | 2.19                     | 0.76              |
| 66:ST:126:GLN:HE22 | 66:ST:129:ARG:HD2  | 1.50                     | 0.76              |
| 12:LD:156:GLY:HA2  | 12:LD:181:PRO:HG3  | 1.68                     | 0.76              |
| 20:LN:124:ASP:OD1  | 20:LN:125:SER:N    | 2.19                     | 0.76              |
| 46:Lo:23:VAL:HG12  | 46:Lo:70:LEU:HD22  | 1.68                     | 0.76              |
| 49:S2:1608:U:OP1   | 65:SS:134:GLN:NE2  | 2.18                     | 0.76              |
| 5:A4:48:A:H61      | 6:B4:33:C:H42      | 1.33                     | 0.76              |
| 8:L5:496:G:N2      | 8:L5:658:C:C2      | 2.54                     | 0.76              |
| 46:Lo:11:PHE:O     | 46:Lo:81:ARG:NH2   | 2.20                     | 0.75              |
| 66:ST:56:ARG:HG2   | 66:ST:103:VAL:HG21 | 1.68                     | 0.75              |
| 46:Lo:103:VAL:O    | 46:Lo:105:GLN:N    | 2.19                     | 0.75              |
| 2:SA:40:LYS:NZ     | 64:SR:101:ASP:OD1  | 2.19                     | 0.75              |
| 54:SG:2:LYS:HB2    | 54:SG:108:VAL:HG22 | 1.69                     | 0.75              |
| 9:L7:51:G:N2       | 17:LJ:12:MET:SD    | 2.60                     | 0.75              |
| 48:Lr:58:LYS:O     | 48:Lr:83:ASN:ND2   | 2.19                     | 0.75              |
| 49:S2:126:G:O2'    | 49:S2:181:A:N3     | 2.20                     | 0.74              |
| 49:S2:1336:C:O2'   | 49:S2:1337:4AC:H6  | 1.87                     | 0.74              |
| 20:LN:96:ARG:NH2   | 20:LN:104:GLU:OE1  | 2.20                     | 0.74              |
| 54:SG:22:ARG:HA    | 54:SG:25:ARG:HE    | 1.53                     | 0.74              |
| 9:L7:72:U:O2       | 9:L7:103:A:N6      | 2.19                     | 0.74              |
| 35:Lc:17:ARG:HH11  | 35:Lc:108:MET:HE1  | 1.53                     | 0.74              |
| 49:S2:1115:U:H3    | 49:S2:1118:C:N4    | 1.85                     | 0.74              |
| 15:LG:176:LYS:HD2  | 40:Li:43:MET:HE1   | 1.68                     | 0.74              |
| 57:SJ:140:GLN:NE2  | 71:SY:64:PHE:O     | 2.20                     | 0.74              |
| 63:SQ:21:ALA:O     | 63:SQ:87:SER:OG    | 2.06                     | 0.74              |
| 8:L5:1372:A:OP1    | 20:LN:202:ARG:NH2  | 2.21                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:Lc:105:ILE:O    | 35:Lc:106:ARG:HG2  | 1.88                     | 0.73              |
| 49:S2:1396:A:O2'   | 49:S2:1398:G:N7    | 2.21                     | 0.73              |
| 49:S2:1285:G:N1    | 80:SM:57:ASP:OD2   | 2.21                     | 0.73              |
| 67:SU:78:ASP:OD2   | 76:Sd:54:LYS:NZ    | 2.18                     | 0.73              |
| 6:B4:74:C:O2'      | 46:Lo:54:PRO:O     | 2.06                     | 0.73              |
| 15:LG:162:ASP:HB2  | 15:LG:163:PRO:HD3  | 1.70                     | 0.73              |
| 8:L5:435:A:O2'     | 81:Le:26:ASP:OD2   | 2.06                     | 0.73              |
| 40:Li:2:ALA:N      | 40:Li:5:TYR:HH     | 1.86                     | 0.73              |
| 15:LG:58:PRO:HD2   | 15:LG:61:ILE:HD12  | 1.70                     | 0.73              |
| 7:D4:27:G:H22      | 7:D4:43:C:H5       | 1.35                     | 0.73              |
| 14:LF:182:TYR:HB3  | 14:LF:200:ARG:HG3  | 1.69                     | 0.73              |
| 19:LM:106:ASP:OD1  | 19:LM:109:ARG:NH1  | 2.21                     | 0.73              |
| 49:S2:1610:G:OP2   | 65:SS:132:ARG:NH1  | 2.21                     | 0.73              |
| 35:Lc:17:ARG:HH12  | 35:Lc:107:SER:CB   | 2.02                     | 0.73              |
| 78:Sf:127:GLY:O    | 80:SM:44:LYS:NZ    | 2.21                     | 0.73              |
| 31:LY:30:MET:HB3   | 31:LY:101:PRO:HG2  | 1.71                     | 0.72              |
| 76:Sd:53:ILE:HD11  | 76:Sd:55:LEU:HD12  | 1.70                     | 0.72              |
| 8:L5:132:G:H2'     | 8:L5:133:C:H4'     | 1.70                     | 0.72              |
| 8:L5:2400:G:H21    | 38:Lg:6:THR:HG22   | 1.54                     | 0.72              |
| 57:SJ:63:LEU:HD11  | 57:SJ:70:ARG:HB2   | 1.70                     | 0.72              |
| 65:SS:12:ILE:HD11  | 65:SS:19:ASN:HB3   | 1.72                     | 0.72              |
| 62:SP:21:ASP:OD2   | 62:SP:24:GLN:NE2   | 2.21                     | 0.72              |
| 64:SR:120:THR:HG22 | 64:SR:121:GLN:H    | 1.55                     | 0.72              |
| 8:L5:2583:C:OP2    | 38:Lg:76:ARG:NH2   | 2.22                     | 0.72              |
| 8:L5:4122:G:N1     | 38:Lg:98:GLU:OE1   | 2.23                     | 0.72              |
| 17:LJ:17:ILE:HD12  | 17:LJ:80:GLU:OE2   | 1.88                     | 0.72              |
| 24:LR:13:SER:OG    | 24:LR:38:ARG:NH2   | 2.23                     | 0.71              |
| 49:S2:1451:G:N7    | 64:SR:44:LYS:NZ    | 2.38                     | 0.71              |
| 66:ST:126:GLN:HE22 | 66:ST:129:ARG:HH11 | 1.39                     | 0.71              |
| 3:LB:246:ARG:NH1   | 8:L5:4525:C:OP1    | 2.23                     | 0.71              |
| 49:S2:94:G:HO2'    | 49:S2:508:A:HO2'   | 1.30                     | 0.71              |
| 49:S2:818:A:OP1    | 57:SJ:80:ARG:NH2   | 2.24                     | 0.71              |
| 60:SN:3:ARG:HB3    | 60:SN:6:ALA:HB3    | 1.72                     | 0.71              |
| 8:L5:3642:A:HO2'   | 41:Lj:2:THR:N      | 1.89                     | 0.71              |
| 31:LY:32:SER:OG    | 31:LY:101:PRO:O    | 2.08                     | 0.71              |
| 13:LE:208:ILE:HG22 | 13:LE:210:LYS:H    | 1.55                     | 0.71              |
| 42:Lk:50:LYS:O     | 42:Lk:54:GLU:HG2   | 1.90                     | 0.71              |
| 63:SQ:9:SER:OG     | 63:SQ:24:HIS:NE2   | 2.23                     | 0.71              |
| 49:S2:687:C:O2'    | 55:SH:116:ARG:NH2  | 2.22                     | 0.71              |
| 67:SU:78:ASP:OD1   | 76:Sd:44:ARG:NH1   | 2.24                     | 0.71              |
| 49:S2:556:U:H4'    | 49:S2:557:U:H5'    | 1.72                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L8:14:OMU:H5''  | 22:LP:123:PRO:HD3  | 1.74                     | 0.70              |
| 20:LN:193:ARG:O    | 20:LN:197:THR:HG23 | 1.91                     | 0.70              |
| 49:S2:1729:U:H3    | 49:S2:1805:G:H1    | 1.38                     | 0.70              |
| 8:L5:438:G:N2      | 37:Lf:23:GLU:OE1   | 2.19                     | 0.70              |
| 19:LM:36:ALA:HB3   | 19:LM:55:MET:HE1   | 1.73                     | 0.70              |
| 49:S2:64:A:H2      | 49:S2:83:A:H62     | 1.39                     | 0.70              |
| 79:Sg:166:VAL:HG12 | 79:Sg:176:VAL:HG22 | 1.74                     | 0.70              |
| 6:B4:68:U:H2'      | 6:B4:69:G:H8       | 1.57                     | 0.70              |
| 11:LC:303:ARG:O    | 23:LQ:38:ARG:NH2   | 2.19                     | 0.70              |
| 13:LE:250:GLN:NE2  | 13:LE:254:ASP:OD2  | 2.24                     | 0.70              |
| 30:LX:121:VAL:HG13 | 30:LX:138:VAL:HG13 | 1.73                     | 0.70              |
| 49:S2:24:C:HO2'    | 49:S2:25:A:H8      | 1.37                     | 0.70              |
| 20:LN:157:LYS:O    | 20:LN:162:ARG:NH1  | 2.24                     | 0.70              |
| 49:S2:1536:G:H2'   | 49:S2:1537:A:H8    | 1.57                     | 0.70              |
| 7:D4:27:G:H1       | 7:D4:43:C:H41      | 1.38                     | 0.70              |
| 3:LB:57:VAL:HG22   | 3:LB:73:VAL:HG12   | 1.74                     | 0.70              |
| 4:SB:172:MET:O     | 4:SB:176:VAL:HG12  | 1.92                     | 0.70              |
| 32:LZ:10:VAL:O     | 32:LZ:83:THR:OG1   | 2.08                     | 0.70              |
| 49:S2:996:A:OP1    | 60:SN:114:ARG:NH2  | 2.25                     | 0.70              |
| 34:Lb:23:LYS:HG2   | 34:Lb:24:PRO:HD2   | 1.73                     | 0.70              |
| 65:SS:89:ASP:OD2   | 65:SS:106:LYS:NZ   | 2.25                     | 0.70              |
| 3:LB:95:THR:HG22   | 8:L5:4910:G:H4'    | 1.73                     | 0.69              |
| 8:L5:1412:G:H2'    | 8:L5:1413:C:H6     | 1.57                     | 0.69              |
| 8:L5:4745:G:H1     | 8:L5:4955:A:H61    | 1.39                     | 0.69              |
| 8:L5:4472:G:O2'    | 44:Lm:100:TYR:O    | 2.11                     | 0.69              |
| 73:Sa:23:CYS:SG    | 73:Sa:26:CYS:N     | 2.65                     | 0.69              |
| 8:L5:3641:U:OP2    | 8:L5:3646:A:N6     | 2.25                     | 0.69              |
| 15:LG:157:ILE:HG22 | 15:LG:201:THR:OG1  | 1.93                     | 0.69              |
| 49:S2:1745:A:H1'   | 54:SG:66:GLY:HA2   | 1.73                     | 0.69              |
| 62:SP:34:MET:HE2   | 62:SP:42:ARG:HG3   | 1.72                     | 0.69              |
| 8:L5:4635:A:H8     | 8:L5:5048:A:H61    | 1.40                     | 0.69              |
| 49:S2:126:G:OP2    | 54:SG:198:ARG:NH1  | 2.25                     | 0.69              |
| 3:LB:220:ILE:HG22  | 3:LB:278:THR:HA    | 1.73                     | 0.69              |
| 8:L5:1178:G:HO2'   | 12:LD:286:SER:HG   | 1.36                     | 0.69              |
| 81:Le:43:ASN:HB3   | 81:Le:46:ARG:HG2   | 1.73                     | 0.69              |
| 3:LB:92:TYR:HB2    | 3:LB:159:VAL:HG13  | 1.75                     | 0.69              |
| 8:L5:2101:C:H2'    | 8:L5:2102:G:C8     | 2.27                     | 0.69              |
| 51:SD:75:LYS:NZ    | 58:SK:20:VAL:O     | 2.24                     | 0.69              |
| 61:SO:118:ALA:O    | 61:SO:122:SER:OG   | 2.08                     | 0.69              |
| 3:LB:258:HIS:NE2   | 8:L5:3878:C:O2     | 2.25                     | 0.69              |
| 8:L5:2318:G:N2     | 8:L5:2321:G:OP2    | 2.21                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L8:94:G:OP2     | 41:Lj:72:ARG:NH1   | 2.26                     | 0.69              |
| 49:S2:830:A:OP2    | 49:S2:846:G:N2     | 2.25                     | 0.69              |
| 60:SN:55:ARG:NH2   | 74:Sb:51:GLN:OE1   | 2.26                     | 0.69              |
| 22:LP:29:THR:HG21  | 22:LP:146:ILE:HD11 | 1.74                     | 0.69              |
| 49:S2:1033:G:N1    | 49:S2:1080:A:O2'   | 2.25                     | 0.69              |
| 78:Sf:128:ALA:HB3  | 80:SM:44:LYS:NZ    | 2.07                     | 0.69              |
| 4:SB:179:ASN:ND2   | 4:SB:183:GLU:OE1   | 2.24                     | 0.69              |
| 8:L5:137:G:H2'     | 8:L5:138:G:H8      | 1.57                     | 0.69              |
| 8:L5:4218:U:OP2    | 26:LT:9:ARG:NH2    | 2.26                     | 0.69              |
| 60:SN:4:MET:SD     | 60:SN:124:ARG:NH2  | 2.65                     | 0.69              |
| 12:LD:51:MET:HE3   | 12:LD:105:LEU:HD23 | 1.73                     | 0.68              |
| 26:LT:43:LYS:O     | 26:LT:58:HIS:ND1   | 2.26                     | 0.68              |
| 49:S2:921:G:H5'    | 74:Sb:21:LYS:HE2   | 1.75                     | 0.68              |
| 49:S2:1612:G:OP1   | 62:SP:18:ARG:NH2   | 2.27                     | 0.68              |
| 49:S2:1623:A:H5''  | 65:SS:133:GLY:HA3  | 1.75                     | 0.68              |
| 66:ST:126:GLN:NE2  | 66:ST:129:ARG:HH11 | 1.91                     | 0.68              |
| 8:L5:1187:G:OP2    | 8:L5:1187:G:N2     | 2.20                     | 0.68              |
| 65:SS:86:ARG:HE    | 65:SS:106:LYS:HD2  | 1.58                     | 0.68              |
| 82:LI:72:ALA:O     | 82:LI:76:MET:HG2   | 1.93                     | 0.68              |
| 8:L5:3736:A:O2'    | 8:L5:3737:A:O5'    | 2.11                     | 0.68              |
| 14:LF:222:LYS:NZ   | 14:LF:224:THR:OG1  | 2.27                     | 0.68              |
| 8:L5:2262:G:OP2    | 48:Lr:98:ARG:NH1   | 2.26                     | 0.68              |
| 8:L5:2469:C:H5     | 8:L5:2471:G:H1     | 1.42                     | 0.68              |
| 79:Sg:256:ILE:HD11 | 79:Sg:270:LEU:HD12 | 1.75                     | 0.68              |
| 3:LB:56:ILE:HG21   | 3:LB:365:LEU:HD22  | 1.76                     | 0.68              |
| 8:L5:1405:C:N4     | 8:L5:1408:G:N3     | 2.41                     | 0.68              |
| 8:L5:4594:U:H2'    | 8:L5:4595:G:H8     | 1.58                     | 0.68              |
| 7:D4:51:U:H3       | 7:D4:63:G:H1       | 0.78                     | 0.68              |
| 8:L5:2502:G:O6     | 30:LX:50:LYS:NZ    | 2.24                     | 0.68              |
| 35:Lc:99:PRO:HB2   | 35:Lc:102:SER:HB3  | 1.76                     | 0.68              |
| 49:S2:30:C:O2'     | 49:S2:596:U:OP1    | 2.10                     | 0.68              |
| 8:L5:2338:C:HO2'   | 48:Lr:13:CYS:HG    | 1.32                     | 0.68              |
| 8:L5:3589:G:N2     | 8:L5:3590:G:O6     | 2.27                     | 0.68              |
| 16:LH:50:LYS:O     | 16:LH:51:LYS:HG2   | 1.94                     | 0.68              |
| 44:Lm:83:ARG:O     | 44:Lm:87:GLN:HG3   | 1.91                     | 0.68              |
| 49:S2:1649:U:H3    | 49:S2:1675:A:H2    | 1.42                     | 0.68              |
| 79:Sg:220:ASP:HB2  | 79:Sg:227:LEU:HD11 | 1.74                     | 0.68              |
| 8:L5:654:C:H4'     | 11:LC:269:LYS:HG3  | 1.75                     | 0.68              |
| 8:L5:2658:G:N2     | 8:L5:2676:A:OP2    | 2.27                     | 0.68              |
| 20:LN:104:GLU:HA   | 20:LN:160:GLU:HG3  | 1.76                     | 0.68              |
| 1:LA:3:ARG:HH12    | 8:L5:1634:A:H62    | 1.41                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:SH:65:PRO:HG2  | 55:SH:68:GLN:HG3   | 1.76                     | 0.67              |
| 3:LB:246:ARG:NH2  | 8:L5:4558:U:OP2    | 2.28                     | 0.67              |
| 2:SA:173:LEU:O    | 2:SA:177:MET:HG2   | 1.95                     | 0.67              |
| 3:LB:19:ARG:NH2   | 8:L5:4623:OMG:OP1  | 2.27                     | 0.67              |
| 8:L5:3765:G:O2'   | 8:L5:3767:C:N4     | 2.27                     | 0.67              |
| 8:L5:4305:G:N7    | 26:LT:87:LYS:NZ    | 2.41                     | 0.67              |
| 49:S2:686:U:O2    | 55:SH:118:ARG:NH2  | 2.27                     | 0.67              |
| 28:LV:50:ASN:ND2  | 90:LV:201:HOH:O    | 2.27                     | 0.67              |
| 49:S2:1272:C:OP2  | 78:Sf:94:LYS:NZ    | 2.27                     | 0.67              |
| 49:S2:1546:G:N2   | 49:S2:1670:C:O2    | 2.28                     | 0.67              |
| 1:LA:207:VAL:HG21 | 8:L5:1633:G:C6     | 2.30                     | 0.67              |
| 8:L5:4340:U:O2    | 86:L5:5286:SPD:N10 | 2.27                     | 0.67              |
| 79:Sg:249:CYS:SG  | 79:Sg:291:TRP:NE1  | 2.66                     | 0.67              |
| 8:L5:308:G:OP2    | 8:L5:308:G:N2      | 2.26                     | 0.67              |
| 8:L5:1480:C:O2'   | 8:L5:1482:G:OP2    | 2.13                     | 0.67              |
| 13:LE:117:PRO:O   | 48:Lr:112:ARG:NH1  | 2.27                     | 0.67              |
| 49:S2:65:C:N4     | 49:S2:169:U:O2'    | 2.28                     | 0.67              |
| 49:S2:1627:C:H5'' | 66:ST:41:LYS:HD2   | 1.76                     | 0.67              |
| 13:LE:47:ASN:HB2  | 13:LE:62:MET:HE2   | 1.77                     | 0.66              |
| 42:Lk:49:ASP:O    | 42:Lk:50:LYS:HG3   | 1.95                     | 0.66              |
| 8:L5:4076:G:OP1   | 15:LG:73:ARG:NH1   | 2.28                     | 0.66              |
| 8:L5:4096:C:N4    | 8:L5:4113:U:O2'    | 2.28                     | 0.66              |
| 28:LV:13:LYS:HB2  | 28:LV:128:LEU:HD11 | 1.77                     | 0.66              |
| 49:S2:1589:A:N3   | 49:S2:1653:U:O2'   | 2.29                     | 0.66              |
| 73:Sa:32:LYS:O    | 73:Sa:37:LYS:NZ    | 2.28                     | 0.66              |
| 8:L5:508:G:O2'    | 8:L5:510:U:OP2     | 2.13                     | 0.66              |
| 8:L5:4140:C:N3    | 8:L5:4145:C:O2'    | 2.24                     | 0.66              |
| 35:Lc:17:ARG:NH1  | 35:Lc:107:SER:CB   | 2.59                     | 0.66              |
| 49:S2:1536:G:H2'  | 49:S2:1537:A:C8    | 2.30                     | 0.66              |
| 3:LB:268:ARG:NH1  | 8:L5:3896:C:O2'    | 2.28                     | 0.66              |
| 16:LH:124:ARG:NH1 | 16:LH:164:ALA:O    | 2.27                     | 0.66              |
| 61:SO:31:CYS:HB2  | 61:SO:93:LEU:HD22  | 1.77                     | 0.66              |
| 78:Sf:136:PHE:CE2 | 78:Sf:137:ASP:OD1  | 2.49                     | 0.66              |
| 8:L5:4648:A:OP1   | 24:LR:62:ARG:NH2   | 2.28                     | 0.66              |
| 19:LM:25:VAL:HG12 | 19:LM:45:VAL:HG21  | 1.78                     | 0.66              |
| 50:SC:201:GLY:N   | 50:SC:221:ASP:OD2  | 2.28                     | 0.66              |
| 3:LB:58:ARG:NH2   | 3:LB:361:GLU:OE2   | 2.29                     | 0.66              |
| 7:D4:25:C:H2'     | 7:D4:26:A:H8       | 1.60                     | 0.66              |
| 8:L5:664:G:N2     | 8:L5:666:G:O6      | 2.24                     | 0.66              |
| 8:L5:1443:A:H2    | 8:L5:2103:G:H1     | 1.40                     | 0.66              |
| 8:L5:1837:A:OP2   | 26:LT:130:ARG:NH1  | 2.28                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:L5:3823:G:OP2   | 8:L5:3823:G:N2    | 2.23                     | 0.66              |
| 52:SE:153:LEU:O   | 52:SE:174:LYS:NZ  | 2.28                     | 0.66              |
| 2:SA:128:ARG:NH2  | 2:SA:151:ASP:O    | 2.29                     | 0.66              |
| 8:L5:1173:G:N1    | 8:L5:1174:A:N3    | 2.43                     | 0.66              |
| 8:L5:4507:A:O2'   | 28:LV:41:SER:OG   | 2.14                     | 0.66              |
| 24:LR:24:LEU:HD23 | 24:LR:32:ILE:HG21 | 1.78                     | 0.66              |
| 28:LV:90:ARG:HB2  | 28:LV:94:VAL:HG23 | 1.78                     | 0.66              |
| 49:S2:857:U:H2'   | 49:S2:858:A:C8    | 2.31                     | 0.66              |
| 52:SE:63:LYS:O    | 52:SE:67:GLN:HG3  | 1.95                     | 0.66              |
| 35:Lc:17:ARG:NE   | 35:Lc:17:ARG:HA   | 2.10                     | 0.66              |
| 35:Lc:105:ILE:O   | 35:Lc:106:ARG:CG  | 2.44                     | 0.66              |
| 49:S2:65:C:H4'    | 54:SG:172:LYS:HD3 | 1.78                     | 0.66              |
| 8:L5:1097:C:H2'   | 8:L5:1098:G:H8    | 1.61                     | 0.65              |
| 16:LH:44:GLU:HG2  | 16:LH:58:ASP:HB2  | 1.76                     | 0.65              |
| 17:LJ:96:LYS:O    | 17:LJ:159:LYS:NZ  | 2.29                     | 0.65              |
| 4:SB:229:MET:HA   | 4:SB:229:MET:HE3  | 1.79                     | 0.65              |
| 8:L5:1412:G:H2'   | 8:L5:1413:C:C6    | 2.30                     | 0.65              |
| 12:LD:278:ASP:OD2 | 12:LD:282:GLN:NE2 | 2.30                     | 0.65              |
| 14:LF:32:ARG:HG2  | 14:LF:36:LYS:HE2  | 1.78                     | 0.65              |
| 49:S2:874:G:H2'   | 49:S2:875:A:H8    | 1.61                     | 0.65              |
| 78:Sf:119:ARG:CG  | 78:Sf:132:MET:HE2 | 2.11                     | 0.65              |
| 19:LM:29:ASP:OD1  | 19:LM:30:VAL:N    | 2.29                     | 0.65              |
| 82:LI:47:PRO:HD2  | 82:LI:141:LYS:HA  | 1.77                     | 0.65              |
| 8:L5:419:A:N3     | 8:L5:1332:C:O2'   | 2.28                     | 0.65              |
| 19:LM:120:ASN:O   | 19:LM:124:LYS:HG3 | 1.96                     | 0.65              |
| 24:LR:15:LEU:HD22 | 24:LR:52:ARG:HB2  | 1.79                     | 0.65              |
| 57:SJ:30:LYS:O    | 57:SJ:34:GLU:HG2  | 1.96                     | 0.65              |
| 8:L5:62:A:N3      | 8:L5:77:U:O2'     | 2.29                     | 0.65              |
| 8:L5:2103:G:H3'   | 8:L5:2104:G:C8    | 2.32                     | 0.65              |
| 49:S2:1829:G:H1'  | 49:S2:1850:MA6:H2 | 1.79                     | 0.65              |
| 62:SP:64:LYS:NZ   | 62:SP:90:VAL:O    | 2.28                     | 0.65              |
| 80:SM:44:LYS:HA   | 80:SM:44:LYS:HE3  | 1.78                     | 0.65              |
| 54:SG:85:ARG:O    | 54:SG:87:ARG:NH1  | 2.28                     | 0.65              |
| 66:ST:40:ALA:HB3  | 66:ST:43:LYS:HG2  | 1.76                     | 0.65              |
| 8:L5:502:C:H5'    | 8:L5:503:C:H3'    | 1.79                     | 0.65              |
| 8:L5:2562:G:N2    | 8:L5:2565:A:OP2   | 2.17                     | 0.65              |
| 20:LN:5:LYS:HG2   | 40:Li:40:VAL:HG11 | 1.78                     | 0.65              |
| 28:LV:10:SER:OG   | 28:LV:11:GLY:N    | 2.29                     | 0.65              |
| 49:S2:165:G:OP2   | 49:S2:165:G:N2    | 2.26                     | 0.65              |
| 78:Sf:107:LYS:HE3 | 78:Sf:109:ASP:OD1 | 1.96                     | 0.65              |
| 8:L5:703:G:H2'    | 8:L5:704:C:H4'    | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:2693:G:OP1    | 42:Lk:35:LYS:NZ    | 2.26                     | 0.65              |
| 8:L5:4992:G:H2'    | 8:L5:4993:G:C8     | 2.31                     | 0.65              |
| 8:L5:1268:G:N7     | 34:Lb:111:ARG:NH2  | 2.43                     | 0.65              |
| 8:L5:1669:A:H4'    | 8:L5:1685:G:H22    | 1.61                     | 0.65              |
| 8:L5:2338:C:O2'    | 48:Lr:13:CYS:SG    | 2.45                     | 0.65              |
| 17:LJ:18:ARG:H     | 17:LJ:134:LEU:HA   | 1.62                     | 0.65              |
| 44:Lm:96:CYS:HB2   | 44:Lm:99:CYS:H     | 1.61                     | 0.65              |
| 53:SF:102:LEU:HD11 | 72:SZ:100:VAL:HG21 | 1.79                     | 0.65              |
| 8:L5:1516:G:O2'    | 18:LL:18:TRP:NE1   | 2.29                     | 0.65              |
| 8:L5:3689:G:O2'    | 8:L5:3818:U:OP2    | 2.15                     | 0.65              |
| 28:LV:87:SER:OG    | 29:LW:19:ARG:NH1   | 2.28                     | 0.65              |
| 56:SI:78:ILE:HA    | 56:SI:104:ILE:HD12 | 1.79                     | 0.65              |
| 28:LV:106:VAL:HA   | 28:LV:112:MET:HA   | 1.78                     | 0.64              |
| 48:Lr:20:ARG:NH2   | 81:Le:84:GLU:OE2   | 2.28                     | 0.64              |
| 55:SH:145:ARG:NH1  | 69:SW:49:GLU:OE1   | 2.29                     | 0.64              |
| 8:L5:4769:G:H5'    | 21:LO:176:ARG:HD3  | 1.79                     | 0.64              |
| 8:L5:4980:C:N3     | 22:LP:69:ARG:NH2   | 2.45                     | 0.64              |
| 10:L8:105:C:H4'    | 10:L8:106:G:H5''   | 1.79                     | 0.64              |
| 49:S2:527:C:O2'    | 57:SJ:121:LYS:NZ   | 2.30                     | 0.64              |
| 52:SE:18:TRP:HH2   | 52:SE:31:PRO:HD3   | 1.62                     | 0.64              |
| 79:Sg:87:LEU:HB2   | 79:Sg:101:PHE:HB2  | 1.80                     | 0.64              |
| 10:L8:52:A:H62     | 43:Ll:27:ILE:HD13  | 1.63                     | 0.64              |
| 8:L5:2102:G:H1'    | 8:L5:2103:G:H8     | 1.62                     | 0.64              |
| 49:S2:924:G:H5'    | 60:SN:4:MET:HE3    | 1.78                     | 0.64              |
| 49:S2:1091:C:O2'   | 69:SW:2:VAL:N      | 2.28                     | 0.64              |
| 3:LB:300:LYS:HB2   | 3:LB:311:ASP:HA    | 1.79                     | 0.64              |
| 4:SB:35:ALA:O      | 4:SB:42:ARG:NH2    | 2.30                     | 0.64              |
| 12:LD:197:LYS:HG3  | 12:LD:202:GLN:HB2  | 1.80                     | 0.64              |
| 57:SJ:31:LEU:HD21  | 57:SJ:103:GLU:HG3  | 1.80                     | 0.64              |
| 8:L5:1351:G:OP1    | 11:LC:33:ARG:NH1   | 2.31                     | 0.64              |
| 10:L8:22:U:OP1     | 31:LY:11:ARG:NH1   | 2.30                     | 0.64              |
| 49:S2:1528:G:O2'   | 49:S2:1666:C:OP1   | 2.14                     | 0.64              |
| 57:SJ:74:GLY:O     | 57:SJ:78:LEU:HD13  | 1.98                     | 0.64              |
| 2:SA:137:ALA:HB1   | 2:SA:142:LEU:HB3   | 1.80                     | 0.64              |
| 8:L5:1411:C:H41    | 34:Lb:48:LYS:HE2   | 1.62                     | 0.64              |
| 8:L5:4298:A:O3'    | 34:Lb:33:LYS:NZ    | 2.26                     | 0.64              |
| 8:L5:4910:G:N2     | 21:LO:106:ASP:O    | 2.31                     | 0.64              |
| 49:S2:640:A:H2'    | 49:S2:641:A:C8     | 2.31                     | 0.64              |
| 49:S2:993:G:OP1    | 49:S2:1131:G:N2    | 2.25                     | 0.64              |
| 78:Sf:103:LEU:O    | 80:SM:36:ARG:NH2   | 2.30                     | 0.64              |
| 30:LX:114:LYS:NZ   | 30:LX:120:ASP:OD1  | 2.31                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:S2:641:A:O2'   | 49:S2:645:C:OP1    | 2.16                     | 0.64              |
| 61:SO:77:ALA:O    | 61:SO:81:VAL:HG23  | 1.98                     | 0.64              |
| 68:SV:35:ASN:OD1  | 68:SV:52:THR:OG1   | 2.14                     | 0.64              |
| 3:LB:224:LYS:NZ   | 8:L5:4626:A:OP2    | 2.26                     | 0.64              |
| 8:L5:655:C:OP1    | 11:LC:268:ARG:NH2  | 2.31                     | 0.64              |
| 49:S2:1209:A:OP1  | 49:S2:1835:A:N6    | 2.31                     | 0.64              |
| 63:SQ:42:ILE:HG22 | 63:SQ:44:PRO:HD2   | 1.80                     | 0.64              |
| 8:L5:4274:A:H2'   | 8:L5:4275:G:C8     | 2.34                     | 0.63              |
| 59:SL:42:LEU:HD13 | 59:SL:72:ILE:HD11  | 1.79                     | 0.63              |
| 26:LT:18:PRO:HG2  | 26:LT:21:LYS:HB2   | 1.80                     | 0.63              |
| 64:SR:37:GLU:OE2  | 79:Sg:106:LYS:NZ   | 2.30                     | 0.63              |
| 49:S2:289:G:OP1   | 52:SE:155:LYS:NZ   | 2.27                     | 0.63              |
| 78:Sf:117:LEU:C   | 78:Sf:118:ARG:HD2  | 2.24                     | 0.63              |
| 13:LE:161:ARG:NH1 | 13:LE:273:SER:OG   | 2.31                     | 0.63              |
| 16:LH:93:ARG:HD2  | 16:LH:143:GLU:HG3  | 1.80                     | 0.63              |
| 43:Ll:24:PRO:HD2  | 43:Ll:27:ILE:HD12  | 1.79                     | 0.63              |
| 49:S2:468:A:OP1   | 54:SG:96:SER:OG    | 2.17                     | 0.63              |
| 49:S2:809:A:C4'   | 52:SE:221:ARG:NH2  | 2.62                     | 0.63              |
| 54:SG:21:GLU:N    | 54:SG:21:GLU:OE2   | 2.32                     | 0.63              |
| 64:SR:98:VAL:HG13 | 64:SR:102:THR:HB   | 1.81                     | 0.63              |
| 27:LU:20:LYS:HB2  | 27:LU:73:THR:HG23  | 1.80                     | 0.63              |
| 49:S2:1115:U:H1'  | 49:S2:1116:C:H2'   | 1.81                     | 0.63              |
| 8:L5:4206:C:OP1   | 26:LT:5:LYS:NZ     | 2.31                     | 0.63              |
| 16:LH:113:GLU:OE1 | 16:LH:115:ARG:NH2  | 2.31                     | 0.63              |
| 19:LM:104:MET:HE3 | 19:LM:109:ARG:HG2  | 1.81                     | 0.63              |
| 8:L5:5066:U:OP1   | 22:LP:43:LYS:NZ    | 2.29                     | 0.63              |
| 34:Lb:47:LYS:HA   | 34:Lb:50:ASN:HD22  | 1.63                     | 0.63              |
| 49:S2:1228:A:H2'  | 49:S2:1229:G:C8    | 2.33                     | 0.63              |
| 80:SM:84:LYS:HA   | 80:SM:87:GLU:HG3   | 1.80                     | 0.63              |
| 2:SA:52:LYS:HB2   | 64:SR:109:LEU:HD11 | 1.81                     | 0.63              |
| 8:L5:3599:A:H2'   | 8:L5:3600:G:C8     | 2.34                     | 0.63              |
| 24:LR:172:ARG:NH1 | 49:S2:909:G:OP1    | 2.32                     | 0.63              |
| 57:SJ:84:ILE:HG13 | 57:SJ:86:VAL:HG13  | 1.79                     | 0.63              |
| 8:L5:86:U:O2'     | 33:La:65:ARG:NH1   | 2.32                     | 0.62              |
| 11:LC:149:GLU:HG2 | 11:LC:151:PRO:HD2  | 1.79                     | 0.62              |
| 31:LY:43:ASN:ND2  | 31:LY:127:GLN:OE1  | 2.32                     | 0.62              |
| 8:L5:109:G:OP2    | 18:LL:74:ARG:NH2   | 2.32                     | 0.62              |
| 8:L5:462:G:H2'    | 8:L5:463:A:C8      | 2.34                     | 0.62              |
| 79:Sg:244:ASN:OD1 | 79:Sg:245:ARG:N    | 2.32                     | 0.62              |
| 7:D4:5:G:H2'      | 7:D4:6:G:C8        | 2.34                     | 0.62              |
| 8:L5:257:C:H2'    | 8:L5:258:G:C8      | 2.34                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:2059:C:O2     | 25:LS:118:ARG:NH2  | 2.31                     | 0.62              |
| 8:L5:4635:A:H2     | 8:L5:4663:G:H21    | 1.46                     | 0.62              |
| 16:LH:137:SER:OG   | 16:LH:143:GLU:HB3  | 1.99                     | 0.62              |
| 36:Ld:24:GLU:HG2   | 36:Ld:87:ARG:HG3   | 1.81                     | 0.62              |
| 49:S2:832:G:O6     | 71:SY:11:LYS:NZ    | 2.33                     | 0.62              |
| 56:SI:110:ARG:NH2  | 56:SI:122:GLY:O    | 2.32                     | 0.62              |
| 67:SU:34:LYS:HZ1   | 67:SU:107:GLU:HG3  | 1.65                     | 0.62              |
| 42:Lk:12:LEU:HB3   | 42:Lk:16:ARG:HH21  | 1.62                     | 0.62              |
| 71:SY:62:THR:HG23  | 71:SY:69:THR:HG22  | 1.81                     | 0.62              |
| 2:SA:74:VAL:HG12   | 2:SA:121:LEU:HB3   | 1.80                     | 0.62              |
| 4:SB:107:ARG:NH2   | 61:SO:133:THR:O    | 2.29                     | 0.62              |
| 8:L5:4327:C:OP1    | 26:LT:70:HIS:NE2   | 2.33                     | 0.62              |
| 35:Lc:36:LYS:O     | 35:Lc:40:GLN:HG2   | 1.98                     | 0.62              |
| 38:Lg:41:ALA:O     | 38:Lg:52:ARG:NH1   | 2.33                     | 0.62              |
| 49:S2:921:G:OP2    | 74:Sb:26:GLN:NE2   | 2.31                     | 0.62              |
| 78:Sf:114:ILE:HG12 | 80:SM:71:GLU:OE2   | 2.00                     | 0.62              |
| 8:L5:2702:C:OP1    | 27:LU:101:ARG:NH2  | 2.33                     | 0.62              |
| 13:LE:244:GLU:O    | 13:LE:248:ILE:HG12 | 1.99                     | 0.62              |
| 46:Lo:78:ARG:O     | 46:Lo:80:LYS:NZ    | 2.33                     | 0.62              |
| 57:SJ:69:ARG:NH1   | 57:SJ:73:GLU:OE2   | 2.28                     | 0.62              |
| 8:L5:3710:G:N2     | 8:L5:3712:A:H62    | 1.97                     | 0.62              |
| 8:L5:3777:G:O2'    | 8:L5:3815:G:O6     | 2.15                     | 0.62              |
| 24:LR:105:LEU:HD23 | 24:LR:138:LEU:HD23 | 1.82                     | 0.62              |
| 49:S2:1061:U:O4    | 49:S2:1849:G:N2    | 2.32                     | 0.62              |
| 7:D4:21:A:N6       | 7:D4:46:G:O2'      | 2.33                     | 0.62              |
| 8:L5:4940:C:OP1    | 13:LE:156:ARG:NH2  | 2.32                     | 0.62              |
| 54:SG:57:ASP:HA    | 54:SG:106:LEU:HA   | 1.81                     | 0.62              |
| 81:Le:85:LEU:HD21  | 81:Le:115:ALA:HB2  | 1.82                     | 0.62              |
| 82:LI:86:HIS:HB3   | 82:LI:139:ARG:HG2  | 1.80                     | 0.62              |
| 8:L5:724:C:OP1     | 11:LC:350:ARG:HD2  | 2.00                     | 0.62              |
| 8:L5:4467:A:O2'    | 8:L5:4510:A:N3     | 2.30                     | 0.61              |
| 11:LC:146:GLU:OE1  | 11:LC:146:GLU:N    | 2.33                     | 0.61              |
| 55:SH:51:ILE:HD12  | 55:SH:176:VAL:HG22 | 1.80                     | 0.61              |
| 6:B4:11:C:H2'      | 6:B4:12:G:H8       | 1.65                     | 0.61              |
| 8:L5:655:C:H2'     | 8:L5:656:C:O4'     | 2.00                     | 0.61              |
| 8:L5:257:C:H2'     | 8:L5:258:G:H8      | 1.65                     | 0.61              |
| 8:L5:3932:U:HO2'   | 8:L5:3933:G:H8     | 1.48                     | 0.61              |
| 8:L5:4274:A:H2'    | 8:L5:4275:G:H8     | 1.64                     | 0.61              |
| 8:L5:5006:U:H4'    | 8:L5:5007:A:H5'    | 1.82                     | 0.61              |
| 21:LO:194:GLU:O    | 21:LO:198:THR:HG23 | 2.00                     | 0.61              |
| 49:S2:1273:C:O2'   | 49:S2:1506:A:N6    | 2.33                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:SB:151:ARG:NH2   | 49:S2:1123:C:OP1   | 2.33                     | 0.61              |
| 8:L5:1564:A:OP1    | 60:SN:140:LYS:NZ   | 2.31                     | 0.61              |
| 8:L5:1661:C:O2'    | 81:Le:36:ARG:NH1   | 2.33                     | 0.61              |
| 18:LL:180:ALA:O    | 18:LL:184:MET:HG3  | 2.00                     | 0.61              |
| 49:S2:1289:U:OP2   | 78:Sf:97:LYS:NZ    | 2.32                     | 0.61              |
| 49:S2:1585:U:O2'   | 49:S2:1586:U:O5'   | 2.19                     | 0.61              |
| 8:L5:2100:A:H2'    | 8:L5:2101:C:C2     | 2.35                     | 0.61              |
| 12:LD:184:ASP:OD2  | 12:LD:187:SER:OG   | 2.18                     | 0.61              |
| 1:LA:54:ARG:NH2    | 8:L5:3680:U:OP1    | 2.34                     | 0.61              |
| 7:D4:37:A:OP1      | 77:Se:74:LYS:N     | 2.33                     | 0.61              |
| 49:S2:1337:4AC:H2' | 49:S2:1338:G:C8    | 2.36                     | 0.61              |
| 51:SD:163:PRO:O    | 51:SD:167:TYR:HB2  | 2.00                     | 0.61              |
| 1:LA:128:ARG:NH1   | 8:L5:3681:G:OP2    | 2.33                     | 0.61              |
| 7:D4:64:A:H4'      | 82:LI:27:PRO:HA    | 1.81                     | 0.61              |
| 8:L5:1326:A2M:OP2  | 8:L5:4445:U:O2'    | 2.18                     | 0.61              |
| 8:L5:1778:C:H5''   | 12:LD:5:LYS:HG2    | 1.82                     | 0.61              |
| 8:L5:1654:G:N2     | 8:L5:1678:C:OP1    | 2.33                     | 0.61              |
| 49:S2:1230:C:OP1   | 65:SS:130:ARG:NH2  | 2.33                     | 0.61              |
| 49:S2:1388:A:H61   | 51:SD:161:GLY:HA3  | 1.65                     | 0.61              |
| 49:S2:1708:C:H2'   | 49:S2:1709:G:H5''  | 1.83                     | 0.61              |
| 79:Sg:197:THR:HG21 | 79:Sg:238:ALA:HA   | 1.82                     | 0.61              |
| 8:L5:1750:G:N2     | 82:LI:193:ASP:OD2  | 2.34                     | 0.61              |
| 18:LL:11:LYS:NZ    | 33:La:52:TYR:OH    | 2.34                     | 0.61              |
| 35:Lc:57:LYS:O     | 35:Lc:61:GLU:HG2   | 1.99                     | 0.61              |
| 50:SC:198:ALA:HB1  | 50:SC:202:THR:HG21 | 1.82                     | 0.61              |
| 8:L5:1095:A:H2     | 8:L5:1200:G:H1     | 1.49                     | 0.61              |
| 8:L5:1095:A:N1     | 8:L5:1200:G:O6     | 2.34                     | 0.61              |
| 43:LI:2:SER:O      | 43:LI:5:LYS:NZ     | 2.34                     | 0.61              |
| 8:L5:677:G:H2'     | 8:L5:678:C:C6      | 2.36                     | 0.60              |
| 8:L5:4363:A:H5''   | 46:Lo:36:GLN:HG2   | 1.83                     | 0.60              |
| 11:LC:283:LYS:NZ   | 23:LQ:22:ASP:OD2   | 2.23                     | 0.60              |
| 18:LL:200:LYS:O    | 18:LL:202:ALA:N    | 2.33                     | 0.60              |
| 35:Lc:17:ARG:HH12  | 35:Lc:107:SER:HB2  | 1.66                     | 0.60              |
| 59:SL:101:ARG:HB2  | 70:SX:10:ALA:HB2   | 1.83                     | 0.60              |
| 8:L5:4124:G:N2     | 15:LG:43:GLN:O     | 2.34                     | 0.60              |
| 51:SD:95:GLY:HA2   | 51:SD:101:GLN:HE21 | 1.64                     | 0.60              |
| 67:SU:22:ILE:HG23  | 67:SU:114:VAL:HG12 | 1.82                     | 0.60              |
| 73:Sa:22:ARG:NH1   | 73:Sa:29:CYS:SG    | 2.74                     | 0.60              |
| 80:SM:42:LEU:HD23  | 80:SM:68:LEU:HB3   | 1.83                     | 0.60              |
| 8:L5:279:A:OP1     | 20:LN:50:ARG:NH1   | 2.34                     | 0.60              |
| 62:SP:100:LYS:HG2  | 62:SP:101:THR:HG23 | 1.82                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:SU:34:LYS:NZ    | 67:SU:107:GLU:HG3  | 2.16                     | 0.60              |
| 7:D4:4:C:H2'       | 7:D4:5:G:C8        | 2.35                     | 0.60              |
| 8:L5:1503:A:H4'    | 8:L5:1504:G:H5'    | 1.84                     | 0.60              |
| 8:L5:2601:A:N6     | 8:L5:2744:A:OP2    | 2.31                     | 0.60              |
| 49:S2:1228:A:H2'   | 49:S2:1229:G:H8    | 1.66                     | 0.60              |
| 8:L5:4238:G:H2'    | 8:L5:4239:A:H8     | 1.67                     | 0.60              |
| 31:LY:8:THR:HG21   | 31:LY:13:LYS:HD3   | 1.83                     | 0.60              |
| 48:Lr:19:LYS:HG2   | 48:Lr:24:THR:HG22  | 1.82                     | 0.60              |
| 49:S2:1563:G:OP1   | 66:ST:121:ARG:NH1  | 2.35                     | 0.60              |
| 4:SB:137:LEU:HG    | 4:SB:215:VAL:HG22  | 1.84                     | 0.60              |
| 8:L5:85:G:O2'      | 8:L5:97:G:O6       | 2.17                     | 0.60              |
| 8:L5:665:C:O2'     | 8:L5:666:G:N7      | 2.35                     | 0.60              |
| 57:SJ:94:LEU:HA    | 57:SJ:97:ILE:HG12  | 1.82                     | 0.60              |
| 18:LL:56:ARG:NH1   | 18:LL:74:ARG:O     | 2.34                     | 0.60              |
| 49:S2:1133:A:H4'   | 73:Sa:13:LYS:HG2   | 1.83                     | 0.60              |
| 72:SZ:65:TYR:CZ    | 72:SZ:76:ARG:HD3   | 2.36                     | 0.60              |
| 36:Ld:20:VAL:HG22  | 36:Ld:91:LYS:HA    | 1.83                     | 0.60              |
| 64:SR:37:GLU:OE1   | 79:Sg:150:TRP:NE1  | 2.34                     | 0.60              |
| 8:L5:693:C:H2'     | 8:L5:694:C:H6      | 1.67                     | 0.60              |
| 8:L5:1398:A:OP1    | 33:La:136:LYS:NZ   | 2.32                     | 0.60              |
| 65:SS:14:ARG:HE    | 65:SS:17:ASN:HA    | 1.65                     | 0.60              |
| 8:L5:1097:C:H2'    | 8:L5:1098:G:C8     | 2.36                     | 0.60              |
| 17:LJ:36:ALA:O     | 17:LJ:39:VAL:HG12  | 2.01                     | 0.59              |
| 35:Lc:28:VAL:HG22  | 35:Lc:95:ALA:HB3   | 1.83                     | 0.59              |
| 53:SF:30:ILE:HG21  | 53:SF:36:GLN:HA    | 1.83                     | 0.59              |
| 8:L5:182:G:N1      | 8:L5:255:C:O2      | 2.35                     | 0.59              |
| 8:L5:2611:A:H5'    | 8:L5:2688:G:H4'    | 1.84                     | 0.59              |
| 8:L5:4405:G:OP2    | 82:LI:7:ARG:NH2    | 2.35                     | 0.59              |
| 11:LC:146:GLU:OE2  | 11:LC:178:ASN:ND2  | 2.33                     | 0.59              |
| 22:LP:22:LEU:HD12  | 22:LP:146:ILE:HD12 | 1.83                     | 0.59              |
| 49:S2:928:G:H2'    | 49:S2:929:G:C8     | 2.37                     | 0.59              |
| 49:S2:1354:G:N2    | 49:S2:1357:A:OP2   | 2.29                     | 0.59              |
| 54:SG:159:ARG:HH21 | 54:SG:171:THR:HG23 | 1.66                     | 0.59              |
| 66:ST:110:LEU:HD23 | 66:ST:112:MET:HE2  | 1.83                     | 0.59              |
| 67:SU:34:LYS:HZ1   | 67:SU:107:GLU:CG   | 2.15                     | 0.59              |
| 67:SU:98:VAL:O     | 67:SU:102:THR:HG23 | 2.03                     | 0.59              |
| 73:Sa:74:CYS:N     | 73:Sa:77:CYS:SG    | 2.75                     | 0.59              |
| 8:L5:693:C:H2'     | 8:L5:694:C:C6      | 2.36                     | 0.59              |
| 8:L5:3615:G:H1'    | 29:LW:44:ARG:HD3   | 1.83                     | 0.59              |
| 42:Lk:24:LYS:HG2   | 42:Lk:67:LYS:NZ    | 2.16                     | 0.59              |
| 63:SQ:116:ASP:HB3  | 63:SQ:119:LEU:HD13 | 1.85                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:Sg:145:GLU:HB2  | 79:Sg:184:LEU:HD11 | 1.83                     | 0.59              |
| 5:A4:46:A:H2'      | 5:A4:47:A:C8       | 2.37                     | 0.59              |
| 7:D4:51:U:O4       | 7:D4:63:G:O6       | 2.21                     | 0.59              |
| 8:L5:2758:G:O2'    | 8:L5:2765:A:N3     | 2.33                     | 0.59              |
| 8:L5:4478:G:O2'    | 8:L5:4602:A:N1     | 2.35                     | 0.59              |
| 12:LD:232:THR:HG22 | 12:LD:234:ASP:H    | 1.67                     | 0.59              |
| 15:LG:207:VAL:HG21 | 15:LG:215:LEU:HD22 | 1.83                     | 0.59              |
| 76:Sd:21:CYS:HB2   | 76:Sd:39:CYS:SG    | 2.42                     | 0.59              |
| 8:L5:3717:A:H2'    | 8:L5:3718:A2M:H8   | 1.84                     | 0.59              |
| 11:LC:293:LEU:O    | 11:LC:299:GLN:NE2  | 2.31                     | 0.59              |
| 55:SH:10:LYS:NZ    | 55:SH:12:ASN:OD1   | 2.29                     | 0.59              |
| 79:Sg:110:SER:OG   | 79:Sg:152:SER:O    | 2.20                     | 0.59              |
| 3:LB:228:TYR:O     | 8:L5:2835:A:O2'    | 2.21                     | 0.59              |
| 8:L5:490:C:H2'     | 8:L5:491:G:H8      | 1.67                     | 0.59              |
| 8:L5:4670:C:O2'    | 8:L5:4672:A:OP2    | 2.20                     | 0.59              |
| 7:D4:53:G:H2'      | 7:D4:54:U:C6       | 2.38                     | 0.59              |
| 10:L8:75:OMG:OP2   | 31:LY:74:TYR:OH    | 2.18                     | 0.59              |
| 54:SG:59:GLN:OE1   | 54:SG:72:ARG:NH2   | 2.36                     | 0.59              |
| 1:LA:244:GLY:HA3   | 8:L5:3746:A:H5''   | 1.85                     | 0.59              |
| 8:L5:715:G:OP1     | 11:LC:321:ASN:ND2  | 2.35                     | 0.59              |
| 8:L5:4162:C:O2     | 15:LG:73:ARG:NH2   | 2.34                     | 0.59              |
| 16:LH:85:THR:HG23  | 16:LH:86:LEU:HG    | 1.85                     | 0.59              |
| 35:Lc:17:ARG:HH11  | 35:Lc:108:MET:CE   | 2.16                     | 0.59              |
| 46:Lo:100:LYS:O    | 46:Lo:102:GLN:NE2  | 2.35                     | 0.59              |
| 49:S2:1387:G:N1    | 51:SD:206:ASP:OD2  | 2.30                     | 0.59              |
| 52:SE:100:ARG:NH2  | 52:SE:121:TYR:O    | 2.34                     | 0.59              |
| 79:Sg:184:LEU:H    | 79:Sg:184:LEU:HD12 | 1.67                     | 0.59              |
| 6:B4:11:C:H2'      | 6:B4:12:G:C8       | 2.37                     | 0.59              |
| 8:L5:4093:G:H2'    | 8:L5:4094:G:C8     | 2.37                     | 0.59              |
| 12:LD:107:ARG:NH1  | 12:LD:169:GLY:O    | 2.34                     | 0.59              |
| 52:SE:151:ASP:HB3  | 52:SE:154:ILE:HG13 | 1.83                     | 0.59              |
| 57:SJ:64:ASP:OD1   | 57:SJ:65:GLU:N     | 2.36                     | 0.59              |
| 8:L5:1364:U:OP2    | 18:LL:36:ARG:NH1   | 2.27                     | 0.59              |
| 8:L5:1443:A:N6     | 8:L5:1444:G:O6     | 2.35                     | 0.59              |
| 8:L5:4882:U:OP1    | 19:LM:117:LYS:NZ   | 2.36                     | 0.59              |
| 15:LG:108:GLN:OE1  | 15:LG:108:GLN:N    | 2.30                     | 0.59              |
| 32:LZ:83:THR:HG22  | 38:Lg:95:PHE:CZ    | 2.38                     | 0.59              |
| 50:SC:161:SER:O    | 50:SC:161:SER:OG   | 2.18                     | 0.59              |
| 70:SX:107:ARG:HD3  | 70:SX:112:VAL:HG12 | 1.83                     | 0.59              |
| 8:L5:666:G:H1'     | 8:L5:667:A:H3'     | 1.84                     | 0.58              |
| 9:L7:54:A:O2'      | 17:LJ:13:ARG:NH1   | 2.36                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:LO:121:PRO:HA   | 21:LO:124:LEU:HD12 | 1.84                     | 0.58              |
| 72:SZ:65:TYR:CE2   | 72:SZ:76:ARG:HD3   | 2.37                     | 0.58              |
| 8:L5:1577:G:O2'    | 8:L5:1612:G:H4'    | 2.03                     | 0.58              |
| 8:L5:1870:C:H2'    | 8:L5:1871:A2M:H8   | 1.85                     | 0.58              |
| 8:L5:3910:C:H2'    | 8:L5:3911:C:C6     | 2.38                     | 0.58              |
| 11:LC:1:MET:HG3    | 11:LC:2:ALA:H      | 1.68                     | 0.58              |
| 15:LG:165:GLU:OE1  | 20:LN:26:ARG:NH1   | 2.29                     | 0.58              |
| 52:SE:115:THR:HG22 | 52:SE:117:GLU:H    | 1.67                     | 0.58              |
| 64:SR:90:ALA:O     | 64:SR:93:GLN:NE2   | 2.36                     | 0.58              |
| 16:LH:31:ARG:NH1   | 16:LH:188:GLN:OE1  | 2.35                     | 0.58              |
| 19:LM:7:VAL:HG23   | 19:LM:27:ILE:HD13  | 1.85                     | 0.58              |
| 76:Sd:15:GLY:O     | 76:Sd:19:ARG:NH1   | 2.36                     | 0.58              |
| 2:SA:189:ILE:HG22  | 2:SA:191:ARG:H     | 1.67                     | 0.58              |
| 52:SE:127:ARG:HH21 | 52:SE:142:HIS:HB2  | 1.68                     | 0.58              |
| 24:LR:107:ARG:O    | 24:LR:111:GLU:HG2  | 2.01                     | 0.58              |
| 46:Lo:2:VAL:N      | 46:Lo:90:HIS:O     | 2.36                     | 0.58              |
| 55:SH:61:ILE:HG13  | 55:SH:93:VAL:HG23  | 1.85                     | 0.58              |
| 82:LI:48:LEU:HB2   | 82:LI:142:LEU:HD23 | 1.84                     | 0.58              |
| 8:L5:1942:A:H2'    | 8:L5:1943:A:C8     | 2.38                     | 0.58              |
| 8:L5:1968:G:H2'    | 8:L5:1969:G:C8     | 2.39                     | 0.58              |
| 8:L5:5064:G:N2     | 22:LP:75:GLN:OE1   | 2.36                     | 0.58              |
| 23:LQ:3:VAL:HG22   | 23:LQ:5:ILE:HG23   | 1.85                     | 0.58              |
| 8:L5:690:C:H2'     | 8:L5:691:C:C6      | 2.38                     | 0.58              |
| 8:L5:2640:G:H2'    | 8:L5:2641:A:C8     | 2.38                     | 0.58              |
| 12:LD:65:ALA:HB2   | 12:LD:74:ILE:HD13  | 1.85                     | 0.58              |
| 32:LZ:66:SER:O     | 32:LZ:66:SER:OG    | 2.19                     | 0.58              |
| 65:SS:36:VAL:HG12  | 65:SS:40:TYR:CD1   | 2.39                     | 0.58              |
| 9:L7:28:C:H1'      | 9:L7:54:A:H61      | 1.68                     | 0.58              |
| 11:LC:143:ARG:NH1  | 11:LC:145:GLU:OE2  | 2.37                     | 0.58              |
| 25:LS:76:LYS:NZ    | 25:LS:100:LEU:O    | 2.36                     | 0.58              |
| 8:L5:423:G:OP1     | 22:LP:62:ARG:NH1   | 2.37                     | 0.58              |
| 8:L5:2019:C:O2'    | 8:L5:2020:U:OP1    | 2.19                     | 0.58              |
| 49:S2:521:A:OP1    | 57:SJ:45:ARG:NH1   | 2.33                     | 0.58              |
| 54:SG:50:VAL:HB    | 54:SG:111:LEU:HD12 | 1.86                     | 0.58              |
| 62:SP:72:LYS:HE2   | 62:SP:106:GLU:HG3  | 1.86                     | 0.58              |
| 64:SR:71:ILE:HG13  | 64:SR:74:GLN:HB2   | 1.86                     | 0.58              |
| 72:SZ:70:PRO:O     | 72:SZ:74:SER:OG    | 2.21                     | 0.58              |
| 1:LA:177:LYS:HB2   | 47:Lp:29:ILE:HD13  | 1.86                     | 0.58              |
| 8:L5:4272:G:OP2    | 8:L5:4272:G:N2     | 2.27                     | 0.58              |
| 8:L5:4347:G:H2'    | 8:L5:4348:A:C8     | 2.38                     | 0.58              |
| 8:L5:4541:G:N2     | 8:L5:4544:A:OP2    | 2.35                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:LU:35:ASP:OD2   | 27:LU:94:ASN:ND2   | 2.36                     | 0.58              |
| 49:S2:919:A:OP1    | 60:SN:20:ARG:NH1   | 2.33                     | 0.58              |
| 63:SQ:53:GLU:OE1   | 63:SQ:85:ARG:NH1   | 2.36                     | 0.58              |
| 79:Sg:201:SER:OG   | 79:Sg:203:ASP:OD1  | 2.22                     | 0.58              |
| 3:LB:222:VAL:O     | 3:LB:343:ARG:NH1   | 2.36                     | 0.57              |
| 8:L5:3910:C:H2'    | 8:L5:3911:C:H6     | 1.69                     | 0.57              |
| 49:S2:507:G:O6     | 71:SY:105:LYS:NZ   | 2.36                     | 0.57              |
| 49:S2:925:G:H1     | 49:S2:1017:U:H3    | 1.52                     | 0.57              |
| 49:S2:981:A:H2'    | 49:S2:982:G:C8     | 2.39                     | 0.57              |
| 52:SE:183:VAL:HG11 | 52:SE:220:THR:HG21 | 1.86                     | 0.57              |
| 6:B4:64:C:H2'      | 6:B4:65:C:H6       | 1.69                     | 0.57              |
| 8:L5:74:G:H5'      | 18:LL:59:VAL:HB    | 1.85                     | 0.57              |
| 8:L5:2520:C:H2'    | 8:L5:2521:G:H8     | 1.68                     | 0.57              |
| 14:LF:132:MET:O    | 14:LF:136:VAL:HG12 | 2.05                     | 0.57              |
| 30:LX:148:ASP:O    | 30:LX:152:LYS:NZ   | 2.34                     | 0.57              |
| 55:SH:44:ASN:OD1   | 55:SH:68:GLN:NE2   | 2.38                     | 0.57              |
| 57:SJ:71:LEU:O     | 57:SJ:75:ASN:ND2   | 2.33                     | 0.57              |
| 3:LB:217:ILE:HD12  | 3:LB:347:LEU:HB3   | 1.86                     | 0.57              |
| 8:L5:1332:C:H2'    | 8:L5:1333:A:H8     | 1.69                     | 0.57              |
| 20:LN:135:ILE:HG23 | 20:LN:142:ILE:HD13 | 1.86                     | 0.57              |
| 49:S2:1115:U:C2    | 49:S2:1118:C:N4    | 2.72                     | 0.57              |
| 54:SG:5:ILE:HG21   | 54:SG:124:LEU:HD21 | 1.86                     | 0.57              |
| 54:SG:162:LEU:HD12 | 54:SG:170:ARG:HG2  | 1.85                     | 0.57              |
| 1:LA:33:ASP:N      | 1:LA:33:ASP:OD1    | 2.36                     | 0.57              |
| 1:LA:51:ASP:HB2    | 1:LA:58:LEU:HD22   | 1.86                     | 0.57              |
| 1:LA:209:HIS:CE1   | 1:LA:235:VAL:HG11  | 2.40                     | 0.57              |
| 2:SA:85:ARG:HH21   | 2:SA:201:LEU:HD12  | 1.69                     | 0.57              |
| 4:SB:89:GLU:OE2    | 4:SB:220:LYS:NZ    | 2.36                     | 0.57              |
| 8:L5:442:G:OP1     | 37:Lf:68:ARG:NH1   | 2.37                     | 0.57              |
| 8:L5:4699:U:H1'    | 8:L5:4700:A:H5''   | 1.87                     | 0.57              |
| 38:Lg:94:ALA:O     | 38:Lg:98:GLU:HG2   | 2.05                     | 0.57              |
| 1:LA:37:ARG:NH2    | 8:L5:4088:C:OP1    | 2.37                     | 0.57              |
| 8:L5:407:A:O2'     | 8:L5:410:A:OP1     | 2.16                     | 0.57              |
| 22:LP:10:ASN:ND2   | 22:LP:13:LYS:HD2   | 2.20                     | 0.57              |
| 35:Lc:19:GLN:CD    | 35:Lc:20:LEU:H     | 2.13                     | 0.57              |
| 38:Lg:10:ARG:NH2   | 43:Ll:3:SER:OG     | 2.37                     | 0.57              |
| 49:S2:1497:G:O6    | 58:SK:25:LYS:NZ    | 2.38                     | 0.57              |
| 49:S2:1745:A:H8    | 54:SG:65:GLN:HG3   | 1.69                     | 0.57              |
| 51:SD:62:LYS:O     | 51:SD:67:ARG:NH2   | 2.35                     | 0.57              |
| 56:SI:65:PHE:O     | 56:SI:109:TYR:OH   | 2.21                     | 0.57              |
| 65:SS:98:VAL:HG11  | 65:SS:106:LYS:HG3  | 1.85                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:Sg:124:SER:OG   | 79:Sg:125:ARG:N    | 2.37                     | 0.57              |
| 8:L5:4594:U:H2'    | 8:L5:4595:G:C8     | 2.39                     | 0.57              |
| 19:LM:81:ASP:N     | 19:LM:81:ASP:OD1   | 2.36                     | 0.57              |
| 30:LX:145:ASP:O    | 30:LX:149:VAL:HG23 | 2.05                     | 0.57              |
| 48:Lr:28:GLU:OE2   | 48:Lr:41:ASN:ND2   | 2.36                     | 0.57              |
| 49:S2:367:U:H4'    | 49:S2:371:A:C8     | 2.39                     | 0.57              |
| 57:SJ:170:PRO:HB3  | 57:SJ:174:LYS:HD2  | 1.86                     | 0.57              |
| 36:Ld:68:LEU:HB3   | 36:Ld:108:TYR:HB2  | 1.86                     | 0.57              |
| 37:Lf:37:ASP:OD1   | 37:Lf:37:ASP:N     | 2.38                     | 0.57              |
| 49:S2:1126:G:OP2   | 64:SR:129:LYS:NZ   | 2.34                     | 0.57              |
| 49:S2:1543:U:OP1   | 63:SQ:37:ARG:NH1   | 2.38                     | 0.57              |
| 55:SH:148:LEU:HA   | 69:SW:42:MET:HE3   | 1.86                     | 0.57              |
| 55:SH:148:LEU:HD22 | 69:SW:49:GLU:HG3   | 1.87                     | 0.57              |
| 57:SJ:106:LEU:HD23 | 57:SJ:109:ARG:HD2  | 1.86                     | 0.57              |
| 73:Sa:2:THR:OG1    | 73:Sa:3:LYS:N      | 2.28                     | 0.57              |
| 2:SA:149:ASN:HB2   | 2:SA:165:ASN:HB2   | 1.87                     | 0.57              |
| 8:L5:2322:G:OP1    | 81:Le:36:ARG:NH2   | 2.38                     | 0.57              |
| 50:SC:194:ARG:HD3  | 50:SC:196:ILE:HD11 | 1.87                     | 0.57              |
| 5:A4:49:G:H1       | 7:D4:36:A:H2       | 1.52                     | 0.57              |
| 11:LC:12:SER:HA    | 11:LC:155:GLU:HG2  | 1.87                     | 0.57              |
| 19:LM:11:ARG:HB3   | 19:LM:27:ILE:HD12  | 1.86                     | 0.57              |
| 49:S2:1025:U:O3'   | 49:S2:1089:G:N2    | 2.37                     | 0.57              |
| 50:SC:116:THR:OG1  | 50:SC:119:GLY:O    | 2.21                     | 0.57              |
| 56:SI:177:SER:HB2  | 56:SI:186:ASP:HB2  | 1.86                     | 0.57              |
| 79:Sg:5:MET:HB2    | 79:Sg:270:LEU:HD21 | 1.86                     | 0.57              |
| 79:Sg:171:ASP:OD1  | 79:Sg:171:ASP:N    | 2.38                     | 0.57              |
| 8:L5:1969:G:H3'    | 8:L5:1970:A:H8     | 1.69                     | 0.56              |
| 20:LN:46:ASP:OD2   | 20:LN:50:ARG:NH2   | 2.37                     | 0.56              |
| 49:S2:1544:C:H2'   | 49:S2:1545:A:H5''  | 1.87                     | 0.56              |
| 51:SD:215:ASP:N    | 51:SD:215:ASP:OD1  | 2.37                     | 0.56              |
| 5:A4:49:G:H22      | 7:D4:36:A:H2       | 1.54                     | 0.56              |
| 8:L5:3710:G:H4'    | 8:L5:3711:A:H5'    | 1.87                     | 0.56              |
| 8:L5:4120:U:O2'    | 38:Lg:93:ARG:NH1   | 2.36                     | 0.56              |
| 8:L5:4260:U:H2'    | 8:L5:4261:C:C6     | 2.39                     | 0.56              |
| 8:L5:4763:U:O2'    | 25:LS:174:THR:OG1  | 2.22                     | 0.56              |
| 15:LG:143:VAL:HG21 | 15:LG:201:THR:HG22 | 1.87                     | 0.56              |
| 16:LH:180:TYR:HB2  | 44:Lm:85:LEU:HD21  | 1.85                     | 0.56              |
| 49:S2:600:G:H2'    | 49:S2:601:OMG:H5'' | 1.85                     | 0.56              |
| 1:LA:27:ALA:O      | 1:LA:128:ARG:NH2   | 2.38                     | 0.56              |
| 8:L5:66:A:O2'      | 8:L5:326:C:O2      | 2.20                     | 0.56              |
| 8:L5:662:C:H2'     | 8:L5:663:G:H8      | 1.69                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:691:C:H2'     | 8:L5:692:A:C8      | 2.41                     | 0.56              |
| 8:L5:2102:G:H1'    | 8:L5:2103:G:C8     | 2.39                     | 0.56              |
| 8:L5:2566:G:H2'    | 8:L5:2567:G:H8     | 1.70                     | 0.56              |
| 8:L5:4313:A:H4'    | 26:LT:71:ALA:HB3   | 1.87                     | 0.56              |
| 14:LF:171:ASP:OD1  | 14:LF:172:ASN:N    | 2.38                     | 0.56              |
| 19:LM:105:THR:OG1  | 19:LM:108:ASP:OD2  | 2.17                     | 0.56              |
| 38:Lg:67:LEU:O     | 38:Lg:72:LYS:NZ    | 2.39                     | 0.56              |
| 49:S2:223:C:H2'    | 49:S2:224:A:C8     | 2.39                     | 0.56              |
| 50:SC:209:VAL:HG13 | 50:SC:210:PRO:HD3  | 1.86                     | 0.56              |
| 54:SG:70:HIS:HB3   | 54:SG:101:ILE:HB   | 1.87                     | 0.56              |
| 64:SR:98:VAL:HG21  | 64:SR:117:LEU:HD22 | 1.86                     | 0.56              |
| 69:SW:51:GLU:OE1   | 74:Sb:8:LEU:HD21   | 2.05                     | 0.56              |
| 74:Sb:35:VAL:HG21  | 74:Sb:63:LEU:HD21  | 1.88                     | 0.56              |
| 8:L5:43:U:O2       | 46:Lo:44:LYS:NZ    | 2.37                     | 0.56              |
| 8:L5:2744:A:H2'    | 8:L5:2745:A:C8     | 2.40                     | 0.56              |
| 8:L5:2898:G:OP1    | 24:LR:104:ARG:NH1  | 2.37                     | 0.56              |
| 19:LM:5:ARG:NE     | 19:LM:59:ASP:OD1   | 2.34                     | 0.56              |
| 25:LS:2:LYS:HD3    | 25:LS:43:ARG:HD2   | 1.87                     | 0.56              |
| 61:SO:136:PRO:HB2  | 61:SO:139:SER:HB3  | 1.88                     | 0.56              |
| 77:Se:75:VAL:O     | 77:Se:76:HIS:ND1   | 2.38                     | 0.56              |
| 8:L5:2566:G:H2'    | 8:L5:2567:G:C8     | 2.41                     | 0.56              |
| 17:LJ:136:ARG:NH1  | 17:LJ:156:ARG:O    | 2.39                     | 0.56              |
| 30:LX:148:ASP:HB3  | 30:LX:152:LYS:NZ   | 2.19                     | 0.56              |
| 56:SI:46:VAL:HG22  | 56:SI:54:LYS:HB3   | 1.87                     | 0.56              |
| 34:Lb:36:ASP:HB3   | 34:Lb:39:PHE:HB3   | 1.88                     | 0.56              |
| 49:S2:604:A:N3     | 49:S2:639:C:O2'    | 2.36                     | 0.56              |
| 49:S2:1171:G:O2'   | 49:S2:1187:G:O6    | 2.23                     | 0.56              |
| 67:SU:81:GLN:NE2   | 76:Sd:56:ASP:OD2   | 2.38                     | 0.56              |
| 78:Sf:117:LEU:O    | 78:Sf:118:ARG:HD2  | 2.06                     | 0.56              |
| 78:Sf:119:ARG:HB3  | 78:Sf:132:MET:HG3  | 1.88                     | 0.56              |
| 82:LI:30:LYS:HD3   | 82:LI:63:GLU:HG3   | 1.87                     | 0.56              |
| 8:L5:2474:G:N2     | 8:L5:2502:G:O2'    | 2.39                     | 0.56              |
| 9:L7:26:C:O2'      | 17:LJ:147:ARG:NH1  | 2.38                     | 0.56              |
| 12:LD:257:PRO:N    | 12:LD:257:PRO:HG2  | 2.01                     | 0.56              |
| 21:LO:178:ARG:O    | 21:LO:182:GLU:HG3  | 2.05                     | 0.56              |
| 24:LR:136:ARG:O    | 24:LR:140:GLU:HG2  | 2.06                     | 0.56              |
| 26:LT:28:ALA:O     | 26:LT:32:ARG:HG2   | 2.06                     | 0.56              |
| 49:S2:96:C:H2'     | 49:S2:97:U:C6      | 2.41                     | 0.56              |
| 49:S2:959:G:OP2    | 61:SO:38:ASN:ND2   | 2.33                     | 0.56              |
| 1:LA:54:ARG:HG3    | 1:LA:56:ALA:H      | 1.70                     | 0.56              |
| 1:LA:108:PRO:O     | 1:LA:111:THR:OG1   | 2.16                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:297:U:O2'     | 20:LN:179:LYS:O    | 2.24                     | 0.56              |
| 8:L5:3811:G:O2'    | 8:L5:3814:U:OP2    | 2.24                     | 0.56              |
| 12:LD:62:CYS:HB3   | 12:LD:105:LEU:HD22 | 1.88                     | 0.56              |
| 20:LN:103:GLU:OE2  | 20:LN:118:SER:OG   | 2.20                     | 0.56              |
| 38:Lg:22:LEU:HD12  | 38:Lg:30:ILE:HG21  | 1.87                     | 0.56              |
| 49:S2:145:G:H2'    | 49:S2:146:G:C8     | 2.41                     | 0.56              |
| 51:SD:5:ILE:HD12   | 51:SD:9:ARG:HG2    | 1.88                     | 0.56              |
| 56:SI:136:ILE:HG13 | 56:SI:137:LEU:H    | 1.71                     | 0.56              |
| 71:SY:41:ARG:NH2   | 71:SY:52:PRO:O     | 2.39                     | 0.56              |
| 80:SM:52:LEU:HD12  | 80:SM:53:ALA:H     | 1.71                     | 0.56              |
| 8:L5:3614:G:O2'    | 8:L5:3615:G:OP1    | 2.15                     | 0.56              |
| 8:L5:4700:A:H2     | 16:LH:69:THR:HG22  | 1.69                     | 0.56              |
| 17:LJ:100:SER:HG   | 17:LJ:131:TYR:HH   | 1.47                     | 0.56              |
| 35:Lc:17:ARG:NH2   | 35:Lc:19:GLN:HE21  | 2.03                     | 0.56              |
| 49:S2:1648:G:N2    | 49:S2:1675:A:OP2   | 2.27                     | 0.56              |
| 70:SX:68:LYS:HB3   | 70:SX:91:LEU:HD22  | 1.88                     | 0.56              |
| 79:Sg:93:THR:HG23  | 79:Sg:94:THR:HG23  | 1.87                     | 0.56              |
| 8:L5:268:G:H2'     | 8:L5:269:G:H8      | 1.71                     | 0.56              |
| 8:L5:2573:A:H1'    | 32:LZ:112:ARG:HH22 | 1.69                     | 0.56              |
| 8:L5:4935:C:H2'    | 8:L5:4936:G:C8     | 2.41                     | 0.56              |
| 17:LJ:65:ASN:ND2   | 46:Lo:102:GLN:OE1  | 2.39                     | 0.56              |
| 8:L5:1210:C:O2'    | 8:L5:1211:G:O5'    | 2.20                     | 0.55              |
| 49:S2:1337:4AC:H2' | 49:S2:1338:G:H8    | 1.70                     | 0.55              |
| 49:S2:1568:C:O2    | 49:S2:1627:C:O2'   | 2.23                     | 0.55              |
| 8:L5:280:G:H5''    | 20:LN:14:LYS:HE2   | 1.88                     | 0.55              |
| 8:L5:2579:G:N2     | 8:L5:2582:A:OP2    | 2.30                     | 0.55              |
| 17:LJ:136:ARG:NH2  | 17:LJ:161:GLU:OE1  | 2.39                     | 0.55              |
| 27:LU:47:ILE:HD12  | 27:LU:63:ILE:HD11  | 1.88                     | 0.55              |
| 49:S2:373:G:OP1    | 59:SL:137:THR:OG1  | 2.19                     | 0.55              |
| 52:SE:221:ARG:HG3  | 52:SE:221:ARG:O    | 2.05                     | 0.55              |
| 56:SI:31:ARG:HH12  | 56:SI:48:VAL:HG12  | 1.70                     | 0.55              |
| 2:SA:85:ARG:HH12   | 2:SA:205:ARG:HD3   | 1.72                     | 0.55              |
| 2:SA:126:ASP:OD1   | 2:SA:165:ASN:ND2   | 2.38                     | 0.55              |
| 8:L5:497:G:H4'     | 8:L5:498:C:H5'     | 1.87                     | 0.55              |
| 8:L5:1324:A:O2'    | 8:L5:1326:A2M:OP1  | 2.23                     | 0.55              |
| 24:LR:90:PRO:HB2   | 24:LR:93:VAL:HG22  | 1.88                     | 0.55              |
| 49:S2:419:G:N2     | 49:S2:661:U:O2     | 2.40                     | 0.55              |
| 49:S2:1661:A:H8    | 76:Sd:14:PHE:HB2   | 1.71                     | 0.55              |
| 59:SL:99:TYR:O     | 59:SL:101:ARG:N    | 2.39                     | 0.55              |
| 8:L5:935:A:N1      | 19:LM:70:GLN:NE2   | 2.48                     | 0.55              |
| 8:L5:1320:U:O2'    | 8:L5:1891:A:N1     | 2.31                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:1523:A:N3     | 8:L5:4389:C:O2'    | 2.34                     | 0.55              |
| 8:L5:4250:G:OP1    | 17:LJ:98:ASN:ND2   | 2.39                     | 0.55              |
| 8:L5:4291:G:H5'    | 8:L5:4293:U:C6     | 2.40                     | 0.55              |
| 30:LX:155:ILE:HG13 | 30:LX:156:ILE:HG23 | 1.88                     | 0.55              |
| 49:S2:1446:A:H5''  | 67:SU:58:THR:HG23  | 1.88                     | 0.55              |
| 49:S2:1599:U:H5''  | 72:SZ:44:LEU:HD12  | 1.89                     | 0.55              |
| 54:SG:57:ASP:HB3   | 54:SG:98:ARG:HD2   | 1.87                     | 0.55              |
| 8:L5:194:C:O2      | 31:LY:121:ARG:NH1  | 2.39                     | 0.55              |
| 35:Lc:48:LEU:HD21  | 35:Lc:60:ILE:HG21  | 1.88                     | 0.55              |
| 37:Lf:39:THR:HG21  | 37:Lf:77:ALA:HB2   | 1.89                     | 0.55              |
| 49:S2:659:G:O2'    | 49:S2:662:G:O2'    | 2.21                     | 0.55              |
| 51:SD:172:VAL:HG13 | 51:SD:185:LYS:HG2  | 1.88                     | 0.55              |
| 8:L5:307:A:N3      | 8:L5:310:G:O2'     | 2.38                     | 0.55              |
| 8:L5:2033:A:O3'    | 25:LS:86:SER:OG    | 2.24                     | 0.55              |
| 8:L5:4238:G:H2'    | 8:L5:4239:A:C8     | 2.41                     | 0.55              |
| 8:L5:4279:A:H5'    | 8:L5:4281:A:H1'    | 1.89                     | 0.55              |
| 12:LD:256:LYS:C    | 12:LD:257:PRO:CG   | 2.75                     | 0.55              |
| 14:LF:220:MET:HE1  | 14:LF:223:LYS:HE3  | 1.88                     | 0.55              |
| 29:LW:56:ARG:HH21  | 29:LW:61:LYS:HB3   | 1.71                     | 0.55              |
| 52:SE:129:ILE:HD11 | 52:SE:139:LEU:HD12 | 1.88                     | 0.55              |
| 57:SJ:78:LEU:HD23  | 57:SJ:92:MET:HG3   | 1.87                     | 0.55              |
| 63:SQ:116:ASP:OD1  | 63:SQ:118:THR:OG1  | 2.21                     | 0.55              |
| 3:LB:252:ALA:HB1   | 8:L5:4524:G:C2     | 2.41                     | 0.55              |
| 8:L5:1563:A:N6     | 49:S2:1028:A:N1    | 2.55                     | 0.55              |
| 8:L5:4322:G:N2     | 8:L5:4325:A:OP2    | 2.33                     | 0.55              |
| 20:LN:38:ARG:HH21  | 20:LN:60:VAL:HG22  | 1.71                     | 0.55              |
| 28:LV:107:ASN:OD1  | 28:LV:108:ASN:N    | 2.40                     | 0.55              |
| 31:LY:44:VAL:HG21  | 31:LY:119:LEU:HD13 | 1.88                     | 0.55              |
| 49:S2:1091:C:OP1   | 60:SN:9:LYS:NZ     | 2.38                     | 0.55              |
| 72:SZ:79:ILE:HB    | 72:SZ:83:LEU:HD23  | 1.88                     | 0.55              |
| 3:LB:121:ASN:OD1   | 8:L5:4987:C:N4     | 2.40                     | 0.55              |
| 8:L5:210:C:OP1     | 31:LY:59:ARG:NH1   | 2.40                     | 0.55              |
| 12:LD:39:GLN:HE21  | 12:LD:46:THR:HB    | 1.71                     | 0.55              |
| 43:Ll:38:ASN:HB3   | 43:Ll:41:ARG:HG3   | 1.89                     | 0.55              |
| 49:S2:349:A:H2'    | 49:S2:350:C:C6     | 2.41                     | 0.55              |
| 49:S2:920:A:OP1    | 69:SW:57:ARG:NE    | 2.38                     | 0.55              |
| 55:SH:46:THR:HG23  | 55:SH:65:PRO:HD3   | 1.88                     | 0.55              |
| 69:SW:42:MET:HB2   | 69:SW:47:ILE:HG13  | 1.88                     | 0.55              |
| 8:L5:662:C:H2'     | 8:L5:663:G:C8      | 2.42                     | 0.55              |
| 8:L5:690:C:OP1     | 48:Lr:87:ARG:NH1   | 2.39                     | 0.55              |
| 49:S2:1124:C:O2'   | 64:SR:126:MET:O    | 2.24                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:130:SER:HB2   | 1:LA:171:GLY:HA3   | 1.88                     | 0.55              |
| 27:LU:63:ILE:O     | 27:LU:63:ILE:HG22  | 2.06                     | 0.55              |
| 49:S2:1218:C:H2'   | 49:S2:1219:C:H6    | 1.71                     | 0.55              |
| 73:Sa:23:CYS:HB2   | 73:Sa:74:CYS:H     | 1.72                     | 0.55              |
| 73:Sa:51:ARG:O     | 73:Sa:55:GLU:HG2   | 2.06                     | 0.55              |
| 4:SB:40:ASN:OD1    | 4:SB:41:ILE:HD13   | 2.06                     | 0.54              |
| 8:L5:17:A:OP1      | 39:Lh:84:ARG:NH2   | 2.28                     | 0.54              |
| 8:L5:92:C:OP1      | 86:L5:5286:SPD:N10 | 2.40                     | 0.54              |
| 8:L5:759:G:H22     | 8:L5:904:C:H2'     | 1.72                     | 0.54              |
| 8:L5:1942:A:H2'    | 8:L5:1943:A:H8     | 1.71                     | 0.54              |
| 16:LH:128:MET:HE1  | 16:LH:146:LEU:HD22 | 1.89                     | 0.54              |
| 49:S2:969:U:O2     | 49:S2:971:G:N1     | 2.40                     | 0.54              |
| 69:SW:90:GLN:OE1   | 69:SW:113:HIS:ND1  | 2.38                     | 0.54              |
| 8:L5:253:G:H2'     | 8:L5:254:G:C8      | 2.42                     | 0.54              |
| 8:L5:977:C:OP2     | 13:LE:59:ARG:NH1   | 2.40                     | 0.54              |
| 13:LE:287:VAL:O    | 19:LM:109:ARG:NH2  | 2.40                     | 0.54              |
| 17:LJ:17:ILE:HD12  | 17:LJ:80:GLU:CD    | 2.32                     | 0.54              |
| 27:LU:18:VAL:N     | 27:LU:75:GLU:OE1   | 2.41                     | 0.54              |
| 36:Ld:36:VAL:HG21  | 36:Ld:44:ARG:HG2   | 1.89                     | 0.54              |
| 50:SC:94:ILE:HG21  | 50:SC:162:ILE:HD12 | 1.89                     | 0.54              |
| 8:L5:490:C:H2'     | 8:L5:491:G:C8      | 2.41                     | 0.54              |
| 8:L5:1604:G:H2'    | 8:L5:1605:G:C8     | 2.43                     | 0.54              |
| 8:L5:1669:A:H4'    | 8:L5:1685:G:N2     | 2.22                     | 0.54              |
| 8:L5:5057:C:H2'    | 8:L5:5058:A:C8     | 2.42                     | 0.54              |
| 11:LC:154:VAL:HG11 | 11:LC:174:LEU:HD11 | 1.89                     | 0.54              |
| 22:LP:23:ARG:HG2   | 22:LP:125:MET:HE1  | 1.90                     | 0.54              |
| 35:Lc:17:ARG:NH1   | 35:Lc:107:SER:OG   | 2.39                     | 0.54              |
| 49:S2:29:G:H4'     | 70:SX:129:SER:HB2  | 1.89                     | 0.54              |
| 49:S2:520:A:O2'    | 49:S2:825:A:N3     | 2.39                     | 0.54              |
| 49:S2:1098:C:H2'   | 49:S2:1099:G:C8    | 2.43                     | 0.54              |
| 60:SN:40:LEU:HD12  | 60:SN:50:ILE:HG23  | 1.88                     | 0.54              |
| 8:L5:1359:G:N2     | 20:LN:204:ARG:OXT  | 2.39                     | 0.54              |
| 8:L5:2297:G:H4'    | 11:LC:242:PRO:HB2  | 1.89                     | 0.54              |
| 8:L5:2781:G:O2'    | 43:Ll:3:SER:O      | 2.25                     | 0.54              |
| 8:L5:4930:C:OP1    | 13:LE:266:GLN:NE2  | 2.39                     | 0.54              |
| 8:L5:5005:G:N2     | 8:L5:5041:G:O2'    | 2.41                     | 0.54              |
| 21:LO:12:ARG:O     | 25:LS:171:ARG:NH2  | 2.40                     | 0.54              |
| 23:LQ:99:LYS:HD2   | 23:LQ:119:LYS:HE2  | 1.89                     | 0.54              |
| 32:LZ:90:PRO:O     | 32:LZ:117:LYS:NZ   | 2.40                     | 0.54              |
| 49:S2:17:C:O2'     | 49:S2:1194:A:N1    | 2.34                     | 0.54              |
| 49:S2:509:G:H4'    | 52:SE:26:VAL:HG11  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1285:G:H3'   | 49:S2:1286:G:H5'   | 1.88                     | 0.54              |
| 49:S2:1546:G:H21   | 49:S2:1670:C:H1'   | 1.73                     | 0.54              |
| 54:SG:84:TYR:OH    | 54:SG:91:GLU:O     | 2.19                     | 0.54              |
| 75:Sc:13:ARG:NH2   | 75:Sc:35:MET:SD    | 2.81                     | 0.54              |
| 80:SM:47:ALA:O     | 80:SM:74:ILE:HD12  | 2.07                     | 0.54              |
| 1:LA:142:GLU:C     | 1:LA:144:LYS:H     | 2.15                     | 0.54              |
| 8:L5:223:G:OP2     | 11:LC:165:LYS:HE2  | 2.08                     | 0.54              |
| 8:L5:462:G:H2'     | 8:L5:463:A:H8      | 1.72                     | 0.54              |
| 8:L5:2573:A:H1'    | 32:LZ:112:ARG:NH2  | 2.22                     | 0.54              |
| 8:L5:4672:A:OP1    | 28:LV:15:ARG:NH2   | 2.40                     | 0.54              |
| 30:LX:152:LYS:HD3  | 30:LX:152:LYS:N    | 2.22                     | 0.54              |
| 49:S2:942:G:H2'    | 49:S2:943:U:C6     | 2.43                     | 0.54              |
| 8:L5:1092:G:H2'    | 8:L5:1093:C:C6     | 2.43                     | 0.54              |
| 8:L5:1244:G:H2'    | 8:L5:1245:C:H6     | 1.73                     | 0.54              |
| 8:L5:4913:G:H4'    | 8:L5:4914:C:O5'    | 2.07                     | 0.54              |
| 18:LL:125:ILE:HD11 | 39:Lh:122:LYS:HB2  | 1.89                     | 0.54              |
| 79:Sg:32:LEU:HG    | 79:Sg:71:ILE:HD11  | 1.89                     | 0.54              |
| 8:L5:2611:A:H2'    | 8:L5:2612:G:C8     | 2.42                     | 0.54              |
| 36:Ld:23:ARG:HG2   | 36:Ld:121:ASN:HA   | 1.90                     | 0.54              |
| 49:S2:126:G:C6     | 54:SG:196:LYS:HG2  | 2.43                     | 0.54              |
| 49:S2:307:G:H1'    | 56:SI:45:THR:HG22  | 1.90                     | 0.54              |
| 49:S2:526:A:OP1    | 77:Se:108:ARG:NH1  | 2.41                     | 0.54              |
| 50:SC:271:ASP:OD1  | 50:SC:271:ASP:N    | 2.40                     | 0.54              |
| 60:SN:57:SER:OG    | 60:SN:58:HIS:ND1   | 2.41                     | 0.54              |
| 78:Sf:128:ALA:HB3  | 80:SM:44:LYS:HZ1   | 1.72                     | 0.54              |
| 8:L5:2263:A:OP1    | 48:Lr:107:ARG:NH1  | 2.32                     | 0.54              |
| 8:L5:2303:C:OP1    | 81:Le:107:ASN:ND2  | 2.36                     | 0.54              |
| 16:LH:90:TYR:CE1   | 16:LH:184:LYS:HG2  | 2.43                     | 0.54              |
| 17:LJ:100:SER:OG   | 17:LJ:131:TYR:OH   | 2.20                     | 0.54              |
| 32:LZ:41:ALA:HB2   | 32:LZ:77:TYR:HE1   | 1.73                     | 0.54              |
| 37:Lf:59:THR:OG1   | 37:Lf:65:ASN:OD1   | 2.24                     | 0.54              |
| 49:S2:612:U:O2'    | 77:Se:84:LYS:NZ    | 2.40                     | 0.54              |
| 52:SE:45:ILE:HB    | 52:SE:80:ILE:HG23  | 1.90                     | 0.54              |
| 8:L5:4239:A:H2'    | 8:L5:4240:G:C8     | 2.43                     | 0.54              |
| 28:LV:126:ALA:HB2  | 28:LV:139:ILE:HD12 | 1.88                     | 0.54              |
| 49:S2:223:C:H2'    | 49:S2:224:A:H8     | 1.73                     | 0.54              |
| 49:S2:1446:A:H1'   | 67:SU:55:ARG:HD2   | 1.90                     | 0.54              |
| 52:SE:95:THR:HG23  | 71:SY:16:ARG:HH12  | 1.73                     | 0.54              |
| 56:SI:79:ILE:HG21  | 56:SI:170:LYS:HE2  | 1.90                     | 0.54              |
| 4:SB:97:LEU:CD2    | 4:SB:229:MET:HE1   | 2.39                     | 0.53              |
| 8:L5:500:G:N3      | 8:L5:504:G:O2'     | 2.37                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:1818:G:OP2    | 8:L5:1818:G:N2     | 2.32                     | 0.53              |
| 8:L5:1968:G:H2'    | 8:L5:1969:G:H8     | 1.72                     | 0.53              |
| 8:L5:2705:G:H22    | 8:L5:2710:C:H5     | 1.56                     | 0.53              |
| 8:L5:4537:C:H2'    | 8:L5:4538:G:C8     | 2.43                     | 0.53              |
| 14:LF:136:VAL:HG22 | 14:LF:136:VAL:O    | 2.07                     | 0.53              |
| 17:LJ:144:LYS:O    | 17:LJ:148:THR:OG1  | 2.26                     | 0.53              |
| 49:S2:67:C:OP2     | 54:SG:172:LYS:NZ   | 2.31                     | 0.53              |
| 49:S2:807:G:H2'    | 49:S2:808:A:H8     | 1.72                     | 0.53              |
| 49:S2:964:A:H2'    | 49:S2:965:U:H6     | 1.72                     | 0.53              |
| 52:SE:199:GLU:OE2  | 52:SE:209:HIS:NE2  | 2.41                     | 0.53              |
| 52:SE:210:VAL:HG13 | 52:SE:218:PHE:CE2  | 2.43                     | 0.53              |
| 67:SU:67:LYS:HG3   | 67:SU:67:LYS:O     | 2.08                     | 0.53              |
| 4:SB:97:LEU:HD21   | 4:SB:229:MET:HE1   | 1.89                     | 0.53              |
| 7:D4:63:G:H2'      | 7:D4:64:A:H8       | 1.73                     | 0.53              |
| 8:L5:1269:G:O2'    | 8:L5:1270:A:O4'    | 2.24                     | 0.53              |
| 8:L5:1426:G:N1     | 8:L5:1458:C:OP2    | 2.28                     | 0.53              |
| 8:L5:3717:A:H2'    | 8:L5:3718:A2M:C8   | 2.39                     | 0.53              |
| 8:L5:4373:G:N7     | 46:Lo:61:LYS:NZ    | 2.56                     | 0.53              |
| 8:L5:4954:G:H2'    | 8:L5:4955:A:C8     | 2.43                     | 0.53              |
| 15:LG:50:ASP:OD1   | 30:LX:40:ILE:HD12  | 2.08                     | 0.53              |
| 18:LL:79:GLU:HG2   | 18:LL:110:LEU:HD11 | 1.91                     | 0.53              |
| 38:Lg:22:LEU:HD12  | 38:Lg:30:ILE:CG2   | 2.38                     | 0.53              |
| 49:S2:847:A:OP1    | 52:SE:108:ARG:NH2  | 2.41                     | 0.53              |
| 51:SD:8:LYS:HB3    | 67:SU:61:LEU:HD21  | 1.90                     | 0.53              |
| 82:LI:51:HIS:CD2   | 82:LI:168:SER:HB2  | 2.42                     | 0.53              |
| 8:L5:661:C:H2'     | 8:L5:662:C:C6      | 2.43                     | 0.53              |
| 8:L5:1932:A:OP1    | 21:LO:49:ARG:NH2   | 2.41                     | 0.53              |
| 11:LC:4:ALA:O      | 11:LC:29:LYS:NZ    | 2.41                     | 0.53              |
| 12:LD:75:VAL:O     | 12:LD:112:ARG:NH1  | 2.42                     | 0.53              |
| 49:S2:377:G:H5'    | 56:SI:98:LYS:HB3   | 1.91                     | 0.53              |
| 49:S2:1114:U:H3    | 49:S2:1119:A:H61   | 1.56                     | 0.53              |
| 52:SE:31:PRO:HA    | 52:SE:81:THR:HB    | 1.90                     | 0.53              |
| 8:L5:2411:C:H2'    | 8:L5:2412:A:H8     | 1.73                     | 0.53              |
| 28:LV:45:ILE:HG21  | 28:LV:53:PRO:HB3   | 1.91                     | 0.53              |
| 32:LZ:5:MET:O      | 32:LZ:28:ASN:ND2   | 2.42                     | 0.53              |
| 36:Ld:57:MET:SD    | 36:Ld:90:ARG:HB2   | 2.49                     | 0.53              |
| 66:ST:28:LEU:HD13  | 66:ST:110:LEU:HD22 | 1.90                     | 0.53              |
| 71:SY:37:LYS:HA    | 71:SY:40:ILE:HD12  | 1.89                     | 0.53              |
| 8:L5:287:U:O2      | 20:LN:93:LYS:NZ    | 2.35                     | 0.53              |
| 8:L5:2588:C:H41    | 38:Lg:70:THR:HG21  | 1.72                     | 0.53              |
| 8:L5:4730:C:H2'    | 8:L5:4731:G:O4'    | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LL:107:THR:HB   | 40:Li:18:THR:HG23  | 1.90                     | 0.53              |
| 49:S2:142:C:N4     | 49:S2:330:G:OP2    | 2.31                     | 0.53              |
| 49:S2:306:C:OP2    | 56:SI:41:ARG:NH1   | 2.42                     | 0.53              |
| 52:SE:54:TYR:O     | 71:SY:15:ASN:ND2   | 2.42                     | 0.53              |
| 66:ST:108:GLU:OE2  | 66:ST:121:ARG:NE   | 2.21                     | 0.53              |
| 80:SM:56:CYS:SG    | 80:SM:62:VAL:HG12  | 2.48                     | 0.53              |
| 3:LB:214:ASP:HB3   | 3:LB:283:LYS:HZ2   | 1.74                     | 0.53              |
| 7:D4:8:U:H1'       | 7:D4:15:G:H1       | 1.74                     | 0.53              |
| 8:L5:67:C:OP2      | 8:L5:312:G:N2      | 2.37                     | 0.53              |
| 8:L5:690:C:H2'     | 8:L5:691:C:H6      | 1.73                     | 0.53              |
| 8:L5:1406:G:O6     | 8:L5:1408:G:O2'    | 2.22                     | 0.53              |
| 8:L5:2499:C:H2'    | 8:L5:2500:U:H6     | 1.72                     | 0.53              |
| 8:L5:2685:C:OP1    | 38:Lg:57:ARG:NH1   | 2.40                     | 0.53              |
| 8:L5:4344:U:H2'    | 8:L5:4345:C:C6     | 2.43                     | 0.53              |
| 21:LO:33:VAL:HG13  | 21:LO:102:LEU:HD12 | 1.90                     | 0.53              |
| 49:S2:659:G:HO2'   | 49:S2:662:G:HO2'   | 1.53                     | 0.53              |
| 49:S2:1130:G:OP2   | 49:S2:1130:G:N2    | 2.37                     | 0.53              |
| 55:SH:17:ASP:OD1   | 55:SH:17:ASP:N     | 2.40                     | 0.53              |
| 61:SO:121:ARG:HH12 | 75:Sc:62:GLU:HB2   | 1.74                     | 0.53              |
| 67:SU:17:ILE:HG12  | 67:SU:94:PRO:HB3   | 1.90                     | 0.53              |
| 8:L5:4874:A:O2'    | 25:LS:170:LYS:NZ   | 2.42                     | 0.53              |
| 9:L7:49:A:H5''     | 12:LD:224:SER:HB3  | 1.91                     | 0.53              |
| 24:LR:163:ARG:NH1  | 49:S2:873:G:OP1    | 2.42                     | 0.53              |
| 25:LS:24:THR:O     | 25:LS:24:THR:OG1   | 2.22                     | 0.53              |
| 49:S2:170:A:OP2    | 54:SG:140:ARG:NH1  | 2.41                     | 0.53              |
| 62:SP:31:GLU:O     | 62:SP:34:MET:HB2   | 2.09                     | 0.53              |
| 75:Sc:61:SER:O     | 75:Sc:62:GLU:HG2   | 2.07                     | 0.53              |
| 11:LC:140:LYS:HE2  | 11:LC:242:PRO:HD2  | 1.90                     | 0.53              |
| 19:LM:16:SER:OG    | 19:LM:54:CYS:O     | 2.27                     | 0.53              |
| 27:LU:33:ILE:HD11  | 27:LU:100:LEU:HD21 | 1.90                     | 0.53              |
| 35:Lc:17:ARG:NH1   | 35:Lc:107:SER:HB2  | 2.20                     | 0.53              |
| 46:Lo:33:LEU:HA    | 46:Lo:38:LYS:HG2   | 1.90                     | 0.53              |
| 49:S2:28:U:H2'     | 49:S2:29:G:H8      | 1.74                     | 0.53              |
| 54:SG:154:ARG:O    | 54:SG:155:GLN:HG2  | 2.09                     | 0.53              |
| 82:LI:200:ILE:HD12 | 82:LI:212:LEU:HD21 | 1.90                     | 0.53              |
| 8:L5:478:G:OP1     | 48:Lr:66:ARG:NH1   | 2.38                     | 0.53              |
| 8:L5:677:G:H2'     | 8:L5:678:C:H6      | 1.73                     | 0.53              |
| 8:L5:1749:A:H2'    | 8:L5:1750:G:C8     | 2.43                     | 0.53              |
| 10:L8:154:G:H3'    | 15:LG:89:ARG:HH22  | 1.73                     | 0.53              |
| 49:S2:952:G:H2'    | 49:S2:953:C:C6     | 2.43                     | 0.53              |
| 63:SQ:32:ILE:HG21  | 63:SQ:39:LEU:HD22  | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:ST:124:THR:HG23 | 66:ST:127:GLY:H    | 1.74                     | 0.53              |
| 75:Sc:21:THR:OG1   | 75:Sc:22:GLY:N     | 2.42                     | 0.53              |
| 79:Sg:218:LEU:HD21 | 79:Sg:228:TYR:CD1  | 2.43                     | 0.53              |
| 2:SA:81:ASN:HA     | 2:SA:84:GLN:NE2    | 2.23                     | 0.53              |
| 8:L5:1533:A:H5'    | 8:L5:1623:A:H61    | 1.73                     | 0.53              |
| 8:L5:2755:A:OP2    | 32:LZ:51:ARG:NH2   | 2.29                     | 0.53              |
| 8:L5:4093:G:H2'    | 8:L5:4094:G:H8     | 1.72                     | 0.53              |
| 10:L8:54:C:H2'     | 10:L8:55:PSU:C6    | 2.43                     | 0.53              |
| 16:LH:117:PHE:O    | 16:LH:120:GLU:HG3  | 2.08                     | 0.53              |
| 49:S2:1204:A:H62   | 49:S2:1694:U:H3    | 1.57                     | 0.53              |
| 50:SC:68:ARG:NH2   | 50:SC:72:ASP:OD1   | 2.42                     | 0.53              |
| 50:SC:78:LEU:HD11  | 50:SC:94:ILE:HD13  | 1.91                     | 0.53              |
| 52:SE:79:ASP:HB3   | 52:SE:82:TYR:HB2   | 1.91                     | 0.53              |
| 60:SN:130:LYS:NZ   | 60:SN:139:TRP:O    | 2.41                     | 0.53              |
| 80:SM:20:GLU:O     | 80:SM:24:THR:OG1   | 2.20                     | 0.53              |
| 3:LB:80:GLU:OE1    | 3:LB:323:TYR:OH    | 2.24                     | 0.52              |
| 8:L5:1933:G:H2'    | 8:L5:1934:A:C8     | 2.44                     | 0.52              |
| 8:L5:2520:C:H2'    | 8:L5:2521:G:C8     | 2.43                     | 0.52              |
| 18:LL:103:ARG:HH11 | 18:LL:105:LYS:HD2  | 1.73                     | 0.52              |
| 40:Li:73:ILE:O     | 40:Li:77:VAL:HG22  | 2.09                     | 0.52              |
| 49:S2:161:U:O2'    | 54:SG:87:ARG:NE    | 2.42                     | 0.52              |
| 49:S2:1077:A:OP1   | 60:SN:106:ARG:NH2  | 2.42                     | 0.52              |
| 55:SH:139:ILE:HG23 | 55:SH:156:VAL:HG13 | 1.90                     | 0.52              |
| 71:SY:102:THR:HG23 | 71:SY:107:ARG:HE   | 1.73                     | 0.52              |
| 2:SA:58:LEU:HD21   | 2:SA:177:MET:HB2   | 1.90                     | 0.52              |
| 3:LB:156:TYR:OH    | 8:L5:4912:G:N2     | 2.42                     | 0.52              |
| 8:L5:513:U:H3      | 8:L5:515:C:H3'     | 1.74                     | 0.52              |
| 8:L5:1970:A:H5'    | 8:L5:2000:G:N1     | 2.24                     | 0.52              |
| 8:L5:2623:A:OP1    | 27:LU:101:ARG:NH1  | 2.42                     | 0.52              |
| 11:LC:138:MET:HG3  | 48:Lr:43:LEU:HD13  | 1.91                     | 0.52              |
| 49:S2:1714:U:H2'   | 49:S2:1715:A:C8    | 2.45                     | 0.52              |
| 50:SC:188:CYS:SG   | 50:SC:238:LYS:HG3  | 2.49                     | 0.52              |
| 56:SI:177:SER:OG   | 56:SI:182:CYS:SG   | 2.67                     | 0.52              |
| 62:SP:68:PRO:HG2   | 62:SP:71:GLU:HB3   | 1.89                     | 0.52              |
| 4:SB:114:VAL:O     | 49:S2:1869:A:N6    | 2.42                     | 0.52              |
| 8:L5:1633:G:H5'    | 8:L5:1634:A:OP1    | 2.09                     | 0.52              |
| 61:SO:54:CYS:SG    | 61:SO:81:VAL:HG13  | 2.50                     | 0.52              |
| 78:Sf:128:ALA:HB3  | 80:SM:44:LYS:HZ2   | 1.74                     | 0.52              |
| 2:SA:199:PRO:HG2   | 2:SA:200:ASP:N     | 2.22                     | 0.52              |
| 3:LB:117:ARG:HG2   | 3:LB:180:LEU:HD12  | 1.91                     | 0.52              |
| 7:D4:63:G:H2'      | 7:D4:64:A:C8       | 2.45                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:382:G:N1      | 8:L5:385:A:OP2     | 2.37                     | 0.52              |
| 8:L5:2303:C:H5''   | 81:Le:104:SER:HB3  | 1.90                     | 0.52              |
| 8:L5:2539:C:H2'    | 8:L5:2540:C:C6     | 2.44                     | 0.52              |
| 8:L5:2611:A:H2'    | 8:L5:2612:G:H8     | 1.73                     | 0.52              |
| 8:L5:3868:G:H22    | 8:L5:3900:G:H1'    | 1.74                     | 0.52              |
| 16:LH:91:LYS:HB2   | 16:LH:183:GLU:HB2  | 1.90                     | 0.52              |
| 49:S2:107:A:H2'    | 49:S2:108:G:C8     | 2.44                     | 0.52              |
| 52:SE:228:ILE:HD11 | 52:SE:236:ILE:HD11 | 1.89                     | 0.52              |
| 71:SY:45:ALA:HB2   | 71:SY:52:PRO:HB3   | 1.92                     | 0.52              |
| 72:SZ:51:ASP:OD1   | 72:SZ:51:ASP:N     | 2.33                     | 0.52              |
| 49:S2:106:C:H2'    | 49:S2:107:A:H8     | 1.73                     | 0.52              |
| 49:S2:368:U:OP1    | 49:S2:369:C:O2'    | 2.28                     | 0.52              |
| 49:S2:433:A:H2'    | 49:S2:434:G:C8     | 2.45                     | 0.52              |
| 49:S2:1013:U:OP1   | 49:S2:1129:G:O2'   | 2.27                     | 0.52              |
| 49:S2:1617:G:N1    | 49:S2:1620:A:OP2   | 2.43                     | 0.52              |
| 57:SJ:32:ILE:HG22  | 57:SJ:37:LEU:HD12  | 1.92                     | 0.52              |
| 66:ST:60:THR:HG23  | 66:ST:75:MET:HE2   | 1.92                     | 0.52              |
| 74:Sb:34:ASP:HB3   | 74:Sb:82:LYS:HE2   | 1.91                     | 0.52              |
| 11:LC:33:ARG:NH2   | 11:LC:35:ASP:OD2   | 2.38                     | 0.52              |
| 28:LV:117:ILE:HB   | 28:LV:136:ALA:HA   | 1.92                     | 0.52              |
| 31:LY:4:ASN:HB3    | 31:LY:7:VAL:HG22   | 1.92                     | 0.52              |
| 49:S2:1256:G:H8    | 67:SU:66:ARG:HB2   | 1.74                     | 0.52              |
| 49:S2:1614:A:H2'   | 49:S2:1615:U:H6    | 1.74                     | 0.52              |
| 65:SS:24:ARG:HB2   | 65:SS:29:ALA:HB2   | 1.91                     | 0.52              |
| 65:SS:108:ARG:NH2  | 65:SS:109:GLU:OE2  | 2.43                     | 0.52              |
| 78:Sf:135:HIS:HB2  | 78:Sf:138:ARG:HG2  | 1.91                     | 0.52              |
| 5:A4:51:U:O2'      | 5:A4:52:U:O2       | 2.24                     | 0.52              |
| 7:D4:53:G:H2'      | 7:D4:54:U:C5       | 2.44                     | 0.52              |
| 19:LM:13:ALA:HB1   | 19:LM:55:MET:HB2   | 1.91                     | 0.52              |
| 48:Lr:90:LEU:HG    | 48:Lr:111:ILE:HG23 | 1.90                     | 0.52              |
| 49:S2:1109:C:O2'   | 49:S2:1110:G:H8    | 1.93                     | 0.52              |
| 49:S2:1360:U:O2'   | 49:S2:1379:A:OP2   | 2.28                     | 0.52              |
| 55:SH:23:ILE:HD13  | 55:SH:87:PHE:HE2   | 1.75                     | 0.52              |
| 60:SN:119:GLU:O    | 60:SN:123:HIS:ND1  | 2.42                     | 0.52              |
| 8:L5:420:A:H62     | 10:L8:14:OMU:H5    | 1.74                     | 0.52              |
| 8:L5:666:G:O6      | 8:L5:668:C:N4      | 2.43                     | 0.52              |
| 8:L5:4992:G:H2'    | 8:L5:4993:G:H8     | 1.71                     | 0.52              |
| 9:L7:12:U:OP2      | 9:L7:67:C:O2'      | 2.26                     | 0.52              |
| 14:LF:171:ASP:OD1  | 14:LF:173:ALA:N    | 2.32                     | 0.52              |
| 16:LH:112:VAL:HB   | 16:LH:126:VAL:HG22 | 1.91                     | 0.52              |
| 20:LN:17:ASP:N     | 20:LN:17:ASP:OD1   | 2.41                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:LV:87:SER:HA    | 28:LV:97:TYR:HB3   | 1.92                     | 0.52              |
| 63:SQ:12:VAL:HG11  | 63:SQ:90:LYS:HB3   | 1.91                     | 0.52              |
| 78:Sf:118:ARG:HB3  | 78:Sf:131:PHE:HB3  | 1.91                     | 0.52              |
| 1:LA:116:LEU:HD12  | 1:LA:117:GLU:H     | 1.75                     | 0.52              |
| 7:D4:4:C:H2'       | 7:D4:5:G:H8        | 1.74                     | 0.52              |
| 12:LD:278:ASP:O    | 12:LD:282:GLN:HG3  | 2.09                     | 0.52              |
| 15:LG:182:CYS:HB2  | 15:LG:222:ILE:HD13 | 1.91                     | 0.52              |
| 33:La:84:GLU:O     | 33:La:88:VAL:HG13  | 2.10                     | 0.52              |
| 49:S2:554:A:H2'    | 49:S2:555:A:C5     | 2.45                     | 0.52              |
| 60:SN:34:LYS:HG2   | 60:SN:74:ILE:HD13  | 1.92                     | 0.52              |
| 65:SS:48:ALA:HB2   | 65:SS:70:ILE:HD12  | 1.91                     | 0.52              |
| 8:L5:737:C:C6      | 8:L5:739:G:H5''    | 2.45                     | 0.52              |
| 20:LN:38:ARG:NH2   | 20:LN:60:VAL:HG22  | 2.25                     | 0.52              |
| 22:LP:103:GLU:HG3  | 22:LP:109:VAL:HG21 | 1.92                     | 0.52              |
| 49:S2:370:G:O2'    | 56:SI:10:LYS:NZ    | 2.43                     | 0.52              |
| 49:S2:586:G:OP1    | 57:SJ:176:LYS:NZ   | 2.37                     | 0.52              |
| 49:S2:1531:A:H4'   | 49:S2:1605:G:H4'   | 1.92                     | 0.52              |
| 57:SJ:78:LEU:HD11  | 57:SJ:94:LEU:HB3   | 1.92                     | 0.52              |
| 3:LB:107:ALA:HB1   | 3:LB:202:GLU:HG3   | 1.92                     | 0.51              |
| 4:SB:124:HIS:HA    | 4:SB:137:LEU:O     | 2.09                     | 0.51              |
| 8:L5:2823:G:N7     | 24:LR:20:LYS:HD2   | 2.25                     | 0.51              |
| 8:L5:4173:G:H2'    | 8:L5:4174:U:C6     | 2.45                     | 0.51              |
| 21:LO:181:ALA:O    | 21:LO:185:VAL:HG22 | 2.10                     | 0.51              |
| 23:LQ:178:ARG:NH2  | 33:La:46:ASP:OD2   | 2.42                     | 0.51              |
| 27:LU:107:LYS:HE2  | 27:LU:108:GLU:HG2  | 1.91                     | 0.51              |
| 49:S2:1549:U:OP2   | 51:SD:8:LYS:NZ     | 2.43                     | 0.51              |
| 52:SE:44:LEU:HD12  | 52:SE:72:ILE:HD11  | 1.92                     | 0.51              |
| 55:SH:157:HIS:HB3  | 55:SH:190:PRO:HG3  | 1.92                     | 0.51              |
| 8:L5:325:U:H2'     | 8:L5:326:C:C6      | 2.46                     | 0.51              |
| 8:L5:4935:C:H2'    | 8:L5:4936:G:H8     | 1.76                     | 0.51              |
| 11:LC:328:LEU:HD22 | 14:LF:187:MET:HG3  | 1.93                     | 0.51              |
| 12:LD:152:ARG:O    | 12:LD:157:ASN:ND2  | 2.43                     | 0.51              |
| 18:LL:146:LEU:O    | 18:LL:148:THR:OG1  | 2.23                     | 0.51              |
| 20:LN:159:ARG:HB2  | 20:LN:164:LEU:HB2  | 1.92                     | 0.51              |
| 28:LV:104:VAL:HG11 | 28:LV:117:ILE:HD11 | 1.93                     | 0.51              |
| 35:Lc:38:ILE:HD11  | 35:Lc:46:VAL:HG21  | 1.93                     | 0.51              |
| 49:S2:1533:A:H2    | 49:S2:1536:G:N3    | 2.07                     | 0.51              |
| 49:S2:1658:G:OP2   | 49:S2:1660:C:N4    | 2.42                     | 0.51              |
| 52:SE:133:THR:HG22 | 52:SE:134:LYS:HG3  | 1.91                     | 0.51              |
| 54:SG:120:ASP:O    | 54:SG:125:THR:OG1  | 2.27                     | 0.51              |
| 80:SM:80:ASP:OD1   | 80:SM:80:ASP:N     | 2.38                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:SB:109:LYS:O     | 4:SB:113:MET:HG2   | 2.10                     | 0.51              |
| 8:L5:1283:G:N1     | 8:L5:2076:G:OP1    | 2.37                     | 0.51              |
| 8:L5:4139:G:H21    | 8:L5:4140:C:H41    | 1.58                     | 0.51              |
| 15:LG:193:LEU:HD12 | 15:LG:194:VAL:HG13 | 1.91                     | 0.51              |
| 28:LV:97:TYR:OH    | 29:LW:37:GLU:OE2   | 2.15                     | 0.51              |
| 56:SI:117:TYR:HD1  | 56:SI:152:ARG:HB3  | 1.75                     | 0.51              |
| 8:L5:139:G:H2'     | 8:L5:140:G:H8      | 1.75                     | 0.51              |
| 8:L5:1967:A:H61    | 8:L5:2020:U:H3     | 1.59                     | 0.51              |
| 25:LS:164:LYS:HB3  | 25:LS:165:PRO:HD3  | 1.91                     | 0.51              |
| 30:LX:73:HIS:CD2   | 30:LX:115:LYS:HG2  | 2.46                     | 0.51              |
| 36:Ld:85:ARG:HD3   | 36:Ld:111:VAL:HG21 | 1.90                     | 0.51              |
| 49:S2:526:A:N6     | 49:S2:588:G:H22    | 2.08                     | 0.51              |
| 49:S2:855:G:HO2'   | 49:S2:856:C:P      | 2.34                     | 0.51              |
| 63:SQ:40:GLU:OE1   | 63:SQ:40:GLU:N     | 2.43                     | 0.51              |
| 72:SZ:65:TYR:OH    | 72:SZ:76:ARG:HD3   | 2.10                     | 0.51              |
| 3:LB:45:ALA:HB3    | 3:LB:183:ILE:HG23  | 1.93                     | 0.51              |
| 48:Lr:65:LYS:O     | 48:Lr:102:TYR:OH   | 2.26                     | 0.51              |
| 49:S2:96:C:H1'     | 49:S2:474:G:H5'    | 1.92                     | 0.51              |
| 49:S2:855:G:O2'    | 49:S2:856:C:O5'    | 2.29                     | 0.51              |
| 49:S2:928:G:H1     | 49:S2:1013:U:H3    | 1.58                     | 0.51              |
| 54:SG:33:ALA:N     | 54:SG:52:ILE:O     | 2.41                     | 0.51              |
| 57:SJ:160:SER:O    | 57:SJ:163:SER:OG   | 2.29                     | 0.51              |
| 65:SS:13:LEU:HB2   | 65:SS:20:ILE:HG12  | 1.91                     | 0.51              |
| 65:SS:15:VAL:HG12  | 65:SS:68:ILE:HD11  | 1.92                     | 0.51              |
| 71:SY:12:PHE:HD1   | 71:SY:23:MET:HG2   | 1.75                     | 0.51              |
| 81:Le:38:PRO:HB2   | 81:Le:46:ARG:HB3   | 1.91                     | 0.51              |
| 1:LA:183:GLY:HA2   | 8:L5:1613:A:H5''   | 1.92                     | 0.51              |
| 8:L5:138:G:H2'     | 8:L5:139:G:H8      | 1.75                     | 0.51              |
| 8:L5:267:G:H2'     | 8:L5:268:G:H8      | 1.76                     | 0.51              |
| 8:L5:978:G:H2'     | 8:L5:979:C:H6      | 1.75                     | 0.51              |
| 8:L5:2526:C:N4     | 30:LX:84:GLU:OE2   | 2.43                     | 0.51              |
| 18:LL:42:LYS:O     | 18:LL:46:ILE:HG12  | 2.09                     | 0.51              |
| 19:LM:92:ALA:HA    | 19:LM:95:ILE:HG12  | 1.91                     | 0.51              |
| 49:S2:562:U:O4'    | 57:SJ:132:GLN:NE2  | 2.44                     | 0.51              |
| 56:SI:86:SER:O     | 56:SI:88:ASN:N     | 2.42                     | 0.51              |
| 8:L5:1217:G:H2'    | 8:L5:1218:G:O4'    | 2.10                     | 0.51              |
| 8:L5:1873:A:OP2    | 34:Lb:5:LYS:NZ     | 2.38                     | 0.51              |
| 8:L5:2765:A:H2'    | 8:L5:2766:A:C8     | 2.46                     | 0.51              |
| 8:L5:2899:C:OP1    | 24:LR:108:ARG:NH2  | 2.43                     | 0.51              |
| 49:S2:443:U:H3     | 49:S2:447:A:H62    | 1.57                     | 0.51              |
| 52:SE:246:LEU:HB2  | 52:SE:250:GLU:HB2  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:SM:31:LEU:HB2   | 80:SM:110:VAL:O    | 2.11                     | 0.51              |
| 80:SM:89:VAL:HG13  | 80:SM:91:LEU:HD13  | 1.92                     | 0.51              |
| 4:SB:127:VAL:HG11  | 4:SB:176:VAL:HG11  | 1.93                     | 0.51              |
| 8:L5:1198:G:H2'    | 8:L5:1199:G:C8     | 2.45                     | 0.51              |
| 8:L5:2704:C:H2'    | 8:L5:2705:G:H8     | 1.75                     | 0.51              |
| 30:LX:81:LEU:HD22  | 30:LX:97:VAL:HG11  | 1.92                     | 0.51              |
| 38:Lg:78:TYR:HB3   | 38:Lg:82:MET:HB2   | 1.92                     | 0.51              |
| 49:S2:1713:C:H2'   | 49:S2:1714:U:C6    | 2.46                     | 0.51              |
| 53:SF:113:VAL:O    | 53:SF:117:ILE:HG23 | 2.11                     | 0.51              |
| 67:SU:44:LYS:C     | 67:SU:46:LYS:H     | 2.19                     | 0.51              |
| 80:SM:32:ALA:HB1   | 80:SM:37:GLU:HB3   | 1.92                     | 0.51              |
| 3:LB:357:ARG:HD2   | 8:L5:4615:C:H5''   | 1.91                     | 0.51              |
| 8:L5:1241:C:O2     | 34:Lb:115:GLY:HA2  | 2.10                     | 0.51              |
| 8:L5:1739:G:N3     | 8:L5:1742:A:N6     | 2.59                     | 0.51              |
| 8:L5:1877:G:O6     | 34:Lb:10:HIS:NE2   | 2.36                     | 0.51              |
| 8:L5:2570:U:H2'    | 8:L5:2571:C:C6     | 2.46                     | 0.51              |
| 16:LH:74:CYS:O     | 16:LH:78:GLN:HG3   | 2.10                     | 0.51              |
| 49:S2:1298:G:H5''  | 62:SP:77:LYS:HB2   | 1.92                     | 0.51              |
| 56:SI:136:ILE:C    | 56:SI:138:ASN:H    | 2.19                     | 0.51              |
| 74:Sb:67:THR:HG22  | 74:Sb:68:GLY:H     | 1.76                     | 0.51              |
| 8:L5:1198:G:H2'    | 8:L5:1199:G:H8     | 1.74                     | 0.51              |
| 8:L5:1290:G:H5''   | 13:LE:219:LYS:HD2  | 1.93                     | 0.51              |
| 8:L5:1521:C:H5'    | 11:LC:95:MET:HE1   | 1.92                     | 0.51              |
| 8:L5:3736:A:O2'    | 8:L5:3737:A:C8     | 2.63                     | 0.51              |
| 8:L5:4174:U:H2'    | 8:L5:4175:G:H8     | 1.75                     | 0.51              |
| 25:LS:29:ARG:HB2   | 26:LT:148:PRO:HB2  | 1.93                     | 0.51              |
| 27:LU:26:THR:O     | 27:LU:30:GLU:HG2   | 2.11                     | 0.51              |
| 49:S2:919:A:OP2    | 60:SN:64:ARG:NH1   | 2.42                     | 0.51              |
| 49:S2:924:G:H21    | 60:SN:87:ASP:CG    | 2.19                     | 0.51              |
| 49:S2:1653:U:H2'   | 49:S2:1654:G:C8    | 2.45                     | 0.51              |
| 3:LB:385:LYS:NZ    | 8:L5:5002:U:OP2    | 2.44                     | 0.50              |
| 8:L5:162:A:H2'     | 8:L5:163:A:C8      | 2.46                     | 0.50              |
| 8:L5:1920:C:H3'    | 8:L5:1921:C:H5''   | 1.92                     | 0.50              |
| 8:L5:4459:U:H2'    | 8:L5:4460:U:C6     | 2.46                     | 0.50              |
| 8:L5:4736:C:H2'    | 8:L5:4737:G:H8     | 1.77                     | 0.50              |
| 23:LQ:79:THR:HB    | 23:LQ:136:THR:HG22 | 1.92                     | 0.50              |
| 52:SE:191:ARG:HH11 | 52:SE:245:ARG:HE   | 1.59                     | 0.50              |
| 71:SY:15:ASN:ND2   | 71:SY:22:GLN:OE1   | 2.43                     | 0.50              |
| 8:L5:1961:G:H21    | 8:L5:2025:A:H62    | 1.58                     | 0.50              |
| 8:L5:3641:U:H5     | 8:L5:3646:A:N7     | 2.09                     | 0.50              |
| 8:L5:4344:U:O2'    | 46:Lo:28:LYS:O     | 2.21                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L8:102:G:OP2    | 10:L8:104:A:O2'    | 2.27                     | 0.50              |
| 17:LJ:22:LEU:HA    | 17:LJ:130:PHE:HB3  | 1.93                     | 0.50              |
| 44:Lm:94:MET:C     | 44:Lm:95:ILE:HD13  | 2.37                     | 0.50              |
| 49:S2:1217:A:H2'   | 49:S2:1218:C:C6    | 2.46                     | 0.50              |
| 49:S2:1286:G:H8    | 49:S2:1286:G:OP2   | 1.95                     | 0.50              |
| 49:S2:1628:C:H2'   | 49:S2:1629:C:C6    | 2.46                     | 0.50              |
| 69:SW:86:LEU:HD21  | 69:SW:113:HIS:HB2  | 1.92                     | 0.50              |
| 2:SA:56:GLU:HG2    | 68:SV:79:VAL:HG13  | 1.93                     | 0.50              |
| 6:B4:18:G:N3       | 6:B4:56:G:N2       | 2.59                     | 0.50              |
| 7:D4:5:G:O2'       | 7:D4:6:G:H5'       | 2.12                     | 0.50              |
| 7:D4:8:U:O2'       | 7:D4:15:G:N2       | 2.44                     | 0.50              |
| 8:L5:1328:G:O2'    | 8:L5:2349:A:OP1    | 2.28                     | 0.50              |
| 31:LY:82:ILE:HG22  | 31:LY:83:GLU:H     | 1.76                     | 0.50              |
| 49:S2:57:U:OP1     | 49:S2:504:G:O2'    | 2.29                     | 0.50              |
| 49:S2:60:A:N3      | 49:S2:316:G:O2'    | 2.36                     | 0.50              |
| 52:SE:136:ILE:HG23 | 52:SE:149:TYR:CZ   | 2.46                     | 0.50              |
| 8:L5:258:G:H2'     | 8:L5:259:C:H6      | 1.76                     | 0.50              |
| 8:L5:3600:G:H2'    | 8:L5:3601:C:C6     | 2.45                     | 0.50              |
| 19:LM:43:THR:O     | 19:LM:43:THR:HG22  | 2.11                     | 0.50              |
| 47:Lp:27:LYS:O     | 47:Lp:31:ILE:HG23  | 2.12                     | 0.50              |
| 49:S2:1863:A:OP2   | 73:Sa:4:LYS:NZ     | 2.43                     | 0.50              |
| 50:SC:125:LYS:HB3  | 50:SC:143:CYS:HB2  | 1.93                     | 0.50              |
| 52:SE:247:THR:HG23 | 52:SE:249:ALA:H    | 1.76                     | 0.50              |
| 57:SJ:83:ARG:HG2   | 57:SJ:150:ARG:HD2  | 1.94                     | 0.50              |
| 7:D4:51:U:O2       | 7:D4:63:G:N2       | 2.30                     | 0.50              |
| 8:L5:352:G:C8      | 11:LC:193:LYS:HD3  | 2.47                     | 0.50              |
| 8:L5:433:A:C2      | 8:L5:3867:A:H4'    | 2.46                     | 0.50              |
| 8:L5:3923:A:H2'    | 8:L5:3924:C:C6     | 2.46                     | 0.50              |
| 49:S2:571:U:O2'    | 71:SY:60:PHE:O     | 2.27                     | 0.50              |
| 49:S2:846:G:OP2    | 52:SE:108:ARG:NH1  | 2.35                     | 0.50              |
| 49:S2:1253:A:OP2   | 49:S2:1526:G:N2    | 2.32                     | 0.50              |
| 49:S2:1345:G:OP1   | 49:S2:1688:C:O2'   | 2.28                     | 0.50              |
| 52:SE:11:ARG:NH1   | 52:SE:20:LEU:HB3   | 2.27                     | 0.50              |
| 55:SH:49:LYS:HG3   | 55:SH:63:PHE:HE1   | 1.75                     | 0.50              |
| 56:SI:103:LEU:HG   | 56:SI:170:LYS:HB3  | 1.92                     | 0.50              |
| 64:SR:14:ARG:HG2   | 64:SR:69:ILE:HG13  | 1.93                     | 0.50              |
| 4:SB:107:ARG:NH1   | 61:SO:135:ILE:HD12 | 2.25                     | 0.50              |
| 7:D4:8:U:H1'       | 7:D4:15:G:N1       | 2.26                     | 0.50              |
| 8:L5:2362:U:H2'    | 8:L5:2363:A2M:H8   | 1.93                     | 0.50              |
| 8:L5:2563:C:H2'    | 8:L5:2564:G:O4'    | 2.11                     | 0.50              |
| 16:LH:44:GLU:CG    | 16:LH:58:ASP:HB2   | 2.41                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LL:116:ARG:NH2  | 18:LL:155:MET:O    | 2.39                     | 0.50              |
| 20:LN:107:GLY:HA3  | 20:LN:160:GLU:OE1  | 2.12                     | 0.50              |
| 49:S2:525:A:OP2    | 77:Se:99:LYS:NZ    | 2.30                     | 0.50              |
| 2:SA:34:MET:HE2    | 2:SA:149:ASN:O     | 2.12                     | 0.50              |
| 8:L5:1690:C:OP2    | 23:LQ:11:ARG:NH2   | 2.39                     | 0.50              |
| 11:LC:14:LYS:N     | 11:LC:14:LYS:HD3   | 2.27                     | 0.50              |
| 35:Lc:17:ARG:HD2   | 35:Lc:108:MET:CE   | 2.39                     | 0.50              |
| 49:S2:1232:U:H2'   | 49:S2:1233:G:H8    | 1.77                     | 0.50              |
| 49:S2:1664:A:O2'   | 49:S2:1665:G:OP1   | 2.21                     | 0.50              |
| 49:S2:1736:G:H2'   | 49:S2:1737:G:H8    | 1.76                     | 0.50              |
| 49:S2:1865:C:OP2   | 73:Sa:5:ARG:NH1    | 2.45                     | 0.50              |
| 52:SE:70:ILE:HD11  | 52:SE:90:ILE:HG22  | 1.94                     | 0.50              |
| 82:LI:189:ARG:NH1  | 82:LI:199:TYR:OH   | 2.45                     | 0.50              |
| 3:LB:59:GLU:HG3    | 3:LB:366:LYS:HD2   | 1.94                     | 0.50              |
| 4:SB:157:GLN:HB2   | 4:SB:160:GLN:HG3   | 1.94                     | 0.50              |
| 8:L5:172:C:H4'     | 8:L5:173:C:H5'     | 1.94                     | 0.50              |
| 8:L5:256:G:H2'     | 8:L5:257:C:C6      | 2.47                     | 0.50              |
| 8:L5:1249:C:H2'    | 8:L5:1250:C:H6     | 1.77                     | 0.50              |
| 8:L5:1504:G:H2'    | 8:L5:1505:C:C6     | 2.46                     | 0.50              |
| 8:L5:4862:G:H2'    | 8:L5:4863:G:C8     | 2.47                     | 0.50              |
| 17:LJ:39:VAL:HG21  | 17:LJ:112:HIS:CD2  | 2.46                     | 0.50              |
| 30:LX:55:ARG:HH11  | 30:LX:55:ARG:HG3   | 1.76                     | 0.50              |
| 39:Lh:88:THR:OG1   | 39:Lh:91:MET:HG2   | 2.12                     | 0.50              |
| 48:Lr:54:ALA:HA    | 48:Lr:61:VAL:HG23  | 1.92                     | 0.50              |
| 49:S2:1395:C:HO2'  | 49:S2:1396:A:C5'   | 2.25                     | 0.50              |
| 50:SC:66:LEU:HD11  | 50:SC:81:ILE:HG12  | 1.94                     | 0.50              |
| 61:SO:34:PHE:HB3   | 61:SO:41:PHE:HB2   | 1.93                     | 0.50              |
| 64:SR:120:THR:HG22 | 64:SR:121:GLN:N    | 2.23                     | 0.50              |
| 79:Sg:64:HIS:HD2   | 79:Sg:83:TRP:HB3   | 1.77                     | 0.50              |
| 79:Sg:304:ASP:O    | 79:Sg:306:LEU:N    | 2.44                     | 0.50              |
| 1:LA:13:GLY:O      | 1:LA:17:ARG:NH1    | 2.45                     | 0.50              |
| 1:LA:177:LYS:HD2   | 47:Lp:29:ILE:HG21  | 1.93                     | 0.50              |
| 8:L5:1731:C:OP1    | 26:LT:100:LYS:NZ   | 2.37                     | 0.50              |
| 12:LD:99:TYR:CD2   | 12:LD:199:ILE:HD13 | 2.47                     | 0.50              |
| 35:Lc:17:ARG:CD    | 35:Lc:108:MET:HE1  | 2.39                     | 0.50              |
| 49:S2:118:C:H1'    | 49:S2:445:A:C5     | 2.47                     | 0.50              |
| 49:S2:311:C:H5'    | 49:S2:312:G:H5''   | 1.94                     | 0.50              |
| 51:SD:122:VAL:O    | 51:SD:126:ILE:HG23 | 2.11                     | 0.50              |
| 59:SL:77:VAL:HG23  | 59:SL:122:ILE:HA   | 1.94                     | 0.50              |
| 62:SP:17:TYR:HB3   | 62:SP:25:LEU:HD11  | 1.93                     | 0.50              |
| 82:LI:85:PHE:HD2   | 82:LI:87:ILE:HG13  | 1.75                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:LB:77:THR:HG21   | 3:LB:337:VAL:HG13  | 1.94                     | 0.49              |
| 8:L5:263:G:N1      | 8:L5:264:C:O2      | 2.45                     | 0.49              |
| 8:L5:3652:A:H2'    | 8:L5:3653:A:C8     | 2.47                     | 0.49              |
| 49:S2:12:U:H2'     | 49:S2:13:C:C6      | 2.46                     | 0.49              |
| 52:SE:126:VAL:HA   | 52:SE:141:THR:HA   | 1.94                     | 0.49              |
| 75:Sc:17:VAL:HG22  | 75:Sc:30:VAL:HG12  | 1.94                     | 0.49              |
| 78:Sf:135:HIS:HB3  | 78:Sf:138:ARG:NH1  | 2.27                     | 0.49              |
| 8:L5:978:G:H2'     | 8:L5:979:C:C6      | 2.47                     | 0.49              |
| 8:L5:2614:C:O2'    | 8:L5:2808:G:OP1    | 2.26                     | 0.49              |
| 8:L5:4504:C:H2'    | 8:L5:4505:C:C6     | 2.46                     | 0.49              |
| 24:LR:7:GLN:OE1    | 24:LR:7:GLN:N      | 2.45                     | 0.49              |
| 49:S2:1862:G:O2'   | 49:S2:1864:U:OP2   | 2.29                     | 0.49              |
| 69:SW:11:LEU:HD12  | 69:SW:74:VAL:HB    | 1.95                     | 0.49              |
| 82:LI:88:ARG:HD2   | 82:LI:90:ARG:HD2   | 1.94                     | 0.49              |
| 3:LB:92:TYR:HB2    | 3:LB:159:VAL:CG1   | 2.43                     | 0.49              |
| 8:L5:422:C:H2'     | 8:L5:423:G:H8      | 1.77                     | 0.49              |
| 8:L5:4537:C:H2'    | 8:L5:4538:G:H8     | 1.76                     | 0.49              |
| 8:L5:4600:G:O2'    | 8:L5:4609:G:O6     | 2.28                     | 0.49              |
| 10:L8:142:U:OP1    | 20:LN:38:ARG:NH2   | 2.44                     | 0.49              |
| 13:LE:150:LEU:HD13 | 13:LE:194:VAL:HG11 | 1.93                     | 0.49              |
| 49:S2:581:U:H4'    | 71:SY:66:GLY:HA2   | 1.94                     | 0.49              |
| 49:S2:1413:G:H2'   | 49:S2:1414:A:H8    | 1.77                     | 0.49              |
| 50:SC:270:THR:O    | 50:SC:274:VAL:HG23 | 2.10                     | 0.49              |
| 52:SE:247:THR:HG22 | 52:SE:250:GLU:HG3  | 1.93                     | 0.49              |
| 55:SH:60:ILE:HG13  | 55:SH:92:VAL:HA    | 1.94                     | 0.49              |
| 57:SJ:78:LEU:O     | 57:SJ:82:VAL:HG13  | 2.11                     | 0.49              |
| 78:Sf:107:LYS:O    | 78:Sf:114:ILE:HA   | 2.13                     | 0.49              |
| 4:SB:58:ALA:O      | 4:SB:62:LEU:HD23   | 2.12                     | 0.49              |
| 5:A4:47:A:N1       | 6:B4:34:A:N1       | 2.60                     | 0.49              |
| 6:B4:52:G:H2'      | 6:B4:53:A:H8       | 1.77                     | 0.49              |
| 8:L5:956:A:H1'     | 8:L5:2076:G:H5''   | 1.93                     | 0.49              |
| 8:L5:2521:G:H4'    | 38:Lg:26:PRO:HD2   | 1.94                     | 0.49              |
| 8:L5:3610:A:H2'    | 8:L5:3611:A:H8     | 1.77                     | 0.49              |
| 8:L5:3715:U:H2'    | 8:L5:3716:C:O4'    | 2.13                     | 0.49              |
| 10:L8:141:C:H2'    | 10:L8:142:U:C6     | 2.47                     | 0.49              |
| 16:LH:43:VAL:HG21  | 16:LH:73:ILE:HD12  | 1.93                     | 0.49              |
| 17:LJ:63:ARG:HD3   | 46:Lo:103:VAL:CG1  | 2.43                     | 0.49              |
| 21:LO:142:ALA:HA   | 21:LO:145:VAL:HG22 | 1.94                     | 0.49              |
| 31:LY:80:ILE:HG23  | 31:LY:101:PRO:HG3  | 1.93                     | 0.49              |
| 42:Lk:56:LEU:HA    | 42:Lk:59:SER:OG    | 2.11                     | 0.49              |
| 49:S2:29:G:H2'     | 49:S2:30:C:C6      | 2.47                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:29:G:OP1     | 70:SX:124:LYS:NZ   | 2.46                     | 0.49              |
| 49:S2:104:A:H62    | 49:S2:356:C:H5     | 1.60                     | 0.49              |
| 49:S2:878:G:O6     | 49:S2:908:A:N1     | 2.46                     | 0.49              |
| 49:S2:1546:G:N3    | 49:S2:1670:C:O2'   | 2.42                     | 0.49              |
| 63:SQ:18:THR:O     | 63:SQ:18:THR:OG1   | 2.28                     | 0.49              |
| 65:SS:85:ASN:OD1   | 65:SS:86:ARG:N     | 2.38                     | 0.49              |
| 67:SU:34:LYS:O     | 67:SU:38:ASP:OD1   | 2.30                     | 0.49              |
| 82:LI:36:LEU:HD13  | 82:LI:73:ASN:OD1   | 2.12                     | 0.49              |
| 2:SA:52:LYS:HB2    | 64:SR:109:LEU:CD1  | 2.41                     | 0.49              |
| 8:L5:711:A:H2'     | 8:L5:712:C:C6      | 2.47                     | 0.49              |
| 8:L5:2086:G:H5''   | 11:LC:306:ARG:HH21 | 1.78                     | 0.49              |
| 8:L5:2758:G:H2'    | 8:L5:2759:G:C5     | 2.48                     | 0.49              |
| 8:L5:3615:G:O3'    | 29:LW:44:ARG:NH1   | 2.45                     | 0.49              |
| 8:L5:3861:A:H2'    | 8:L5:3862:A:H8     | 1.75                     | 0.49              |
| 21:LO:126:VAL:HG13 | 21:LO:127:VAL:HG13 | 1.93                     | 0.49              |
| 35:Lc:17:ARG:C     | 35:Lc:19:GLN:H     | 2.20                     | 0.49              |
| 35:Lc:21:VAL:HG23  | 35:Lc:22:MET:H     | 1.77                     | 0.49              |
| 49:S2:996:A:H5''   | 60:SN:7:PRO:HG3    | 1.95                     | 0.49              |
| 49:S2:1232:U:H2'   | 49:S2:1233:G:C8    | 2.47                     | 0.49              |
| 49:S2:1337:4AC:P   | 76:Sd:44:ARG:HH22  | 2.35                     | 0.49              |
| 50:SC:275:LYS:HG3  | 50:SC:276:THR:HG23 | 1.95                     | 0.49              |
| 52:SE:191:ARG:NH1  | 52:SE:245:ARG:HE   | 2.10                     | 0.49              |
| 55:SH:101:LEU:HB2  | 55:SH:116:ARG:HD3  | 1.93                     | 0.49              |
| 71:SY:27:VAL:HG21  | 71:SY:35:VAL:HG21  | 1.93                     | 0.49              |
| 79:Sg:44:LYS:NZ    | 79:Sg:56:GLN:OE1   | 2.30                     | 0.49              |
| 82:LI:51:HIS:HD2   | 82:LI:168:SER:HB2  | 1.76                     | 0.49              |
| 8:L5:1719:A:H2'    | 8:L5:1720:C:C6     | 2.48                     | 0.49              |
| 8:L5:2704:C:H2'    | 8:L5:2705:G:C8     | 2.48                     | 0.49              |
| 8:L5:4638:U:H2'    | 8:L5:4639:G:N3     | 2.27                     | 0.49              |
| 8:L5:4967:A:H2'    | 8:L5:4968:A:C8     | 2.47                     | 0.49              |
| 10:L8:26:C:O2'     | 11:LC:53:ALA:O     | 2.28                     | 0.49              |
| 16:LH:126:VAL:HG21 | 16:LH:161:ILE:HG12 | 1.95                     | 0.49              |
| 19:LM:99:GLU:O     | 19:LM:103:LYS:HG2  | 2.11                     | 0.49              |
| 21:LO:151:ALA:O    | 21:LO:155:THR:HG23 | 2.13                     | 0.49              |
| 36:Ld:92:ARG:HA    | 36:Ld:102:LEU:HD13 | 1.94                     | 0.49              |
| 41:Lj:20:ARG:NH2   | 41:Lj:39:TYR:OH    | 2.41                     | 0.49              |
| 49:S2:644:OMG:H5'  | 57:SJ:41:ARG:HH22  | 1.77                     | 0.49              |
| 51:SD:95:GLY:HA2   | 51:SD:101:GLN:NE2  | 2.27                     | 0.49              |
| 82:LI:76:MET:HE2   | 82:LI:138:ILE:HG21 | 1.95                     | 0.49              |
| 4:SB:52:THR:HB     | 4:SB:58:ALA:H      | 1.77                     | 0.49              |
| 8:L5:1296:G:H2'    | 8:L5:1297:U:C6     | 2.47                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:L5:1339:U:H2'   | 8:L5:1340:OMC:C6   | 2.48                     | 0.49              |
| 8:L5:3861:A:H2'   | 8:L5:3862:A:C8     | 2.48                     | 0.49              |
| 8:L5:4584:A:H2'   | 8:L5:4585:U:O4'    | 2.13                     | 0.49              |
| 10:L8:144:U:H2'   | 10:L8:145:C:C6     | 2.48                     | 0.49              |
| 12:LD:128:ASP:OD1 | 12:LD:129:GLU:N    | 2.42                     | 0.49              |
| 21:LO:121:PRO:HD3 | 25:LS:168:THR:HG22 | 1.95                     | 0.49              |
| 34:Lb:94:ASP:OD1  | 34:Lb:94:ASP:N     | 2.44                     | 0.49              |
| 49:S2:588:G:H4'   | 49:S2:589:G:H5'    | 1.95                     | 0.49              |
| 49:S2:829:C:OP1   | 52:SE:22:LYS:HG2   | 2.13                     | 0.49              |
| 49:S2:1798:C:H2'  | 49:S2:1799:G:O4'   | 2.12                     | 0.49              |
| 8:L5:742:G:N2     | 8:L5:743:G:O6      | 2.46                     | 0.49              |
| 8:L5:1349:G:OP1   | 23:LQ:15:ARG:NH2   | 2.46                     | 0.49              |
| 8:L5:1739:G:H2'   | 8:L5:1740:C:C6     | 2.48                     | 0.49              |
| 12:LD:235:MET:O   | 12:LD:238:GLU:HG2  | 2.12                     | 0.49              |
| 24:LR:157:ASP:OD1 | 24:LR:158:GLN:N    | 2.45                     | 0.49              |
| 36:Ld:18:ASN:O    | 36:Ld:90:ARG:NH1   | 2.45                     | 0.49              |
| 49:S2:677:G:OP1   | 60:SN:120:SER:OG   | 2.31                     | 0.49              |
| 50:SC:70:VAL:HG21 | 50:SC:93:ILE:HG23  | 1.95                     | 0.49              |
| 78:Sf:121:CYS:HB2 | 78:Sf:132:MET:HG2  | 1.94                     | 0.49              |
| 8:L5:1333:A:H2'   | 8:L5:1334:A:C8     | 2.48                     | 0.49              |
| 8:L5:4336:A:H5''  | 8:L5:4337:C:H5'    | 1.95                     | 0.49              |
| 8:L5:4967:A:H2'   | 8:L5:4968:A:H8     | 1.77                     | 0.49              |
| 24:LR:3:MET:HE1   | 24:LR:5:ARG:NE     | 2.28                     | 0.49              |
| 38:Lg:5:LEU:HD23  | 38:Lg:5:LEU:H      | 1.76                     | 0.49              |
| 41:Lj:56:ARG:O    | 41:Lj:57:THR:CG2   | 2.59                     | 0.49              |
| 49:S2:1849:G:HO2' | 49:S2:1850:MA6:H8  | 1.77                     | 0.49              |
| 50:SC:173:LYS:HB3 | 68:SV:3:ASN:HA     | 1.95                     | 0.49              |
| 55:SH:9:VAL:N     | 55:SH:24:SER:OG    | 2.46                     | 0.49              |
| 55:SH:30:LEU:O    | 55:SH:34:SER:OG    | 2.27                     | 0.49              |
| 75:Sc:51:ARG:N    | 75:Sc:54:ASP:OD2   | 2.35                     | 0.49              |
| 8:L5:308:G:O6     | 20:LN:12:ARG:NH1   | 2.46                     | 0.49              |
| 8:L5:1969:G:H3'   | 8:L5:1970:A:C8     | 2.46                     | 0.49              |
| 8:L5:2664:G:OP1   | 24:LR:110:ARG:NH1  | 2.46                     | 0.49              |
| 8:L5:4251:A:C2    | 17:LJ:127:GLY:HA3  | 2.47                     | 0.49              |
| 8:L5:4563:U:H2'   | 8:L5:4564:A:H8     | 1.78                     | 0.49              |
| 12:LD:51:MET:HE1  | 12:LD:166:ALA:HB2  | 1.94                     | 0.49              |
| 17:LJ:44:THR:OG1  | 17:LJ:45:GLY:N     | 2.45                     | 0.49              |
| 20:LN:9:GLU:HB2   | 40:Li:44:ILE:HG13  | 1.94                     | 0.49              |
| 31:LY:37:GLU:HG3  | 31:LY:38:LEU:N     | 2.27                     | 0.49              |
| 36:Ld:64:ILE:HG23 | 36:Ld:68:LEU:HD21  | 1.94                     | 0.49              |
| 49:S2:845:G:H2'   | 49:S2:846:G:C8     | 2.48                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1189:A:H2'   | 49:S2:1190:A:H8    | 1.78                     | 0.49              |
| 49:S2:1221:G:O2'   | 49:S2:1676:U:O2    | 2.25                     | 0.49              |
| 54:SG:181:THR:HG22 | 54:SG:184:VAL:HG23 | 1.95                     | 0.49              |
| 60:SN:46:THR:HG22  | 60:SN:86:GLU:OE1   | 2.12                     | 0.49              |
| 65:SS:22:GLY:HA2   | 65:SS:56:ALA:HB3   | 1.94                     | 0.49              |
| 79:Sg:218:LEU:HD11 | 79:Sg:228:TYR:CZ   | 2.47                     | 0.49              |
| 18:LL:43:ALA:O     | 18:LL:149:GLN:NE2  | 2.35                     | 0.48              |
| 49:S2:855:G:O2'    | 49:S2:856:C:H6     | 1.94                     | 0.48              |
| 79:Sg:163:PRO:HB2  | 79:Sg:179:LEU:HB2  | 1.95                     | 0.48              |
| 2:SA:148:CYS:SG    | 2:SA:160:ALA:HB1   | 2.53                     | 0.48              |
| 8:L5:73:A:OP1      | 18:LL:106:SER:OG   | 2.31                     | 0.48              |
| 8:L5:1802:A:N3     | 26:LT:130:ARG:NH2  | 2.59                     | 0.48              |
| 8:L5:2848:G:N2     | 8:L5:3839:G:OP2    | 2.39                     | 0.48              |
| 8:L5:3736:A:HO2'   | 8:L5:3737:A:H8     | 1.58                     | 0.48              |
| 8:L5:3925:OMU:HM23 | 8:L5:3925:OMU:H1'  | 1.52                     | 0.48              |
| 10:L8:66:A:H2'     | 10:L8:67:U:C6      | 2.48                     | 0.48              |
| 13:LE:141:ARG:NH2  | 13:LE:191:GLN:O    | 2.47                     | 0.48              |
| 28:LV:107:ASN:HB3  | 28:LV:111:GLU:HG2  | 1.95                     | 0.48              |
| 34:Lb:91:ARG:HB2   | 34:Lb:94:ASP:OD1   | 2.12                     | 0.48              |
| 49:S2:4:C:H4'      | 50:SC:207:ALA:HB2  | 1.94                     | 0.48              |
| 49:S2:209:A:H2'    | 49:S2:210:U:O4'    | 2.14                     | 0.48              |
| 50:SC:234:GLY:O    | 50:SC:238:LYS:HG2  | 2.13                     | 0.48              |
| 60:SN:46:THR:O     | 60:SN:50:ILE:HG13  | 2.13                     | 0.48              |
| 1:LA:186:TYR:HB2   | 1:LA:196:TRP:CZ3   | 2.48                     | 0.48              |
| 3:LB:13:SER:HB2    | 8:L5:4622:A:H4'    | 1.94                     | 0.48              |
| 8:L5:371:A:N3      | 8:L5:1531:U:O2'    | 2.45                     | 0.48              |
| 8:L5:425:U:H2'     | 8:L5:426:A:H8      | 1.77                     | 0.48              |
| 8:L5:444:G:H2'     | 8:L5:445:U:C6      | 2.48                     | 0.48              |
| 8:L5:2079:G:H2'    | 8:L5:2080:U:C6     | 2.47                     | 0.48              |
| 8:L5:2458:C:H1'    | 8:L5:3671:G:H21    | 1.78                     | 0.48              |
| 8:L5:2601:A:OP1    | 38:Lg:40:LYS:NZ    | 2.38                     | 0.48              |
| 8:L5:3701:OMC:H4'  | 8:L5:3702:A:O5'    | 2.13                     | 0.48              |
| 16:LH:15:ASN:OD1   | 16:LH:16:VAL:HG23  | 2.13                     | 0.48              |
| 16:LH:93:ARG:NH1   | 44:Lm:82:LEU:HD21  | 2.28                     | 0.48              |
| 25:LS:69:GLU:HG3   | 25:LS:101:THR:HG22 | 1.95                     | 0.48              |
| 27:LU:28:PRO:HB2   | 27:LU:34:MET:HB2   | 1.95                     | 0.48              |
| 38:Lg:60:ARG:HA    | 38:Lg:60:ARG:HD2   | 1.70                     | 0.48              |
| 50:SC:132:ASP:C    | 50:SC:132:ASP:OD1  | 2.56                     | 0.48              |
| 61:SO:84:ARG:HH11  | 61:SO:88:LEU:HD21  | 1.77                     | 0.48              |
| 82:LI:206:LEU:HD23 | 82:LI:210:ARG:HH21 | 1.79                     | 0.48              |
| 8:L5:162:A:H2'     | 8:L5:163:A:H8      | 1.77                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:364:G:C6      | 41:Lj:52:LYS:HE3   | 2.47                     | 0.48              |
| 8:L5:1478:C:H2'    | 8:L5:1479:G:H8     | 1.78                     | 0.48              |
| 8:L5:1912:G:N2     | 21:LO:87:MET:SD    | 2.86                     | 0.48              |
| 8:L5:2323:C:H2'    | 8:L5:2324:C:H6     | 1.78                     | 0.48              |
| 8:L5:2324:C:O2'    | 81:Le:98:GLU:OE1   | 2.32                     | 0.48              |
| 8:L5:3845:A:H2'    | 8:L5:3846:C:C6     | 2.49                     | 0.48              |
| 17:LJ:108:GLY:HA2  | 17:LJ:129:ASP:HA   | 1.96                     | 0.48              |
| 32:LZ:83:THR:HG22  | 38:Lg:95:PHE:CE1   | 2.47                     | 0.48              |
| 49:S2:15:U:H2'     | 49:S2:16:G:O4'     | 2.13                     | 0.48              |
| 49:S2:809:A:H4'    | 52:SE:221:ARG:NH2  | 2.28                     | 0.48              |
| 49:S2:1405:A:H2'   | 49:S2:1406:G:O4'   | 2.13                     | 0.48              |
| 52:SE:183:VAL:CG1  | 52:SE:220:THR:HG21 | 2.43                     | 0.48              |
| 54:SG:141:ILE:HD13 | 54:SG:157:VAL:HG12 | 1.95                     | 0.48              |
| 56:SI:161:LEU:O    | 56:SI:165:GLN:HG2  | 2.12                     | 0.48              |
| 59:SL:134:LEU:HB2  | 59:SL:138:VAL:HG23 | 1.96                     | 0.48              |
| 67:SU:56:MET:HB2   | 67:SU:86:LYS:HB3   | 1.95                     | 0.48              |
| 69:SW:23:ARG:HG3   | 74:Sb:4:ALA:HB2    | 1.94                     | 0.48              |
| 3:LB:3:HIS:HB2     | 8:L5:4516:G:N7     | 2.28                     | 0.48              |
| 3:LB:291:TYR:CE1   | 3:LB:299:ILE:HG22  | 2.49                     | 0.48              |
| 4:SB:127:VAL:HG21  | 4:SB:176:VAL:HG13  | 1.96                     | 0.48              |
| 8:L5:186:G:H4'     | 8:L5:187:U:H5'     | 1.95                     | 0.48              |
| 8:L5:3809:G:OP2    | 8:L5:3809:G:N2     | 2.32                     | 0.48              |
| 8:L5:4691:A:H5'    | 16:LH:71:ARG:HE    | 1.78                     | 0.48              |
| 32:LZ:16:GLY:O     | 32:LZ:19:SER:OG    | 2.30                     | 0.48              |
| 32:LZ:112:ARG:O    | 32:LZ:112:ARG:HD3  | 2.13                     | 0.48              |
| 49:S2:1005:G:H2'   | 49:S2:1006:C:H6    | 1.77                     | 0.48              |
| 65:SS:28:PHE:HE1   | 65:SS:38:ARG:HD3   | 1.77                     | 0.48              |
| 71:SY:21:LYS:HB2   | 71:SY:75:ILE:HB    | 1.94                     | 0.48              |
| 8:L5:364:G:N7      | 41:Lj:55:ARG:NH1   | 2.61                     | 0.48              |
| 8:L5:1371:A:N1     | 10:L8:28:C:O2'     | 2.46                     | 0.48              |
| 8:L5:1617:G:H1'    | 8:L5:2513:A:N6     | 2.29                     | 0.48              |
| 8:L5:2017:A:H2'    | 8:L5:2017:A:N3     | 2.28                     | 0.48              |
| 8:L5:2847:G:H1'    | 28:LV:21:PRO:HD2   | 1.95                     | 0.48              |
| 35:Lc:103:ASP:O    | 35:Lc:107:SER:HB3  | 2.14                     | 0.48              |
| 49:S2:562:U:O2'    | 49:S2:563:G:H8     | 1.97                     | 0.48              |
| 49:S2:958:G:H2'    | 49:S2:959:G:C8     | 2.48                     | 0.48              |
| 49:S2:1628:C:H2'   | 49:S2:1629:C:H6    | 1.79                     | 0.48              |
| 56:SI:88:ASN:O     | 56:SI:88:ASN:ND2   | 2.46                     | 0.48              |
| 65:SS:125:HIS:NE2  | 65:SS:131:VAL:HG21 | 2.29                     | 0.48              |
| 71:SY:79:LEU:C     | 71:SY:81:TYR:H     | 2.22                     | 0.48              |
| 74:Sb:83:GLN:OE1   | 74:Sb:83:GLN:N     | 2.46                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:SB:165:ARG:HG2   | 4:SB:169:MET:HE2   | 1.96                     | 0.48              |
| 7:D4:66:U:H2'      | 7:D4:67:C:C6       | 2.49                     | 0.48              |
| 8:L5:280:G:OP1     | 20:LN:47:LYS:HE2   | 2.14                     | 0.48              |
| 8:L5:1079:C:H2'    | 8:L5:1080:C:H6     | 1.79                     | 0.48              |
| 8:L5:1345:A:H2'    | 8:L5:1346:C:C6     | 2.49                     | 0.48              |
| 8:L5:4126:C:H5''   | 8:L5:4127:A:H5''   | 1.95                     | 0.48              |
| 20:LN:80:THR:OG1   | 20:LN:80:THR:O     | 2.32                     | 0.48              |
| 24:LR:175:GLU:O    | 24:LR:176:ARG:HG2  | 2.14                     | 0.48              |
| 25:LS:99:ASP:OD1   | 25:LS:100:LEU:N    | 2.45                     | 0.48              |
| 48:Lr:51:VAL:HG12  | 48:Lr:62:VAL:HG22  | 1.95                     | 0.48              |
| 49:S2:190:G:H5''   | 56:SI:145:ILE:HD12 | 1.96                     | 0.48              |
| 49:S2:528:A:H2'    | 49:S2:529:A:C8     | 2.48                     | 0.48              |
| 80:SM:54:SER:OG    | 80:SM:80:ASP:CA    | 2.47                     | 0.48              |
| 1:LA:183:GLY:CA    | 8:L5:1613:A:H5''   | 2.44                     | 0.48              |
| 8:L5:1857:C:H2'    | 8:L5:1858:A:C8     | 2.49                     | 0.48              |
| 8:L5:2580:U:OP1    | 32:LZ:36:ARG:NH1   | 2.35                     | 0.48              |
| 8:L5:4771:C:H2'    | 8:L5:4772:C:C6     | 2.49                     | 0.48              |
| 17:LJ:30:GLY:O     | 17:LJ:34:THR:HG23  | 2.14                     | 0.48              |
| 19:LM:108:ASP:HB3  | 21:LO:199:HIS:NE2  | 2.29                     | 0.48              |
| 21:LO:113:ASP:OD1  | 21:LO:114:LYS:HG3  | 2.13                     | 0.48              |
| 44:Lm:96:CYS:CB    | 44:Lm:99:CYS:H     | 2.26                     | 0.48              |
| 49:S2:569:A:H2'    | 49:S2:570:C:O4'    | 2.14                     | 0.48              |
| 49:S2:1158:G:O3'   | 69:SW:76:SER:OG    | 2.19                     | 0.48              |
| 49:S2:1839:U:H2'   | 49:S2:1840:U:C6    | 2.49                     | 0.48              |
| 61:SO:45:THR:HA    | 61:SO:52:THR:HA    | 1.96                     | 0.48              |
| 66:ST:65:TYR:HB2   | 66:ST:123:LEU:HD22 | 1.96                     | 0.48              |
| 67:SU:40:ILE:HG23  | 67:SU:44:LYS:HE2   | 1.96                     | 0.48              |
| 69:SW:102:ILE:H    | 69:SW:113:HIS:HD2  | 1.61                     | 0.48              |
| 70:SX:40:PRO:O     | 70:SX:77:ASN:ND2   | 2.46                     | 0.48              |
| 1:LA:175:ILE:HD13  | 8:L5:3683:C:O4'    | 2.13                     | 0.48              |
| 8:L5:1443:A:H61    | 8:L5:2104:G:N2     | 2.11                     | 0.48              |
| 8:L5:2529:A:O2'    | 8:L5:2531:C:OP2    | 2.32                     | 0.48              |
| 8:L5:3723:A2M:HM'3 | 8:L5:3723:A2M:H1'  | 1.63                     | 0.48              |
| 8:L5:4918:C:H2'    | 8:L5:4919:G:C8     | 2.49                     | 0.48              |
| 9:L7:23:A:H2'      | 9:L7:24:C:C6       | 2.48                     | 0.48              |
| 10:L8:8:U:H2'      | 10:L8:9:A:C8       | 2.49                     | 0.48              |
| 11:LC:13:GLU:HG3   | 11:LC:14:LYS:HD3   | 1.96                     | 0.48              |
| 12:LD:210:TYR:HA   | 12:LD:213:GLU:HG2  | 1.95                     | 0.48              |
| 24:LR:172:ARG:HH12 | 49:S2:909:G:P      | 2.37                     | 0.48              |
| 49:S2:957:A:H2'    | 49:S2:958:G:H21    | 1.79                     | 0.48              |
| 51:SD:7:LYS:HD3    | 67:SU:25:THR:HG21  | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:SE:62:LYS:HB2   | 52:SE:80:ILE:HD11  | 1.95                     | 0.48              |
| 53:SF:204:ARG:CZ   | 75:Sc:60:GLU:HG2   | 2.44                     | 0.48              |
| 79:Sg:246:TYR:HD2  | 79:Sg:262:GLU:HG2  | 1.78                     | 0.48              |
| 2:SA:85:ARG:NH1    | 2:SA:205:ARG:HD3   | 2.28                     | 0.48              |
| 2:SA:154:LEU:HD22  | 2:SA:157:VAL:HG21  | 1.96                     | 0.48              |
| 8:L5:4:G:H2'       | 8:L5:5:A:H8        | 1.79                     | 0.48              |
| 8:L5:2103:G:H2'    | 8:L5:2103:G:N3     | 2.29                     | 0.48              |
| 37:Lf:45:LYS:HA    | 37:Lf:107:PRO:HD2  | 1.94                     | 0.48              |
| 39:Lh:34:ALA:HA    | 39:Lh:37:THR:HG22  | 1.96                     | 0.48              |
| 49:S2:1109:C:HO2'  | 49:S2:1110:G:H8    | 1.61                     | 0.48              |
| 62:SP:29:SER:OG    | 62:SP:30:TYR:N     | 2.47                     | 0.48              |
| 71:SY:109:GLU:HB3  | 71:SY:113:ARG:NH2  | 2.29                     | 0.48              |
| 2:SA:41:ARG:NH1    | 49:S2:1126:G:OP1   | 2.22                     | 0.47              |
| 8:L5:126:C:H2'     | 8:L5:127:G:H8      | 1.79                     | 0.47              |
| 8:L5:175:C:H2'     | 8:L5:176:G:H8      | 1.78                     | 0.47              |
| 8:L5:175:C:H2'     | 8:L5:176:G:C8      | 2.49                     | 0.47              |
| 8:L5:418:A:N6      | 10:L8:16:G:H1'     | 2.29                     | 0.47              |
| 8:L5:2745:A:H2'    | 8:L5:2746:A:H8     | 1.79                     | 0.47              |
| 8:L5:4137:C:H2'    | 8:L5:4138:C:C6     | 2.49                     | 0.47              |
| 8:L5:4612:C:C2     | 16:LH:120:GLU:HB3  | 2.49                     | 0.47              |
| 10:L8:14:OMU:HM23  | 10:L8:14:OMU:H1'   | 1.55                     | 0.47              |
| 15:LG:175:ARG:HD3  | 15:LG:230:TYR:CD2  | 2.49                     | 0.47              |
| 49:S2:1745:A:C8    | 54:SG:65:GLN:HG3   | 2.49                     | 0.47              |
| 61:SO:94:HIS:HA    | 61:SO:127:GLY:O    | 2.13                     | 0.47              |
| 62:SP:106:GLU:OE1  | 62:SP:108:LYS:HE3  | 2.14                     | 0.47              |
| 3:LB:29:VAL:HG22   | 3:LB:220:ILE:HD11  | 1.96                     | 0.47              |
| 3:LB:168:MET:HA    | 3:LB:171:LEU:HD12  | 1.95                     | 0.47              |
| 8:L5:1521:C:OP1    | 11:LC:100:ARG:NH2  | 2.46                     | 0.47              |
| 8:L5:1964:A:N6     | 8:L5:2023:C:O2'    | 2.42                     | 0.47              |
| 8:L5:2545:U:H3'    | 8:L5:2546:G:H4'    | 1.95                     | 0.47              |
| 49:S2:1005:G:H2'   | 49:S2:1006:C:C6    | 2.48                     | 0.47              |
| 51:SD:76:ARG:O     | 51:SD:76:ARG:NH1   | 2.41                     | 0.47              |
| 55:SH:10:LYS:O     | 55:SH:10:LYS:HG3   | 2.13                     | 0.47              |
| 70:SX:128:VAL:HG23 | 70:SX:133:LEU:HD11 | 1.95                     | 0.47              |
| 79:Sg:195:LEU:HA   | 79:Sg:211:GLY:HA3  | 1.96                     | 0.47              |
| 2:SA:42:LYS:HG3    | 2:SA:48:ILE:HD11   | 1.96                     | 0.47              |
| 8:L5:4694:G:OP1    | 8:L5:4694:G:N2     | 2.48                     | 0.47              |
| 17:LJ:19:LYS:HE2   | 17:LJ:133:VAL:HG11 | 1.97                     | 0.47              |
| 21:LO:38:CYS:O     | 21:LO:138:LEU:HD21 | 2.14                     | 0.47              |
| 24:LR:163:ARG:HD3  | 49:S2:871:U:H1'    | 1.95                     | 0.47              |
| 49:S2:388:U:H2'    | 49:S2:389:A:H8     | 1.79                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 49:S2:1158:G:H5''  | 69:SW:76:SER:HB2  | 1.95                     | 0.47              |
| 49:S2:1614:A:H2'   | 49:S2:1615:U:C6   | 2.50                     | 0.47              |
| 8:L5:171:U:H5''    | 8:L5:172:C:C5     | 2.49                     | 0.47              |
| 8:L5:1448:G:H2'    | 8:L5:1449:C:H6    | 1.79                     | 0.47              |
| 8:L5:2517:A:N3     | 8:L5:2539:C:O2'   | 2.47                     | 0.47              |
| 8:L5:2602:G:H2'    | 8:L5:2603:C:C6    | 2.50                     | 0.47              |
| 8:L5:2667:C:O4'    | 24:LR:96:MET:HG2  | 2.15                     | 0.47              |
| 8:L5:3586:G:H2'    | 8:L5:3586:G:N3    | 2.28                     | 0.47              |
| 8:L5:4212:A:N1     | 26:LT:3:ASN:ND2   | 2.47                     | 0.47              |
| 8:L5:4260:U:H2'    | 8:L5:4261:C:H6    | 1.79                     | 0.47              |
| 8:L5:4723:A:H2'    | 8:L5:4724:A:C8    | 2.50                     | 0.47              |
| 10:L8:60:G:O6      | 10:L8:96:C:O2'    | 2.26                     | 0.47              |
| 12:LD:164:LYS:HG2  | 12:LD:195:HIS:CE1 | 2.49                     | 0.47              |
| 51:SD:142:LEU:HD12 | 51:SD:148:LYS:HG3 | 1.96                     | 0.47              |
| 78:Sf:123:SER:HB3  | 78:Sf:126:CYS:HB2 | 1.96                     | 0.47              |
| 1:LA:223:SER:HB3   | 8:L5:3748:A:O2'   | 2.14                     | 0.47              |
| 4:SB:65:ARG:HH12   | 61:SO:51:GLU:HG3  | 1.80                     | 0.47              |
| 8:L5:23:C:H2'      | 8:L5:24:G:O4'     | 2.14                     | 0.47              |
| 8:L5:138:G:H2'     | 8:L5:139:G:C8     | 2.49                     | 0.47              |
| 8:L5:491:G:H2'     | 8:L5:492:U:H6     | 1.79                     | 0.47              |
| 8:L5:1199:G:H2'    | 8:L5:1200:G:C8    | 2.48                     | 0.47              |
| 8:L5:1244:G:H2'    | 8:L5:1245:C:C6    | 2.49                     | 0.47              |
| 8:L5:1669:A:P      | 34:Lb:18:ARG:HH12 | 2.38                     | 0.47              |
| 8:L5:2803:U:H2'    | 8:L5:2804:OMC:H6  | 1.78                     | 0.47              |
| 8:L5:3917:A:H2'    | 8:L5:3918:G:H8    | 1.79                     | 0.47              |
| 8:L5:4940:C:O2'    | 13:LE:246:ARG:NH2 | 2.47                     | 0.47              |
| 21:LO:19:LEU:O     | 21:LO:23:VAL:HG13 | 2.15                     | 0.47              |
| 31:LY:52:ASP:HB2   | 31:LY:110:LYS:HG2 | 1.96                     | 0.47              |
| 49:S2:1650:A:H2'   | 49:S2:1651:A:O4'  | 2.14                     | 0.47              |
| 49:S2:1736:G:H2'   | 49:S2:1737:G:C8   | 2.49                     | 0.47              |
| 54:SG:98:ARG:NH1   | 54:SG:101:ILE:O   | 2.43                     | 0.47              |
| 61:SO:113:GLN:OE1  | 73:Sa:46:GLU:N    | 2.47                     | 0.47              |
| 63:SQ:6:PRO:O      | 63:SQ:27:ARG:NH2  | 2.48                     | 0.47              |
| 67:SU:68:THR:O     | 76:Sd:40:ARG:NH1  | 2.41                     | 0.47              |
| 79:Sg:218:LEU:HD21 | 79:Sg:228:TYR:CE1 | 2.49                     | 0.47              |
| 79:Sg:223:GLU:OE1  | 79:Sg:225:LYS:HE3 | 2.14                     | 0.47              |
| 4:SB:28:LYS:HD3    | 4:SB:48:LEU:HD12  | 1.97                     | 0.47              |
| 8:L5:423:G:H2'     | 8:L5:424:U:C6     | 2.50                     | 0.47              |
| 8:L5:1443:A:C5     | 8:L5:1444:G:N7    | 2.83                     | 0.47              |
| 8:L5:1890:G:OP2    | 8:L5:1890:G:N2    | 2.38                     | 0.47              |
| 13:LE:213:THR:HG22 | 13:LE:214:ASP:H   | 1.78                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:LH:53:LYS:HD3   | 16:LH:53:LYS:HA    | 1.63                     | 0.47              |
| 33:La:71:PRO:HG2   | 33:La:108:TYR:HA   | 1.96                     | 0.47              |
| 49:S2:964:A:H2'    | 49:S2:965:U:C6     | 2.48                     | 0.47              |
| 49:S2:1259:A:H1'   | 49:S2:1264:C:H42   | 1.80                     | 0.47              |
| 49:S2:1849:G:O2'   | 49:S2:1850:MA6:O5' | 2.29                     | 0.47              |
| 50:SC:168:GLY:N    | 50:SC:179:THR:O    | 2.37                     | 0.47              |
| 52:SE:80:ILE:HG22  | 52:SE:81:THR:HG23  | 1.96                     | 0.47              |
| 52:SE:141:THR:OG1  | 52:SE:143:ASP:OD1  | 2.33                     | 0.47              |
| 54:SG:48:TYR:HE1   | 54:SG:116:LYS:HG3  | 1.80                     | 0.47              |
| 58:SK:16:PHE:HE2   | 58:SK:89:ILE:HG22  | 1.79                     | 0.47              |
| 81:Le:35:TRP:CZ2   | 81:Le:56:PRO:HD2   | 2.50                     | 0.47              |
| 1:LA:58:LEU:HD23   | 1:LA:75:LEU:HD12   | 1.96                     | 0.47              |
| 3:LB:257:TRP:CD1   | 3:LB:257:TRP:C     | 2.93                     | 0.47              |
| 6:B4:37:A:O2'      | 49:S2:1058:A:OP1   | 2.27                     | 0.47              |
| 8:L5:99:A:H4'      | 20:LN:181:HIS:CD2  | 2.50                     | 0.47              |
| 8:L5:198:A:OP2     | 31:LY:126:ARG:NH2  | 2.48                     | 0.47              |
| 8:L5:919:C:H2'     | 8:L5:920:C:H6      | 1.80                     | 0.47              |
| 8:L5:1197:C:H2'    | 8:L5:1198:G:C8     | 2.50                     | 0.47              |
| 8:L5:1326:A2M:HM'3 | 8:L5:1326:A2M:H1'  | 1.67                     | 0.47              |
| 8:L5:1443:A:N1     | 8:L5:2103:G:O6     | 2.47                     | 0.47              |
| 8:L5:1450:C:H2'    | 8:L5:1451:G:O4'    | 2.14                     | 0.47              |
| 8:L5:1865:G:N2     | 8:L5:1868:A:OP2    | 2.42                     | 0.47              |
| 8:L5:2306:G:H1'    | 8:L5:2332:A:N6     | 2.30                     | 0.47              |
| 8:L5:2809:G:O2'    | 8:L5:4644:G:OP1    | 2.28                     | 0.47              |
| 8:L5:2844:A:O2'    | 8:L5:4631:G:H4'    | 2.15                     | 0.47              |
| 8:L5:3673:C:OP2    | 20:LN:67:ARG:NH2   | 2.43                     | 0.47              |
| 8:L5:3934:G:H2'    | 8:L5:3935:C:C6     | 2.49                     | 0.47              |
| 8:L5:4305:G:C6     | 26:LT:80:VAL:HG11  | 2.50                     | 0.47              |
| 8:L5:4745:G:H1     | 8:L5:4955:A:N6     | 2.10                     | 0.47              |
| 8:L5:4891:G:N2     | 19:LM:118:MET:HE1  | 2.29                     | 0.47              |
| 15:LG:147:VAL:HG12 | 15:LG:179:VAL:HG11 | 1.97                     | 0.47              |
| 18:LL:119:GLU:O    | 18:LL:123:LYS:HG2  | 2.14                     | 0.47              |
| 20:LN:158:HIS:HB3  | 20:LN:161:MET:HG3  | 1.97                     | 0.47              |
| 24:LR:95:TRP:CH2   | 24:LR:99:MET:HE3   | 2.50                     | 0.47              |
| 30:LX:55:ARG:HG3   | 30:LX:55:ARG:NH1   | 2.30                     | 0.47              |
| 39:Lh:80:PRO:HD2   | 39:Lh:83:LEU:HD12  | 1.97                     | 0.47              |
| 49:S2:26:U:H2'     | 49:S2:27:A2M:H8    | 1.97                     | 0.47              |
| 52:SE:18:TRP:CH2   | 52:SE:31:PRO:HD3   | 2.47                     | 0.47              |
| 55:SH:18:GLU:O     | 55:SH:21:SER:OG    | 2.31                     | 0.47              |
| 57:SJ:111:GLN:OE1  | 57:SJ:127:ARG:HB2  | 2.14                     | 0.47              |
| 59:SL:126:VAL:HG13 | 59:SL:142:VAL:HG13 | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:Sc:40:ARG:HH21  | 75:Sc:42:ILE:HD11  | 1.80                     | 0.47              |
| 3:LB:252:ALA:HB3   | 8:L5:4457:U:O2     | 2.15                     | 0.47              |
| 4:SB:75:GLN:HG3    | 4:SB:76:ASN:H      | 1.79                     | 0.47              |
| 8:L5:179:G:H2'     | 8:L5:180:C:C6      | 2.50                     | 0.47              |
| 8:L5:1098:G:H2'    | 8:L5:1099:C:C6     | 2.49                     | 0.47              |
| 8:L5:1443:A:C2     | 8:L5:2103:G:N1     | 2.74                     | 0.47              |
| 8:L5:1541:C:O2'    | 8:L5:2448:G:N3     | 2.48                     | 0.47              |
| 8:L5:4323:A:C2     | 12:LD:146:LEU:HD23 | 2.50                     | 0.47              |
| 8:L5:4535:A:H2'    | 8:L5:4536:OMC:H6   | 1.79                     | 0.47              |
| 8:L5:4970:C:C2     | 8:L5:4971:A:C8     | 3.02                     | 0.47              |
| 12:LD:60:ILE:HB    | 12:LD:80:ALA:HB2   | 1.97                     | 0.47              |
| 12:LD:256:LYS:HA   | 12:LD:257:PRO:HG2  | 1.97                     | 0.47              |
| 30:LX:94:ASN:ND2   | 30:LX:94:ASN:O     | 2.48                     | 0.47              |
| 35:Lc:98:ASP:C     | 35:Lc:98:ASP:OD2   | 2.58                     | 0.47              |
| 49:S2:168:C:O2'    | 54:SG:131:ARG:O    | 2.31                     | 0.47              |
| 49:S2:455:A:H2'    | 49:S2:456:C:C6     | 2.50                     | 0.47              |
| 63:SQ:112:LEU:HD22 | 63:SQ:119:LEU:HD23 | 1.97                     | 0.47              |
| 67:SU:62:ARG:HB3   | 67:SU:62:ARG:HH11  | 1.80                     | 0.47              |
| 79:Sg:11:LEU:HB2   | 79:Sg:307:VAL:HB   | 1.96                     | 0.47              |
| 82:LI:36:LEU:HD13  | 82:LI:73:ASN:CG    | 2.40                     | 0.47              |
| 8:L5:492:U:H2'     | 8:L5:493:G:C8      | 2.50                     | 0.47              |
| 8:L5:908:G:H2'     | 8:L5:909:A:H8      | 1.79                     | 0.47              |
| 8:L5:1173:G:C2     | 8:L5:1174:A:H1'    | 2.50                     | 0.47              |
| 8:L5:1175:A:H2'    | 8:L5:1176:C:O4'    | 2.15                     | 0.47              |
| 8:L5:1857:C:H2'    | 8:L5:1858:A:H8     | 1.80                     | 0.47              |
| 22:LP:36:ILE:HG21  | 22:LP:48:LEU:HD21  | 1.97                     | 0.47              |
| 31:LY:30:MET:SD    | 31:LY:78:TYR:HA    | 2.55                     | 0.47              |
| 34:Lb:32:LEU:HD13  | 34:Lb:43:MET:HE1   | 1.97                     | 0.47              |
| 49:S2:24:C:O2'     | 49:S2:25:A:H8      | 1.96                     | 0.47              |
| 49:S2:455:A:H2'    | 49:S2:456:C:H6     | 1.80                     | 0.47              |
| 49:S2:573:U:O2     | 49:S2:576:A2M:H8   | 2.15                     | 0.47              |
| 49:S2:1162:C:H2'   | 49:S2:1163:C:O4'   | 2.14                     | 0.47              |
| 53:SF:52:SER:O     | 53:SF:52:SER:OG    | 2.30                     | 0.47              |
| 65:SS:68:ILE:HA    | 65:SS:71:MET:HE2   | 1.96                     | 0.47              |
| 72:SZ:73:VAL:HG21  | 72:SZ:88:LEU:HD21  | 1.96                     | 0.47              |
| 3:LB:47:LEU:HD23   | 3:LB:346:THR:HG22  | 1.96                     | 0.47              |
| 8:L5:1686:C:O2'    | 34:Lb:18:ARG:NH1   | 2.48                     | 0.47              |
| 8:L5:2875:C:OP1    | 47:Lp:23:ARG:NH2   | 2.47                     | 0.47              |
| 8:L5:4239:A:H2'    | 8:L5:4240:G:H8     | 1.80                     | 0.47              |
| 42:Lk:24:LYS:HG2   | 42:Lk:67:LYS:HZ2   | 1.78                     | 0.47              |
| 49:S2:1500:G:H2'   | 49:S2:1501:C:C6    | 2.49                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 49:S2:1539:U:OP1    | 66:ST:44:GLU:N     | 2.48                     | 0.47              |
| 57:SJ:28:GLU:O      | 57:SJ:32:ILE:HG23  | 2.15                     | 0.47              |
| 61:SO:136:PRO:CB    | 61:SO:139:SER:HB3  | 2.44                     | 0.47              |
| 68:SV:17:CYS:HB2    | 68:SV:56:CYS:HB3   | 1.97                     | 0.47              |
| 8:L5:38:A:H5''      | 33:La:35:ALA:HB2   | 1.97                     | 0.46              |
| 8:L5:1332:C:H2'     | 8:L5:1333:A:C8     | 2.49                     | 0.46              |
| 8:L5:1840:G:H5''    | 14:LF:113:ARG:HD3  | 1.97                     | 0.46              |
| 8:L5:1932:A:H2'     | 8:L5:1933:G:C8     | 2.50                     | 0.46              |
| 8:L5:2709:C:H5'     | 24:LR:43:LYS:NZ    | 2.30                     | 0.46              |
| 8:L5:3938:G:H4'     | 8:L5:3939:G:O5'    | 2.15                     | 0.46              |
| 9:L7:3:C:H2'        | 9:L7:4:U:C6        | 2.50                     | 0.46              |
| 9:L7:66:G:OP1       | 12:LD:10:LYS:NZ    | 2.39                     | 0.46              |
| 32:LZ:76:ASN:OD1    | 32:LZ:77:TYR:N     | 2.48                     | 0.46              |
| 47:Lp:16:THR:O      | 47:Lp:16:THR:OG1   | 2.30                     | 0.46              |
| 49:S2:811:A:H2'     | 49:S2:812:A:C8     | 2.50                     | 0.46              |
| 49:S2:1203:G:H2'    | 49:S2:1204:A:N3    | 2.30                     | 0.46              |
| 49:S2:1215:C:O2'    | 49:S2:1645:C:OP2   | 2.34                     | 0.46              |
| 58:SK:32:HIS:NE2    | 58:SK:34:GLU:OE1   | 2.48                     | 0.46              |
| 61:SO:56:VAL:HG13   | 61:SO:60:MET:HE2   | 1.96                     | 0.46              |
| 72:SZ:56:ASP:HA     | 72:SZ:59:CYS:SG    | 2.55                     | 0.46              |
| 1:LA:5:ILE:HG12     | 1:LA:8:GLN:HB2     | 1.97                     | 0.46              |
| 4:SB:225:LEU:HD23   | 4:SB:225:LEU:HA    | 1.76                     | 0.46              |
| 8:L5:3626:G:H2'     | 8:L5:3627:OMG:O4'  | 2.15                     | 0.46              |
| 8:L5:4887:C:H42     | 8:L5:4932:U:H3     | 1.63                     | 0.46              |
| 20:LN:45:PRO:O      | 20:LN:49:ARG:HG3   | 2.15                     | 0.46              |
| 36:Ld:24:GLU:OE1    | 36:Ld:109:VAL:HG11 | 2.15                     | 0.46              |
| 48:Lr:75:THR:O      | 48:Lr:75:THR:HG23  | 2.15                     | 0.46              |
| 8:L5:271:C:H2'      | 8:L5:272:U:H6      | 1.80                     | 0.46              |
| 8:L5:2897:G:C4      | 8:L5:3603:G:N2     | 2.83                     | 0.46              |
| 8:L5:4475:G:OP2     | 16:LH:173:ARG:NH2  | 2.44                     | 0.46              |
| 8:L5:4625:C:O2'     | 8:L5:4626:A:H5'    | 2.16                     | 0.46              |
| 8:L5:4752:U:H4'     | 21:LO:4:VAL:HG21   | 1.97                     | 0.46              |
| 13:LE:150:LEU:HB3   | 13:LE:194:VAL:HG13 | 1.97                     | 0.46              |
| 18:LL:111:GLN:O     | 18:LL:115:GLN:HG2  | 2.14                     | 0.46              |
| 20:LN:68:ARG:HA     | 20:LN:98:LEU:HD21  | 1.96                     | 0.46              |
| 25:LS:69:GLU:OE2    | 25:LS:102:THR:N    | 2.40                     | 0.46              |
| 49:S2:5:U:H2'       | 49:S2:6:G:H8       | 1.80                     | 0.46              |
| 49:S2:1442:OMU:HM23 | 49:S2:1442:OMU:H1' | 1.50                     | 0.46              |
| 49:S2:1500:G:H2'    | 49:S2:1501:C:H6    | 1.79                     | 0.46              |
| 49:S2:1512:C:H5''   | 76:Sd:8:TRP:HZ3    | 1.79                     | 0.46              |
| 49:S2:1741:U:H2'    | 49:S2:1742:C:O4'   | 2.14                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:D4:48:C:H2'     | 7:D4:59:U:H1'      | 1.98                     | 0.46              |
| 8:L5:406:C:O2'    | 8:L5:407:A:OP1     | 2.29                     | 0.46              |
| 8:L5:1308:C:H2'   | 8:L5:1309:C:C6     | 2.51                     | 0.46              |
| 8:L5:1816:C:C6    | 34:Lb:42:ASN:OD1   | 2.68                     | 0.46              |
| 8:L5:1866:U:OP1   | 82:LI:4:ARG:NH1    | 2.44                     | 0.46              |
| 8:L5:2415:U:H2'   | 8:L5:2416:G:C8     | 2.51                     | 0.46              |
| 8:L5:2591:A:H2'   | 8:L5:2592:U:H6     | 1.81                     | 0.46              |
| 8:L5:3599:A:H2'   | 8:L5:3600:G:H8     | 1.77                     | 0.46              |
| 8:L5:3619:G:H22   | 8:L5:3624:A:H1'    | 1.80                     | 0.46              |
| 8:L5:4243:C:OP2   | 8:L5:4264:G:N1     | 2.42                     | 0.46              |
| 15:LG:182:CYS:SG  | 15:LG:183:ILE:N    | 2.88                     | 0.46              |
| 25:LS:107:THR:O   | 25:LS:111:ARG:HG2  | 2.14                     | 0.46              |
| 29:LW:52:THR:O    | 29:LW:56:ARG:HG2   | 2.15                     | 0.46              |
| 54:SG:192:ILE:O   | 54:SG:196:LYS:HG3  | 2.15                     | 0.46              |
| 59:SL:15:THR:HG22 | 59:SL:15:THR:O     | 2.16                     | 0.46              |
| 59:SL:92:TYR:OH   | 59:SL:107:LYS:NZ   | 2.48                     | 0.46              |
| 62:SP:109:PRO:O   | 62:SP:112:ILE:HG12 | 2.16                     | 0.46              |
| 67:SU:34:LYS:HE3  | 67:SU:107:GLU:OE2  | 2.15                     | 0.46              |
| 69:SW:102:ILE:H   | 69:SW:113:HIS:CD2  | 2.33                     | 0.46              |
| 74:Sb:6:ASP:O     | 74:Sb:8:LEU:N      | 2.48                     | 0.46              |
| 80:SM:65:VAL:O    | 80:SM:69:CYS:HB2   | 2.14                     | 0.46              |
| 2:SA:135:THR:O    | 2:SA:138:SER:OG    | 2.32                     | 0.46              |
| 7:D4:39:U:H2'     | 7:D4:40:C:C6       | 2.51                     | 0.46              |
| 8:L5:271:C:H2'    | 8:L5:272:U:C6      | 2.49                     | 0.46              |
| 8:L5:655:C:P      | 11:LC:268:ARG:NH2  | 2.88                     | 0.46              |
| 8:L5:1416:G:H2'   | 8:L5:1417:C:H6     | 1.81                     | 0.46              |
| 8:L5:1447:C:O2'   | 8:L5:1448:G:H5'    | 2.16                     | 0.46              |
| 8:L5:1958:A:O2'   | 8:L5:2025:A:N1     | 2.46                     | 0.46              |
| 8:L5:1962:A:OP2   | 8:L5:2024:G:N2     | 2.41                     | 0.46              |
| 8:L5:3672:G:H3'   | 8:L5:3673:C:H5''   | 1.98                     | 0.46              |
| 8:L5:3718:A2M:H2  | 8:L5:3934:G:O4'    | 2.15                     | 0.46              |
| 8:L5:4563:U:H2'   | 8:L5:4564:A:C8     | 2.50                     | 0.46              |
| 10:L8:155:C:P     | 15:LG:89:ARG:HH12  | 2.38                     | 0.46              |
| 49:S2:949:G:H2'   | 49:S2:950:C:C6     | 2.51                     | 0.46              |
| 51:SD:41:VAL:HB   | 51:SD:46:THR:HG23  | 1.98                     | 0.46              |
| 81:Le:44:ARG:CZ   | 81:Le:52:GLN:HE22  | 2.29                     | 0.46              |
| 82:LI:170:LYS:HA  | 82:LI:177:ASN:HA   | 1.97                     | 0.46              |
| 8:L5:106:A:O2'    | 8:L5:335:A:N3      | 2.47                     | 0.46              |
| 8:L5:375:G:OP1    | 11:LC:62:THR:HG23  | 2.16                     | 0.46              |
| 8:L5:1249:C:H2'   | 8:L5:1250:C:C6     | 2.51                     | 0.46              |
| 8:L5:2469:C:H5'   | 8:L5:2470:C:OP2    | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L8:47:C:H1'     | 10:L8:61:A:H2'     | 1.96                     | 0.46              |
| 12:LD:208:MET:O    | 12:LD:212:MET:HG2  | 2.15                     | 0.46              |
| 19:LM:23:LYS:HB3   | 19:LM:43:THR:HG21  | 1.97                     | 0.46              |
| 21:LO:85:ARG:HG3   | 21:LO:99:LEU:HD22  | 1.97                     | 0.46              |
| 32:LZ:52:LYS:O     | 32:LZ:65:ARG:NH2   | 2.47                     | 0.46              |
| 34:Lb:110:ALA:O    | 34:Lb:114:LYS:HG2  | 2.15                     | 0.46              |
| 37:Lf:43:LEU:HD23  | 37:Lf:43:LEU:HA    | 1.78                     | 0.46              |
| 49:S2:496:C:H5'    | 52:SE:29:PRO:HA    | 1.98                     | 0.46              |
| 56:SI:161:LEU:HA   | 56:SI:164:GLU:OE2  | 2.15                     | 0.46              |
| 6:B4:68:U:H2'      | 6:B4:69:G:C8       | 2.45                     | 0.46              |
| 8:L5:52:G:H4'      | 8:L5:1529:G:H4'    | 1.97                     | 0.46              |
| 8:L5:960:A:N6      | 13:LE:125:LEU:O    | 2.47                     | 0.46              |
| 8:L5:1397:A:OP1    | 33:La:132:ARG:HD3  | 2.15                     | 0.46              |
| 8:L5:2264:C:H2'    | 8:L5:2265:G:O4'    | 2.15                     | 0.46              |
| 8:L5:2630:U:O4     | 27:LU:89:LYS:NZ    | 2.48                     | 0.46              |
| 8:L5:3656:A:H2'    | 8:L5:3657:U:H6     | 1.80                     | 0.46              |
| 8:L5:3732:A:H2'    | 8:L5:3733:A:C8     | 2.51                     | 0.46              |
| 8:L5:3932:U:O2'    | 8:L5:3933:G:H8     | 1.97                     | 0.46              |
| 8:L5:4147:G:H2'    | 8:L5:4148:C:C6     | 2.51                     | 0.46              |
| 11:LC:10:VAL:O     | 11:LC:18:SER:OG    | 2.26                     | 0.46              |
| 11:LC:186:SER:OG   | 11:LC:187:GLN:N    | 2.43                     | 0.46              |
| 49:S2:945:U:H2'    | 49:S2:946:U:C6     | 2.51                     | 0.46              |
| 56:SI:103:LEU:HD12 | 56:SI:103:LEU:HA   | 1.83                     | 0.46              |
| 57:SJ:84:ILE:HA    | 57:SJ:150:ARG:HG2  | 1.98                     | 0.46              |
| 64:SR:20:TYR:HD2   | 64:SR:23:ARG:HD3   | 1.79                     | 0.46              |
| 65:SS:26:ILE:O     | 65:SS:30:ILE:HG12  | 2.15                     | 0.46              |
| 67:SU:24:LEU:HD23  | 67:SU:112:VAL:HG22 | 1.97                     | 0.46              |
| 79:Sg:256:ILE:HG12 | 79:Sg:270:LEU:HB2  | 1.98                     | 0.46              |
| 3:LB:55:HIS:NE2    | 3:LB:369:ASP:OD2   | 2.49                     | 0.46              |
| 8:L5:711:A:N3      | 13:LE:136:HIS:HE1  | 2.14                     | 0.46              |
| 8:L5:1079:C:H2'    | 8:L5:1080:C:C6     | 2.50                     | 0.46              |
| 8:L5:1656:U:OP2    | 33:La:26:ARG:NH2   | 2.33                     | 0.46              |
| 8:L5:2652:G:N2     | 47:Lp:58:GLY:O     | 2.48                     | 0.46              |
| 8:L5:3823:G:H2'    | 8:L5:3824:A:C8     | 2.51                     | 0.46              |
| 8:L5:4261:C:O2'    | 17:LJ:102:THR:HG21 | 2.15                     | 0.46              |
| 8:L5:4458:C:H2'    | 8:L5:4459:U:C6     | 2.51                     | 0.46              |
| 13:LE:46:ARG:C     | 13:LE:62:MET:HE1   | 2.41                     | 0.46              |
| 15:LG:157:ILE:HG22 | 15:LG:201:THR:HG1  | 1.81                     | 0.46              |
| 20:LN:28:TRP:O     | 20:LN:32:GLN:HG2   | 2.16                     | 0.46              |
| 49:S2:550:C:H2'    | 49:S2:551:U:C6     | 2.51                     | 0.46              |
| 55:SH:145:ARG:HB2  | 69:SW:51:GLU:HG3   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 59:SL:104:LYS:HE3 | 70:SX:8:ARG:HH21   | 1.80                     | 0.46              |
| 75:Sc:46:VAL:HG12 | 75:Sc:56:LEU:HD21  | 1.97                     | 0.46              |
| 78:Sf:138:ARG:HD2 | 78:Sf:147:THR:CG2  | 2.45                     | 0.46              |
| 81:Le:98:GLU:HG3  | 81:Le:123:THR:OG1  | 2.16                     | 0.46              |
| 82:LI:69:ARG:NH2  | 82:LI:70:ILE:HG13  | 2.31                     | 0.46              |
| 2:SA:50:ASN:O     | 2:SA:54:THR:HG23   | 2.16                     | 0.46              |
| 6:B4:20:A:N6      | 6:B4:45:G:H1'      | 2.31                     | 0.46              |
| 8:L5:1448:G:H2'   | 8:L5:1449:C:C6     | 2.50                     | 0.46              |
| 8:L5:1786:A:H2'   | 8:L5:1789:C:C5     | 2.51                     | 0.46              |
| 8:L5:1811:G:H2'   | 8:L5:1812:C:C6     | 2.50                     | 0.46              |
| 8:L5:4538:G:H2'   | 8:L5:4539:U:C6     | 2.51                     | 0.46              |
| 15:LG:217:LYS:HB3 | 15:LG:217:LYS:HE2  | 1.70                     | 0.46              |
| 17:LJ:40:LEU:HD23 | 17:LJ:40:LEU:HA    | 1.84                     | 0.46              |
| 19:LM:40:GLY:H    | 19:LM:45:VAL:HG23  | 1.81                     | 0.46              |
| 19:LM:43:THR:O    | 19:LM:43:THR:CG2   | 2.64                     | 0.46              |
| 32:LZ:16:GLY:O    | 38:Lg:76:ARG:HG3   | 2.16                     | 0.46              |
| 48:Lr:58:LYS:O    | 48:Lr:58:LYS:HG3   | 2.16                     | 0.46              |
| 49:S2:1093:A:H2'  | 49:S2:1094:C:C6    | 2.50                     | 0.46              |
| 49:S2:1630:A:H5'' | 65:SS:37:GLY:H     | 1.81                     | 0.46              |
| 50:SC:132:ASP:OD1 | 50:SC:134:ASN:N    | 2.36                     | 0.46              |
| 51:SD:132:LYS:HB2 | 51:SD:189:MET:HG2  | 1.98                     | 0.46              |
| 2:SA:70:ASN:HB3   | 2:SA:73:ASP:OD2    | 2.16                     | 0.46              |
| 3:LB:56:ILE:HD12  | 3:LB:368:ILE:HA    | 1.98                     | 0.46              |
| 3:LB:288:GLY:HA3  | 3:LB:330:PHE:CE1   | 2.51                     | 0.46              |
| 8:L5:644:G:H2'    | 8:L5:645:G:O4'     | 2.16                     | 0.46              |
| 8:L5:1202:C:N3    | 8:L5:1203:G:O2'    | 2.47                     | 0.46              |
| 8:L5:1625:OMG:N1  | 8:L5:3918:G:OP1    | 2.42                     | 0.46              |
| 8:L5:2080:U:H2'   | 8:L5:2081:C:C6     | 2.51                     | 0.46              |
| 8:L5:3873:G:H2'   | 8:L5:3874:G:C8     | 2.52                     | 0.46              |
| 8:L5:4481:U:H2'   | 8:L5:4482:U:H6     | 1.81                     | 0.46              |
| 10:L8:54:C:H2'    | 10:L8:55:PSU:H6    | 1.81                     | 0.46              |
| 15:LG:191:GLY:HA2 | 15:LG:194:VAL:HG22 | 1.98                     | 0.46              |
| 17:LJ:22:LEU:HB3  | 17:LJ:128:LEU:HD21 | 1.98                     | 0.46              |
| 17:LJ:80:GLU:OE1  | 17:LJ:80:GLU:HA    | 2.16                     | 0.46              |
| 25:LS:7:LEU:O     | 25:LS:103:ALA:HB1  | 2.16                     | 0.46              |
| 33:La:37:GLY:H    | 33:La:41:HIS:HB2   | 1.80                     | 0.46              |
| 49:S2:807:G:H2'   | 49:S2:808:A:C8     | 2.50                     | 0.46              |
| 49:S2:1541:G:P    | 66:ST:56:ARG:HH21  | 2.39                     | 0.46              |
| 49:S2:1588:A:HO2' | 49:S2:1589:A:H8    | 1.57                     | 0.46              |
| 58:SK:74:GLU:OE2  | 58:SK:74:GLU:N     | 2.45                     | 0.46              |
| 59:SL:124:ASP:OD1 | 59:SL:147:LYS:HA   | 2.16                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 69:SW:86:LEU:HB3   | 69:SW:117:ARG:NH2 | 2.31                     | 0.46              |
| 6:B4:8:U:O4        | 6:B4:14:A:N7      | 2.49                     | 0.45              |
| 8:L5:318:A:H2'     | 8:L5:319:A:H8     | 1.81                     | 0.45              |
| 8:L5:1396:G:O2'    | 8:L5:1468:C:O2'   | 2.31                     | 0.45              |
| 8:L5:4273:A:H2'    | 8:L5:4274:A:C8    | 2.51                     | 0.45              |
| 8:L5:4292:A:O2'    | 46:Lo:8:ARG:NH2   | 2.49                     | 0.45              |
| 8:L5:4425:G:OP1    | 44:Lm:100:TYR:OH  | 2.29                     | 0.45              |
| 8:L5:4578:G:H2'    | 8:L5:4579:U:C6    | 2.51                     | 0.45              |
| 32:LZ:77:TYR:CD2   | 35:Lc:39:ARG:HD3  | 2.51                     | 0.45              |
| 33:La:38:LEU:O     | 33:La:42:ARG:NH1  | 2.49                     | 0.45              |
| 35:Lc:18:LEU:O     | 35:Lc:19:GLN:C    | 2.59                     | 0.45              |
| 49:S2:344:U:H2'    | 49:S2:345:U:C6    | 2.51                     | 0.45              |
| 49:S2:570:C:O2     | 71:SY:34:THR:OG1  | 2.25                     | 0.45              |
| 49:S2:1531:A:H2'   | 49:S2:1532:C:C6   | 2.51                     | 0.45              |
| 50:SC:166:ARG:O    | 50:SC:181:PRO:HD3 | 2.16                     | 0.45              |
| 58:SK:29:MET:HE3   | 58:SK:29:MET:HB2  | 1.85                     | 0.45              |
| 58:SK:41:PRO:HD2   | 58:SK:44:HIS:ND1  | 2.30                     | 0.45              |
| 59:SL:125:ILE:HD13 | 59:SL:148:ALA:HB2 | 1.98                     | 0.45              |
| 78:Sf:118:ARG:CB   | 78:Sf:131:PHE:HB3 | 2.45                     | 0.45              |
| 6:B4:57:A:O2'      | 6:B4:59:A:OP2     | 2.21                     | 0.45              |
| 6:B4:61:C:H2'      | 6:B4:62:A:H8      | 1.80                     | 0.45              |
| 19:LM:3:PHE:H      | 25:LS:175:PHE:HZ  | 1.63                     | 0.45              |
| 31:LY:36:LYS:O     | 31:LY:40:GLN:NE2  | 2.48                     | 0.45              |
| 32:LZ:77:TYR:HD2   | 35:Lc:39:ARG:HD3  | 1.81                     | 0.45              |
| 48:Lr:3:ALA:O      | 48:Lr:44:ILE:HD11 | 2.16                     | 0.45              |
| 49:S2:682:U:O2'    | 69:SW:4:MET:SD    | 2.69                     | 0.45              |
| 52:SE:192:ILE:HG13 | 52:SE:243:GLY:HA3 | 1.99                     | 0.45              |
| 54:SG:95:LYS:HB3   | 54:SG:95:LYS:HE3  | 1.73                     | 0.45              |
| 55:SH:50:GLU:OE1   | 55:SH:60:ILE:HG22 | 2.16                     | 0.45              |
| 79:Sg:108:VAL:HA   | 79:Sg:124:SER:HA  | 1.98                     | 0.45              |
| 1:LA:200:ARG:HE    | 1:LA:200:ARG:HB2  | 1.54                     | 0.45              |
| 2:SA:81:ASN:HA     | 2:SA:84:GLN:HE22  | 1.81                     | 0.45              |
| 7:D4:9:A:OP2       | 7:D4:13:C:N4      | 2.48                     | 0.45              |
| 8:L5:1248:C:H2'    | 8:L5:1249:C:C6    | 2.51                     | 0.45              |
| 8:L5:2370:A:N1     | 8:L5:2390:G:O2'   | 2.44                     | 0.45              |
| 8:L5:2494:U:O2'    | 8:L5:2495:U:O4'   | 2.31                     | 0.45              |
| 10:L8:140:C:H2'    | 10:L8:141:C:C6    | 2.52                     | 0.45              |
| 10:L8:154:G:H5''   | 15:LG:89:ARG:NH1  | 2.32                     | 0.45              |
| 14:LF:157:ARG:NH2  | 14:LF:248:ASN:O   | 2.36                     | 0.45              |
| 49:S2:311:C:H5'    | 49:S2:312:G:C5'   | 2.47                     | 0.45              |
| 49:S2:428:OMU:H4'  | 49:S2:429:C:OP2   | 2.11                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:448:A:H5''   | 56:SI:25:ARG:HA    | 1.98                     | 0.45              |
| 49:S2:1407:U:H2'   | 49:S2:1408:U:C6    | 2.52                     | 0.45              |
| 49:S2:1597:C:H4'   | 49:S2:1603:G:O6    | 2.16                     | 0.45              |
| 51:SD:220:THR:HG23 | 51:SD:222:PRO:HD3  | 1.98                     | 0.45              |
| 56:SI:67:TRP:CD1   | 56:SI:191:GLU:OE2  | 2.70                     | 0.45              |
| 65:SS:34:LYS:HE2   | 65:SS:34:LYS:HB3   | 1.69                     | 0.45              |
| 68:SV:77:GLY:HA2   | 68:SV:81:LYS:NZ    | 2.31                     | 0.45              |
| 80:SM:40:LYS:O     | 80:SM:44:LYS:HG2   | 2.15                     | 0.45              |
| 4:SB:168:MET:HG2   | 4:SB:197:ILE:HD13  | 1.98                     | 0.45              |
| 8:L5:171:U:H5''    | 8:L5:172:C:H5      | 1.82                     | 0.45              |
| 8:L5:270:U:H2'     | 8:L5:271:C:C6      | 2.52                     | 0.45              |
| 8:L5:491:G:H2'     | 8:L5:492:U:C6      | 2.52                     | 0.45              |
| 8:L5:1662:C:H2'    | 8:L5:1663:C:C6     | 2.51                     | 0.45              |
| 8:L5:3697:U:H5''   | 8:L5:3698:G:H5'    | 1.97                     | 0.45              |
| 8:L5:4137:C:H2'    | 8:L5:4138:C:H6     | 1.81                     | 0.45              |
| 9:L7:12:U:O3'      | 9:L7:109:U:O2'     | 2.34                     | 0.45              |
| 11:LC:146:GLU:HG2  | 11:LC:175:LYS:HB3  | 1.97                     | 0.45              |
| 28:LV:84:GLN:HG2   | 28:LV:86:LYS:H     | 1.80                     | 0.45              |
| 49:S2:317:C:OP2    | 54:SG:183:ARG:NH1  | 2.47                     | 0.45              |
| 49:S2:601:OMG:H1'  | 49:S2:601:OMG:HM23 | 1.71                     | 0.45              |
| 49:S2:1643:U:H2'   | 49:S2:1644:C:C6    | 2.51                     | 0.45              |
| 52:SE:35:PRO:HD2   | 52:SE:83:PRO:HG2   | 1.98                     | 0.45              |
| 1:LA:8:GLN:O       | 8:L5:3668:C:H5'    | 2.17                     | 0.45              |
| 1:LA:30:ARG:O      | 1:LA:163:ARG:NH1   | 2.40                     | 0.45              |
| 7:D4:6:G:H1'       | 7:D4:7:A:C8        | 2.52                     | 0.45              |
| 8:L5:398:A2M:H8    | 8:L5:398:A2M:OP2   | 2.15                     | 0.45              |
| 8:L5:919:C:H2'     | 8:L5:920:C:C6      | 2.51                     | 0.45              |
| 8:L5:1730:U:H2'    | 8:L5:1731:C:C6     | 2.52                     | 0.45              |
| 8:L5:2499:C:H2'    | 8:L5:2500:U:C6     | 2.51                     | 0.45              |
| 8:L5:2539:C:H2'    | 8:L5:2540:C:H6     | 1.80                     | 0.45              |
| 8:L5:2702:C:H4'    | 27:LU:103:VAL:HG11 | 1.99                     | 0.45              |
| 8:L5:3736:A:O2'    | 8:L5:3737:A:H8     | 1.99                     | 0.45              |
| 8:L5:4688:C:H2'    | 8:L5:4689:U:C6     | 2.52                     | 0.45              |
| 13:LE:201:ILE:HG13 | 13:LE:203:ILE:HG23 | 1.99                     | 0.45              |
| 14:LF:154:ILE:HD11 | 14:LF:194:ILE:HD12 | 1.98                     | 0.45              |
| 49:S2:10:G:H21     | 50:SC:114:LYS:HA   | 1.81                     | 0.45              |
| 49:S2:1678:A2M:O2' | 49:S2:1679:A:H5'   | 2.16                     | 0.45              |
| 51:SD:72:VAL:HG21  | 58:SK:70:TYR:HE1   | 1.81                     | 0.45              |
| 56:SI:6:ASP:OD1    | 56:SI:9:HIS:ND1    | 2.49                     | 0.45              |
| 56:SI:137:LEU:O    | 56:SI:137:LEU:HD12 | 2.15                     | 0.45              |
| 58:SK:60:GLU:HB2   | 58:SK:69:TRP:CD1   | 2.51                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:SS:35:GLY:O     | 65:SS:97:GLN:NE2   | 2.49                     | 0.45              |
| 2:SA:12:GLU:O      | 2:SA:15:VAL:HG12   | 2.17                     | 0.45              |
| 3:LB:240:LEU:HB2   | 3:LB:248:LEU:HA    | 1.99                     | 0.45              |
| 3:LB:300:LYS:HG3   | 3:LB:304:SER:OG    | 2.17                     | 0.45              |
| 8:L5:268:G:H2'     | 8:L5:269:G:C8      | 2.52                     | 0.45              |
| 8:L5:1481:C:H5''   | 8:L5:1482:G:OP2    | 2.16                     | 0.45              |
| 8:L5:1895:G:O2'    | 8:L5:1907:A:N3     | 2.42                     | 0.45              |
| 8:L5:2521:G:H5'    | 8:L5:2640:G:H1'    | 1.99                     | 0.45              |
| 8:L5:4174:U:H2'    | 8:L5:4175:G:C8     | 2.51                     | 0.45              |
| 8:L5:4342:C:O3'    | 46:Lo:37:GLY:HA3   | 2.16                     | 0.45              |
| 14:LF:127:LYS:HB2  | 26:LT:133:ALA:HB3  | 1.99                     | 0.45              |
| 16:LH:151:ILE:HA   | 16:LH:154:VAL:HG22 | 1.99                     | 0.45              |
| 21:LO:41:ILE:HB    | 21:LO:138:LEU:HD22 | 1.98                     | 0.45              |
| 32:LZ:68:ILE:O     | 32:LZ:115:LYS:NZ   | 2.40                     | 0.45              |
| 49:S2:1491:G:H2'   | 49:S2:1492:U:C6    | 2.52                     | 0.45              |
| 63:SQ:19:ALA:HB2   | 63:SQ:75:GLY:HA3   | 1.98                     | 0.45              |
| 63:SQ:21:ALA:HB2   | 63:SQ:72:VAL:HG23  | 1.98                     | 0.45              |
| 3:LB:44:THR:HG21   | 3:LB:186:ASN:HD22  | 1.81                     | 0.45              |
| 4:SB:176:VAL:HG23  | 4:SB:184:VAL:HG21  | 1.98                     | 0.45              |
| 8:L5:1390:G:N2     | 8:L5:1393:G:OP2    | 2.39                     | 0.45              |
| 8:L5:2361:G:O2'    | 8:L5:3859:G:O6     | 2.29                     | 0.45              |
| 8:L5:2439:G:H5'    | 8:L5:2778:G:OP2    | 2.17                     | 0.45              |
| 8:L5:2811:G:N2     | 8:L5:2814:C:OP2    | 2.39                     | 0.45              |
| 8:L5:4088:C:H2'    | 8:L5:4089:G:H8     | 1.82                     | 0.45              |
| 8:L5:4190:U:O2'    | 8:L5:4382:G:OP2    | 2.34                     | 0.45              |
| 8:L5:4415:A:OP1    | 82:LI:154:ARG:NH1  | 2.50                     | 0.45              |
| 8:L5:4621:C:OP1    | 28:LV:48:ARG:HD2   | 2.17                     | 0.45              |
| 10:L8:60:G:OP1     | 30:LX:68:ARG:NH2   | 2.49                     | 0.45              |
| 10:L8:141:C:H5''   | 20:LN:60:VAL:HG21  | 1.99                     | 0.45              |
| 12:LD:223:PHE:HB3  | 12:LD:226:TYR:HB2  | 1.98                     | 0.45              |
| 49:S2:558:G:H2'    | 49:S2:559:G:C8     | 2.51                     | 0.45              |
| 49:S2:1438:A:H2'   | 49:S2:1439:A:C8    | 2.52                     | 0.45              |
| 52:SE:204:SER:OG   | 52:SE:205:PHE:N    | 2.41                     | 0.45              |
| 79:Sg:104:HIS:NE2  | 79:Sg:122:SER:OG   | 2.46                     | 0.45              |
| 81:Le:91:CYS:HB2   | 81:Le:95:TYR:HD2   | 1.81                     | 0.45              |
| 82:LI:191:ILE:HG12 | 82:LI:200:ILE:HG13 | 1.98                     | 0.45              |
| 8:L5:2634:C:H2'    | 8:L5:2635:U:H6     | 1.81                     | 0.45              |
| 8:L5:2765:A:H2'    | 8:L5:2766:A:H8     | 1.82                     | 0.45              |
| 8:L5:2803:U:H2'    | 8:L5:2804:OMC:C6   | 2.52                     | 0.45              |
| 8:L5:4265:U:N3     | 12:LD:17:GLN:O     | 2.50                     | 0.45              |
| 8:L5:4377:G:O6     | 33:La:42:ARG:NH2   | 2.49                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L8:13:G:O2'     | 22:LP:121:LYS:O    | 2.35                     | 0.45              |
| 18:LL:162:LYS:H    | 18:LL:162:LYS:HG2  | 1.56                     | 0.45              |
| 49:S2:107:A:H2'    | 49:S2:108:G:H8     | 1.81                     | 0.45              |
| 49:S2:322:C:H2'    | 49:S2:323:C:C6     | 2.52                     | 0.45              |
| 49:S2:508:A:H3'    | 49:S2:509:G:H8     | 1.81                     | 0.45              |
| 49:S2:1016:U:O2    | 49:S2:1016:U:H2'   | 2.16                     | 0.45              |
| 49:S2:1521:C:OP1   | 65:SS:124:ARG:NH1  | 2.50                     | 0.45              |
| 49:S2:1664:A:HO2'  | 49:S2:1665:G:P     | 2.39                     | 0.45              |
| 49:S2:1845:A:H2'   | 49:S2:1846:G:C8    | 2.51                     | 0.45              |
| 58:SK:80:ARG:NH1   | 58:SK:89:ILE:O     | 2.49                     | 0.45              |
| 59:SL:68:ILE:HG21  | 59:SL:143:LEU:HD11 | 1.99                     | 0.45              |
| 68:SV:65:SER:O     | 68:SV:69:ILE:HG12  | 2.16                     | 0.45              |
| 75:Sc:18:LEU:O     | 75:Sc:29:GLN:HB3   | 2.16                     | 0.45              |
| 82:LI:140:THR:OG1  | 82:LI:141:LYS:N    | 2.50                     | 0.45              |
| 3:LB:55:HIS:C      | 3:LB:56:ILE:HD13   | 2.42                     | 0.45              |
| 8:L5:1081:C:N4     | 8:L5:1082:C:H41    | 2.15                     | 0.45              |
| 8:L5:1906:U:H2'    | 8:L5:1907:A:H8     | 1.81                     | 0.45              |
| 8:L5:2587:A:OP2    | 38:Lg:70:THR:OG1   | 2.23                     | 0.45              |
| 8:L5:2668:G:OP1    | 24:LR:128:LYS:NZ   | 2.50                     | 0.45              |
| 8:L5:4211:C:OP1    | 87:L5:5287:PUT:N1  | 2.43                     | 0.45              |
| 8:L5:4438:U:H2'    | 8:L5:4439:U:O4'    | 2.17                     | 0.45              |
| 12:LD:256:LYS:C    | 12:LD:257:PRO:HG2  | 2.40                     | 0.45              |
| 26:LT:147:GLU:HG3  | 26:LT:148:PRO:HD2  | 1.98                     | 0.45              |
| 49:S2:563:G:N7     | 57:SJ:172:ARG:NH2  | 2.65                     | 0.45              |
| 49:S2:1189:A:H2'   | 49:S2:1190:A:C8    | 2.52                     | 0.45              |
| 49:S2:1797:U:H2'   | 49:S2:1798:C:C6    | 2.51                     | 0.45              |
| 57:SJ:102:ILE:HG22 | 57:SJ:106:LEU:HD12 | 1.99                     | 0.45              |
| 59:SL:22:ARG:HD3   | 59:SL:22:ARG:H     | 1.80                     | 0.45              |
| 62:SP:87:PRO:O     | 62:SP:90:VAL:HG12  | 2.17                     | 0.45              |
| 4:SB:182:LYS:HG3   | 4:SB:231:LEU:HD22  | 1.98                     | 0.45              |
| 8:L5:119:G:N3      | 15:LG:132:ARG:NH1  | 2.64                     | 0.45              |
| 8:L5:1669:A:OP1    | 34:Lb:11:ASN:ND2   | 2.49                     | 0.45              |
| 8:L5:1821:G:H2'    | 8:L5:1821:G:N3     | 2.31                     | 0.45              |
| 8:L5:2458:C:O2     | 8:L5:3671:G:N2     | 2.49                     | 0.45              |
| 8:L5:2562:G:N2     | 8:L5:2564:G:H3'    | 2.32                     | 0.45              |
| 8:L5:2755:A:OP1    | 32:LZ:65:ARG:NH1   | 2.48                     | 0.45              |
| 8:L5:4481:U:H2'    | 8:L5:4482:U:C6     | 2.51                     | 0.45              |
| 8:L5:4535:A:H2'    | 8:L5:4536:OMC:C6   | 2.51                     | 0.45              |
| 14:LF:41:MET:HA    | 14:LF:41:MET:HE3   | 1.99                     | 0.45              |
| 16:LH:129:ARG:HG2  | 16:LH:157:SER:HB3  | 1.99                     | 0.45              |
| 36:Ld:53:ALA:HA    | 36:Ld:88:LEU:HD21  | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:Lm:94:MET:O     | 44:Lm:95:ILE:HD13  | 2.17                     | 0.45              |
| 49:S2:846:G:C4     | 52:SE:19:MET:HE3   | 2.51                     | 0.45              |
| 49:S2:1373:C:O2'   | 64:SR:10:LYS:HE3   | 2.17                     | 0.45              |
| 50:SC:105:GLU:OE1  | 50:SC:212:LYS:HD3  | 2.17                     | 0.45              |
| 52:SE:230:LYS:HE3  | 52:SE:230:LYS:HB2  | 1.70                     | 0.45              |
| 57:SJ:110:LEU:HG   | 57:SJ:130:ILE:HD11 | 1.98                     | 0.45              |
| 57:SJ:137:VAL:HG21 | 57:SJ:147:PHE:CE2  | 2.52                     | 0.45              |
| 1:LA:173:GLY:O     | 47:Lp:69:TRP:NE1   | 2.48                     | 0.44              |
| 8:L5:2459:G:H2'    | 8:L5:2461:G:OP2    | 2.17                     | 0.44              |
| 9:L7:43:U:H4'      | 17:LJ:143:ASP:O    | 2.17                     | 0.44              |
| 10:L8:19:C:H2'     | 10:L8:20:A:C8      | 2.52                     | 0.44              |
| 11:LC:259:LYS:HG2  | 11:LC:263:LEU:HD13 | 1.98                     | 0.44              |
| 18:LL:58:ILE:HG12  | 18:LL:116:ARG:HE   | 1.82                     | 0.44              |
| 23:LQ:22:ASP:O     | 23:LQ:26:ARG:HG3   | 2.17                     | 0.44              |
| 24:LR:165:LYS:HE2  | 24:LR:165:LYS:HB3  | 1.90                     | 0.44              |
| 27:LU:101:ARG:HB2  | 27:LU:115:PHE:HE1  | 1.82                     | 0.44              |
| 49:S2:14:C:H2'     | 49:S2:15:U:C6      | 2.52                     | 0.44              |
| 49:S2:1236:G:H2'   | 49:S2:1237:C:C6    | 2.52                     | 0.44              |
| 53:SF:68:ILE:HD11  | 53:SF:151:ILE:HD11 | 1.99                     | 0.44              |
| 54:SG:3:LEU:HD22   | 54:SG:18:VAL:HG21  | 1.97                     | 0.44              |
| 54:SG:135:PRO:HG2  | 54:SG:141:ILE:HG12 | 1.99                     | 0.44              |
| 66:ST:129:ARG:O    | 66:ST:133:ARG:HG3  | 2.17                     | 0.44              |
| 71:SY:57:VAL:HB    | 71:SY:60:PHE:CE2   | 2.52                     | 0.44              |
| 81:Le:105:SER:O    | 81:Le:109:LYS:HG3  | 2.16                     | 0.44              |
| 3:LB:252:ALA:HB1   | 8:L5:4524:G:N3     | 2.32                     | 0.44              |
| 3:LB:348:ARG:HH12  | 3:LB:351:LEU:HG    | 1.82                     | 0.44              |
| 4:SB:32:ASP:OD1    | 4:SB:43:ASN:ND2    | 2.50                     | 0.44              |
| 4:SB:49:VAL:HG11   | 4:SB:62:LEU:HD21   | 1.99                     | 0.44              |
| 7:D4:11:C:H2'      | 7:D4:12:U:C6       | 2.52                     | 0.44              |
| 8:L5:135:G:P       | 8:L5:135:G:H8      | 2.40                     | 0.44              |
| 8:L5:1633:G:O6     | 8:L5:3918:G:O2'    | 2.30                     | 0.44              |
| 8:L5:3610:A:H2'    | 8:L5:3611:A:C8     | 2.51                     | 0.44              |
| 8:L5:4344:U:H2'    | 8:L5:4345:C:H6     | 1.81                     | 0.44              |
| 9:L7:35:U:O2       | 9:L7:45:U:O2'      | 2.33                     | 0.44              |
| 10:L8:7:U:H2'      | 10:L8:8:U:C6       | 2.52                     | 0.44              |
| 21:LO:10:ASP:CG    | 21:LO:37:ARG:HH21  | 2.25                     | 0.44              |
| 33:La:75:LEU:HD11  | 33:La:133:ALA:HA   | 1.99                     | 0.44              |
| 36:Ld:59:THR:OG1   | 36:Ld:104:THR:OG1  | 2.30                     | 0.44              |
| 40:Li:84:LYS:HE3   | 40:Li:84:LYS:HB3   | 1.67                     | 0.44              |
| 49:S2:1139:C:H2'   | 49:S2:1140:G:O4'   | 2.18                     | 0.44              |
| 49:S2:1649:U:N3    | 49:S2:1675:A:H2    | 2.14                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:SE:73:ASP:HA    | 52:SE:164:LEU:HD13 | 1.99                     | 0.44              |
| 52:SE:206:ASP:OD1  | 52:SE:206:ASP:N    | 2.51                     | 0.44              |
| 80:SM:41:ALA:HB1   | 80:SM:46:GLN:HB2   | 2.00                     | 0.44              |
| 2:SA:110:ASN:ND2   | 49:S2:1351:G:O4'   | 2.51                     | 0.44              |
| 8:L5:97:G:N7       | 18:LL:13:HIS:NE2   | 2.61                     | 0.44              |
| 8:L5:485:C:H3'     | 8:L5:486:C:H5''    | 2.00                     | 0.44              |
| 8:L5:1214:C:O4'    | 34:Lb:91:ARG:NH2   | 2.50                     | 0.44              |
| 8:L5:1316:OMG:H1'  | 8:L5:1316:OMG:HM23 | 1.73                     | 0.44              |
| 8:L5:2079:G:H2'    | 8:L5:2080:U:H6     | 1.82                     | 0.44              |
| 8:L5:2323:C:H2'    | 8:L5:2324:C:C6     | 2.52                     | 0.44              |
| 8:L5:3611:A:H2     | 8:L5:5016:A:C8     | 2.36                     | 0.44              |
| 8:L5:4474:A:OP2    | 8:L5:4476:C:N4     | 2.47                     | 0.44              |
| 9:L7:3:C:H2'       | 9:L7:4:U:H6        | 1.81                     | 0.44              |
| 12:LD:280:VAL:HG12 | 12:LD:284:LYS:HD2  | 1.99                     | 0.44              |
| 15:LG:143:VAL:O    | 15:LG:147:VAL:HG13 | 2.17                     | 0.44              |
| 21:LO:81:TRP:HB2   | 21:LO:104:VAL:HG21 | 2.00                     | 0.44              |
| 22:LP:39:MET:HG2   | 22:LP:43:LYS:HD3   | 1.99                     | 0.44              |
| 49:S2:561:A:O2'    | 49:S2:562:U:H5'    | 2.17                     | 0.44              |
| 49:S2:943:U:C2     | 49:S2:944:A:C8     | 3.06                     | 0.44              |
| 49:S2:1542:C:C2    | 49:S2:1543:U:H5    | 2.36                     | 0.44              |
| 54:SG:48:TYR:CD1   | 54:SG:116:LYS:HA   | 2.52                     | 0.44              |
| 58:SK:15:LEU:O     | 58:SK:19:GLY:HA2   | 2.17                     | 0.44              |
| 64:SR:27:ASP:HB3   | 64:SR:30:THR:HG22  | 1.98                     | 0.44              |
| 66:ST:96:SER:HB3   | 66:ST:99:VAL:HG12  | 1.99                     | 0.44              |
| 78:Sf:132:MET:HE3  | 78:Sf:139:HIS:HB3  | 1.98                     | 0.44              |
| 79:Sg:76:GLN:O     | 79:Sg:92:LEU:HB2   | 2.17                     | 0.44              |
| 8:L5:25:A:C8       | 8:L5:341:G:C8      | 3.05                     | 0.44              |
| 8:L5:262:G:H2'     | 8:L5:263:G:C8      | 2.53                     | 0.44              |
| 8:L5:318:A:H2'     | 8:L5:319:A:C8      | 2.52                     | 0.44              |
| 8:L5:1333:A:H2'    | 8:L5:1334:A:H8     | 1.81                     | 0.44              |
| 8:L5:4593:C:H2'    | 8:L5:4594:U:H6     | 1.83                     | 0.44              |
| 16:LH:89:ARG:HH21  | 16:LH:187:VAL:HG13 | 1.82                     | 0.44              |
| 20:LN:121:VAL:HG11 | 20:LN:131:GLU:HG3  | 1.99                     | 0.44              |
| 42:Lk:33:LYS:HG2   | 42:Lk:46:VAL:HG22  | 1.99                     | 0.44              |
| 49:S2:146:G:O2'    | 49:S2:147:A:H5'    | 2.17                     | 0.44              |
| 49:S2:963:A:H2'    | 49:S2:964:A:C8     | 2.53                     | 0.44              |
| 49:S2:1374:C:H2'   | 49:S2:1375:G:O4'   | 2.18                     | 0.44              |
| 49:S2:1406:G:H2'   | 49:S2:1407:U:C6    | 2.53                     | 0.44              |
| 49:S2:1620:A:H1'   | 49:S2:1624:U:OP2   | 2.17                     | 0.44              |
| 49:S2:1752:C:H2'   | 49:S2:1753:C:O4'   | 2.17                     | 0.44              |
| 49:S2:1801:A:H2'   | 49:S2:1802:C:H6    | 1.83                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:SG:164:LYS:O    | 54:SG:164:LYS:HD3  | 2.18                     | 0.44              |
| 66:ST:51:ASN:HB3   | 66:ST:54:TYR:HD2   | 1.83                     | 0.44              |
| 69:SW:3:ARG:HD3    | 69:SW:6:VAL:HG12   | 1.99                     | 0.44              |
| 69:SW:62:VAL:HG21  | 74:Sb:8:LEU:HD13   | 1.99                     | 0.44              |
| 79:Sg:156:PHE:HE1  | 79:Sg:179:LEU:HD11 | 1.82                     | 0.44              |
| 1:LA:137:ILE:HD11  | 1:LA:149:LYS:HB2   | 1.99                     | 0.44              |
| 3:LB:121:ASN:HD22  | 3:LB:124:LYS:HB2   | 1.82                     | 0.44              |
| 4:SB:42:ARG:HH11   | 4:SB:42:ARG:HG3    | 1.82                     | 0.44              |
| 8:L5:272:U:H2'     | 8:L5:273:U:C6      | 2.53                     | 0.44              |
| 8:L5:1189:G:H2'    | 8:L5:1190:C:C6     | 2.52                     | 0.44              |
| 8:L5:1447:C:C2'    | 8:L5:1448:G:H5'    | 2.48                     | 0.44              |
| 8:L5:2020:U:H2'    | 8:L5:2021:G:H8     | 1.83                     | 0.44              |
| 8:L5:2461:G:H5'    | 20:LN:104:GLU:OE2  | 2.18                     | 0.44              |
| 8:L5:4323:A:H2     | 12:LD:146:LEU:HD23 | 1.83                     | 0.44              |
| 8:L5:4759:C:H2'    | 8:L5:4760:G:C8     | 2.52                     | 0.44              |
| 8:L5:5002:U:H2'    | 8:L5:5003:U:C6     | 2.52                     | 0.44              |
| 13:LE:126:LEU:HD23 | 13:LE:126:LEU:HA   | 1.88                     | 0.44              |
| 19:LM:23:LYS:HB3   | 19:LM:43:THR:CG2   | 2.47                     | 0.44              |
| 22:LP:32:THR:HG21  | 22:LP:87:SER:HB3   | 2.00                     | 0.44              |
| 24:LR:3:MET:HE1    | 24:LR:5:ARG:HE     | 1.83                     | 0.44              |
| 52:SE:200:ARG:O    | 52:SE:200:ARG:HG3  | 2.18                     | 0.44              |
| 55:SH:69:LEU:HD22  | 55:SH:96:ALA:HB2   | 1.98                     | 0.44              |
| 79:Sg:273:GLU:H    | 79:Sg:273:GLU:CD   | 2.23                     | 0.44              |
| 82:LI:206:LEU:O    | 82:LI:210:ARG:HG2  | 2.18                     | 0.44              |
| 3:LB:184:GLN:OE1   | 3:LB:186:ASN:ND2   | 2.50                     | 0.44              |
| 4:SB:225:LEU:O     | 4:SB:229:MET:HG2   | 2.17                     | 0.44              |
| 8:L5:28:C:OP1      | 20:LN:187:SER:OG   | 2.35                     | 0.44              |
| 8:L5:65:A:N6       | 8:L5:75:G:H1'      | 2.33                     | 0.44              |
| 8:L5:139:G:H2'     | 8:L5:140:G:C8      | 2.52                     | 0.44              |
| 8:L5:1646:A:O2'    | 41:Lj:49:TRP:O     | 2.35                     | 0.44              |
| 8:L5:2295:C:H2'    | 8:L5:2296:G:H8     | 1.81                     | 0.44              |
| 8:L5:2619:G:OP1    | 27:LU:79:SER:OG    | 2.34                     | 0.44              |
| 8:L5:4253:A:H4'    | 8:L5:4254:G:O5'    | 2.18                     | 0.44              |
| 14:LF:196:THR:O    | 14:LF:196:THR:OG1  | 2.35                     | 0.44              |
| 23:LQ:18:PRO:HD3   | 23:LQ:52:PHE:CD1   | 2.53                     | 0.44              |
| 25:LS:29:ARG:HE    | 26:LT:150:LEU:HD13 | 1.83                     | 0.44              |
| 30:LX:72:ASP:N     | 30:LX:72:ASP:OD1   | 2.48                     | 0.44              |
| 31:LY:30:MET:HE2   | 31:LY:75:ARG:HG2   | 1.99                     | 0.44              |
| 49:S2:21:U:O2      | 57:SJ:17:ARG:NH2   | 2.50                     | 0.44              |
| 49:S2:1201:U:H2'   | 49:S2:1202:U:C6    | 2.53                     | 0.44              |
| 49:S2:1521:C:H5''  | 65:SS:129:LEU:HD22 | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:SG:144:LEU:HD23 | 54:SG:145:PHE:CD1  | 2.53                     | 0.44              |
| 55:SH:10:LYS:NZ    | 55:SH:46:THR:O     | 2.45                     | 0.44              |
| 58:SK:74:GLU:CD    | 58:SK:74:GLU:H     | 2.22                     | 0.44              |
| 74:Sb:5:LYS:HG3    | 74:Sb:7:LEU:CD2    | 2.48                     | 0.44              |
| 79:Sg:153:CYS:HB3  | 79:Sg:198:VAL:HG12 | 1.98                     | 0.44              |
| 1:LA:20:VAL:HA     | 1:LA:23:ARG:HG3    | 1.98                     | 0.44              |
| 1:LA:117:GLU:HB2   | 1:LA:122:ASP:OD1   | 2.18                     | 0.44              |
| 2:SA:38:ILE:HD13   | 2:SA:47:TYR:HD2    | 1.83                     | 0.44              |
| 4:SB:38:MET:H      | 4:SB:38:MET:HG3    | 1.51                     | 0.44              |
| 6:B4:26:C:H2'      | 6:B4:27:U:C6       | 2.53                     | 0.44              |
| 7:D4:46:G:H3'      | 7:D4:47:U:H5''     | 1.99                     | 0.44              |
| 8:L5:258:G:H2'     | 8:L5:259:C:C6      | 2.51                     | 0.44              |
| 8:L5:1209:U:O2'    | 8:L5:1211:G:H5''   | 2.18                     | 0.44              |
| 8:L5:1445:U:H2'    | 8:L5:1446:C:C5     | 2.53                     | 0.44              |
| 8:L5:4376:A:O2'    | 33:La:42:ARG:NH1   | 2.51                     | 0.44              |
| 8:L5:4646:U:OP2    | 24:LR:62:ARG:NH1   | 2.33                     | 0.44              |
| 10:L8:94:G:C6      | 41:Lj:84:PRO:HG3   | 2.52                     | 0.44              |
| 11:LC:316:LYS:HB2  | 11:LC:324:ILE:HD12 | 2.00                     | 0.44              |
| 17:LJ:10:ASN:HB3   | 17:LJ:13:ARG:HG2   | 2.00                     | 0.44              |
| 20:LN:108:ARG:CZ   | 20:LN:161:MET:HE1  | 2.48                     | 0.44              |
| 25:LS:30:MET:HE1   | 25:LS:47:PHE:HB3   | 2.00                     | 0.44              |
| 47:Lp:22:LEU:O     | 47:Lp:26:VAL:HG12  | 2.18                     | 0.44              |
| 49:S2:27:A2M:HM'3  | 49:S2:27:A2M:H1'   | 1.78                     | 0.44              |
| 49:S2:1336:C:O2'   | 49:S2:1337:4AC:O5' | 2.34                     | 0.44              |
| 49:S2:1407:U:H2'   | 49:S2:1408:U:H6    | 1.82                     | 0.44              |
| 49:S2:1407:U:HO2'  | 63:SQ:11:GLN:HE22  | 1.61                     | 0.44              |
| 50:SC:179:THR:OG1  | 50:SC:221:ASP:O    | 2.27                     | 0.44              |
| 80:SM:81:ASP:CB    | 80:SM:84:LYS:HB2   | 2.47                     | 0.44              |
| 81:Le:22:ARG:HB3   | 81:Le:25:SER:HB3   | 1.99                     | 0.44              |
| 4:SB:120:MET:HE3   | 4:SB:142:PHE:CE2   | 2.53                     | 0.44              |
| 8:L5:1188:C:H2'    | 8:L5:1189:G:H8     | 1.83                     | 0.44              |
| 8:L5:1416:G:H2'    | 8:L5:1417:C:C6     | 2.53                     | 0.44              |
| 8:L5:1847:C:H2'    | 8:L5:1848:C:C6     | 2.53                     | 0.44              |
| 8:L5:4589:A:N1     | 8:L5:4621:C:O2'    | 2.44                     | 0.44              |
| 11:LC:293:LEU:HD22 | 23:LQ:34:PHE:CD2   | 2.53                     | 0.44              |
| 18:LL:123:LYS:HB2  | 39:Lh:122:LYS:O    | 2.18                     | 0.44              |
| 22:LP:69:ARG:HA    | 22:LP:80:GLN:HA    | 2.00                     | 0.44              |
| 32:LZ:30:ASP:OD1   | 32:LZ:30:ASP:N     | 2.34                     | 0.44              |
| 36:Ld:57:MET:HG3   | 36:Ld:88:LEU:HD23  | 1.99                     | 0.44              |
| 48:Lr:49:VAL:HG11  | 48:Lr:97:ILE:HD11  | 1.99                     | 0.44              |
| 49:S2:90:G:H2'     | 49:S2:91:A:O4'     | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1849:G:O2'   | 49:S2:1850:MA6:P   | 2.76                     | 0.44              |
| 54:SG:72:ARG:HE    | 54:SG:72:ARG:HB2   | 1.57                     | 0.44              |
| 57:SJ:82:VAL:HG12  | 57:SJ:87:LEU:HB3   | 2.00                     | 0.44              |
| 66:ST:65:TYR:CD1   | 66:ST:65:TYR:C     | 2.95                     | 0.44              |
| 76:Sd:53:ILE:CD1   | 76:Sd:55:LEU:HD12  | 2.46                     | 0.44              |
| 1:LA:132:ASN:O     | 1:LA:169:VAL:HG12  | 2.18                     | 0.44              |
| 6:B4:8:U:H3        | 6:B4:14:A:H62      | 1.66                     | 0.44              |
| 8:L5:106:A:H2'     | 8:L5:107:G:O4'     | 2.18                     | 0.44              |
| 8:L5:756:G:H2'     | 8:L5:757:G:H8      | 1.83                     | 0.44              |
| 8:L5:2308:A:N3     | 10:L8:19:C:O2'     | 2.48                     | 0.44              |
| 8:L5:2845:A:H61    | 8:L5:3843:C:H42    | 1.65                     | 0.44              |
| 8:L5:3760:A2M:H4'  | 8:L5:3761:C:H5''   | 1.99                     | 0.44              |
| 8:L5:3933:G:H2'    | 8:L5:3934:G:H8     | 1.83                     | 0.44              |
| 8:L5:4536:OMC:HM22 | 8:L5:4537:C:O4'    | 2.18                     | 0.44              |
| 8:L5:4607:A:H8     | 8:L5:4607:A:O5'    | 2.01                     | 0.44              |
| 46:Lo:26:TYR:HB3   | 46:Lo:67:VAL:HB    | 2.00                     | 0.44              |
| 49:S2:140:C:H42    | 49:S2:313:A:H61    | 1.64                     | 0.44              |
| 49:S2:472:C:H4'    | 49:S2:474:G:OP1    | 2.17                     | 0.44              |
| 49:S2:1243:U:H2'   | 49:S2:1244:U:O4'   | 2.18                     | 0.44              |
| 49:S2:1438:A:H2'   | 49:S2:1439:A:H8    | 1.83                     | 0.44              |
| 52:SE:206:ASP:HB2  | 52:SE:222:LEU:HD23 | 1.99                     | 0.44              |
| 53:SF:163:PHE:CD2  | 53:SF:164:ARG:HG3  | 2.53                     | 0.44              |
| 64:SR:67:ARG:HG2   | 64:SR:68:GLY:N     | 2.33                     | 0.44              |
| 3:LB:261:ARG:HB3   | 8:L5:4564:A:O2'    | 2.18                     | 0.43              |
| 8:L5:2622:G:O6     | 27:LU:81:ARG:NH1   | 2.51                     | 0.43              |
| 23:LQ:178:ARG:HA   | 23:LQ:184:ARG:O    | 2.18                     | 0.43              |
| 37:Lf:18:LEU:HG    | 37:Lf:19:ARG:HG3   | 2.00                     | 0.43              |
| 49:S2:605:A:HO2'   | 49:S2:638:C:HO2'   | 1.66                     | 0.43              |
| 49:S2:1511:U:H2'   | 49:S2:1512:C:C6    | 2.54                     | 0.43              |
| 50:SC:233:LEU:HD23 | 50:SC:233:LEU:O    | 2.18                     | 0.43              |
| 75:Sc:10:LYS:HD2   | 75:Sc:34:PHE:HE2   | 1.83                     | 0.43              |
| 79:Sg:188:HIS:HD2  | 79:Sg:219:TRP:CD2  | 2.36                     | 0.43              |
| 1:LA:106:THR:HG22  | 1:LA:106:THR:O     | 2.18                     | 0.43              |
| 7:D4:55:U:O2'      | 7:D4:57:G:N7       | 2.46                     | 0.43              |
| 8:L5:425:U:H2'     | 8:L5:426:A:C8      | 2.53                     | 0.43              |
| 8:L5:3614:G:HO2'   | 8:L5:3615:G:P      | 2.36                     | 0.43              |
| 11:LC:150:LEU:HB3  | 11:LC:151:PRO:HD3  | 2.00                     | 0.43              |
| 12:LD:256:LYS:HA   | 12:LD:257:PRO:CG   | 2.48                     | 0.43              |
| 17:LJ:93:GLU:HB2   | 17:LJ:175:LEU:HD11 | 2.00                     | 0.43              |
| 19:LM:7:VAL:HG21   | 19:LM:52:PHE:CE1   | 2.53                     | 0.43              |
| 22:LP:126:ARG:HG3  | 22:LP:140:MET:SD   | 2.59                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:LY:48:PRO:O     | 31:LY:115:ARG:NH2  | 2.36                     | 0.43              |
| 49:S2:120:U:H1'    | 52:SE:33:THR:O     | 2.18                     | 0.43              |
| 49:S2:1335:G:O2'   | 49:S2:1336:C:H5'   | 2.18                     | 0.43              |
| 51:SD:64:ARG:O     | 51:SD:68:GLU:HG3   | 2.18                     | 0.43              |
| 52:SE:19:MET:HB3   | 52:SE:19:MET:HE2   | 1.57                     | 0.43              |
| 54:SG:5:ILE:CG2    | 54:SG:124:LEU:HD21 | 2.48                     | 0.43              |
| 61:SO:61:LYS:HD2   | 61:SO:76:LEU:HB3   | 2.00                     | 0.43              |
| 73:Sa:74:CYS:SG    | 73:Sa:77:CYS:N     | 2.78                     | 0.43              |
| 76:Sd:16:GLN:O     | 76:Sd:27:ARG:HD3   | 2.18                     | 0.43              |
| 4:SB:57:ILE:HG22   | 4:SB:59:SER:H      | 1.83                     | 0.43              |
| 5:A4:46:A:H2'      | 5:A4:47:A:H8       | 1.81                     | 0.43              |
| 6:B4:52:G:H2'      | 6:B4:53:A:C8       | 2.53                     | 0.43              |
| 7:D4:18:G:H4'      | 7:D4:60:U:C5       | 2.54                     | 0.43              |
| 8:L5:346:G:OP1     | 31:LY:8:THR:HG23   | 2.18                     | 0.43              |
| 8:L5:1879:C:O2'    | 8:L5:1891:A:N3     | 2.50                     | 0.43              |
| 8:L5:2580:U:O2'    | 32:LZ:79:HIS:ND1   | 2.47                     | 0.43              |
| 8:L5:4154:G:H2'    | 8:L5:4155:C:C6     | 2.54                     | 0.43              |
| 11:LC:134:PRO:O    | 11:LC:138:MET:HG2  | 2.17                     | 0.43              |
| 13:LE:281:ILE:HG23 | 13:LE:286:LEU:HD11 | 1.99                     | 0.43              |
| 16:LH:37:ASP:C     | 16:LH:37:ASP:OD1   | 2.61                     | 0.43              |
| 17:LJ:40:LEU:O     | 17:LJ:44:THR:HG23  | 2.18                     | 0.43              |
| 17:LJ:159:LYS:O    | 17:LJ:163:MET:HG3  | 2.18                     | 0.43              |
| 24:LR:8:LYS:HE3    | 24:LR:24:LEU:HD13  | 2.01                     | 0.43              |
| 37:Lf:5:LEU:HD23   | 37:Lf:5:LEU:HA     | 1.85                     | 0.43              |
| 43:Ll:21:ARG:HG2   | 43:Ll:22:PRO:HD2   | 2.00                     | 0.43              |
| 49:S2:656:G:N2     | 49:S2:663:C:H5''   | 2.33                     | 0.43              |
| 49:S2:1059:G:O6    | 49:S2:1060:A:N6    | 2.51                     | 0.43              |
| 58:SK:52:LEU:HB3   | 58:SK:58:VAL:HG22  | 2.00                     | 0.43              |
| 61:SO:57:THR:OG1   | 61:SO:60:MET:HG3   | 2.19                     | 0.43              |
| 61:SO:98:ARG:HE    | 61:SO:134:PRO:HD3  | 1.83                     | 0.43              |
| 77:Se:98:LYS:HA    | 77:Se:98:LYS:HD3   | 1.66                     | 0.43              |
| 78:Sf:143:LYS:HB3  | 78:Sf:143:LYS:HE3  | 1.78                     | 0.43              |
| 82:LI:38:ARG:NH1   | 82:LI:45:GLU:OE1   | 2.48                     | 0.43              |
| 82:LI:184:MET:HE2  | 82:LI:189:ARG:CD   | 2.48                     | 0.43              |
| 3:LB:117:ARG:NH2   | 3:LB:178:ALA:O     | 2.41                     | 0.43              |
| 6:B4:33:C:H2'      | 6:B4:34:A:C8       | 2.53                     | 0.43              |
| 8:L5:454:U:H2'     | 8:L5:455:C:C6      | 2.53                     | 0.43              |
| 8:L5:682:G:H2'     | 8:L5:683:C:C6      | 2.54                     | 0.43              |
| 8:L5:1391:A:N3     | 8:L5:4364:G:O2'    | 2.39                     | 0.43              |
| 8:L5:2265:G:OP1    | 48:Lr:35:ARG:NH2   | 2.32                     | 0.43              |
| 8:L5:2399:G:O2'    | 8:L5:2822:G:O2'    | 2.35                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:L5:5001:U:H2'   | 8:L5:5002:U:O4'    | 2.18                     | 0.43              |
| 9:L7:63:C:H1'     | 12:LD:280:VAL:HG11 | 1.99                     | 0.43              |
| 10:L8:69:U:H2'    | 10:L8:70:G:O4'     | 2.18                     | 0.43              |
| 29:LW:20:ARG:HE   | 29:LW:20:ARG:HB2   | 1.68                     | 0.43              |
| 49:S2:1109:C:O2'  | 49:S2:1110:G:O4'   | 2.33                     | 0.43              |
| 52:SE:211:LYS:HB3 | 52:SE:211:LYS:HE2  | 1.87                     | 0.43              |
| 54:SG:32:MET:HE2  | 54:SG:65:GLN:HB2   | 2.01                     | 0.43              |
| 60:SN:26:LEU:HD21 | 60:SN:60:VAL:HG12  | 1.99                     | 0.43              |
| 67:SU:61:LEU:HD22 | 67:SU:82:MET:HE2   | 2.00                     | 0.43              |
| 3:LB:80:GLU:CD    | 3:LB:326:VAL:HG23  | 2.43                     | 0.43              |
| 3:LB:214:ASP:HB3  | 3:LB:283:LYS:NZ    | 2.33                     | 0.43              |
| 3:LB:238:LYS:HE2  | 3:LB:238:LYS:HB2   | 1.76                     | 0.43              |
| 5:A4:51:U:O2'     | 5:A4:52:U:O4'      | 2.36                     | 0.43              |
| 8:L5:2413:U:H2'   | 8:L5:2414:G:H8     | 1.81                     | 0.43              |
| 8:L5:2676:A:OP2   | 8:L5:2676:A:H8     | 2.02                     | 0.43              |
| 8:L5:4642:U:H2'   | 8:L5:4643:G:C8     | 2.53                     | 0.43              |
| 8:L5:4875:G:H2'   | 25:LS:169:THR:HB   | 2.00                     | 0.43              |
| 8:L5:5004:C:H2'   | 8:L5:5005:G:O4'    | 2.18                     | 0.43              |
| 12:LD:289:ARG:HD3 | 12:LD:293:ARG:NH2  | 2.33                     | 0.43              |
| 14:LF:75:ALA:HB2  | 26:LT:140:PHE:CE2  | 2.53                     | 0.43              |
| 16:LH:20:LEU:HD12 | 16:LH:47:LEU:HB2   | 2.01                     | 0.43              |
| 17:LJ:59:SER:C    | 17:LJ:61:GLY:H     | 2.27                     | 0.43              |
| 19:LM:52:PHE:CD1  | 19:LM:55:MET:HE3   | 2.54                     | 0.43              |
| 27:LU:19:LEU:HD13 | 27:LU:77:PRO:HA    | 2.00                     | 0.43              |
| 27:LU:56:LEU:HB3  | 27:LU:61:VAL:HB    | 2.01                     | 0.43              |
| 33:La:82:VAL:HG13 | 33:La:101:ILE:HG23 | 1.99                     | 0.43              |
| 49:S2:59:U:H5''   | 49:S2:503:C:N4     | 2.34                     | 0.43              |
| 57:SJ:29:LEU:HD23 | 77:Se:115:PHE:HE2  | 1.83                     | 0.43              |
| 57:SJ:179:LYS:HD2 | 57:SJ:179:LYS:HA   | 1.77                     | 0.43              |
| 4:SB:48:LEU:HD23  | 4:SB:48:LEU:H      | 1.84                     | 0.43              |
| 8:L5:424:U:H2'    | 8:L5:425:U:C6      | 2.53                     | 0.43              |
| 8:L5:683:C:H2'    | 8:L5:684:G:O4'     | 2.19                     | 0.43              |
| 8:L5:2624:G:H2'   | 8:L5:2625:U:H6     | 1.84                     | 0.43              |
| 8:L5:2675:G:H4'   | 8:L5:2676:A:O5'    | 2.18                     | 0.43              |
| 8:L5:3619:G:H5''  | 8:L5:3620:G:H5''   | 2.01                     | 0.43              |
| 8:L5:4661:G:H2'   | 8:L5:4662:C:C6     | 2.54                     | 0.43              |
| 10:L8:64:U:C2     | 10:L8:65:A:C8      | 3.07                     | 0.43              |
| 14:LF:92:VAL:HG13 | 14:LF:142:TRP:HB3  | 2.00                     | 0.43              |
| 17:LJ:143:ASP:N   | 17:LJ:143:ASP:OD1  | 2.52                     | 0.43              |
| 25:LS:164:LYS:HD2 | 25:LS:164:LYS:HA   | 1.87                     | 0.43              |
| 31:LY:82:ILE:HG22 | 31:LY:83:GLU:N     | 2.34                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:Lc:99:PRO:CB    | 35:Lc:102:SER:HB3  | 2.47                     | 0.43              |
| 42:Lk:31:ASN:HB3   | 42:Lk:48:THR:HG22  | 2.00                     | 0.43              |
| 49:S2:1100:A:OP1   | 64:SR:129:LYS:HE3  | 2.18                     | 0.43              |
| 49:S2:1164:G:O2'   | 49:S2:1165:G:H5'   | 2.18                     | 0.43              |
| 49:S2:1199:A:H2'   | 49:S2:1200:A:C8    | 2.54                     | 0.43              |
| 49:S2:1288:OMU:HN3 | 49:S2:1311:C:H42   | 1.67                     | 0.43              |
| 57:SJ:78:LEU:HD11  | 57:SJ:94:LEU:CB    | 2.48                     | 0.43              |
| 70:SX:94:ILE:HD13  | 70:SX:125:VAL:HG23 | 2.00                     | 0.43              |
| 75:Sc:35:MET:HE3   | 75:Sc:35:MET:HB3   | 1.76                     | 0.43              |
| 82:LI:200:ILE:HG21 | 82:LI:212:LEU:CD2  | 2.48                     | 0.43              |
| 7:D4:24:G:H2'      | 7:D4:25:C:C6       | 2.53                     | 0.43              |
| 8:L5:1341:U:H2'    | 8:L5:1342:A:C8     | 2.54                     | 0.43              |
| 8:L5:1341:U:H2'    | 8:L5:1342:A:H8     | 1.84                     | 0.43              |
| 8:L5:1971:C:C2     | 8:L5:2000:G:H2'    | 2.54                     | 0.43              |
| 8:L5:3700:C:O2'    | 8:L5:3774:A:N3     | 2.45                     | 0.43              |
| 8:L5:4705:A:H2'    | 8:L5:4706:G:O4'    | 2.19                     | 0.43              |
| 10:L8:153:C:H5'    | 15:LG:185:LYS:HD3  | 2.00                     | 0.43              |
| 15:LG:180:PRO:HG2  | 15:LG:219:VAL:HG13 | 2.00                     | 0.43              |
| 16:LH:41:ILE:HD12  | 16:LH:73:ILE:HD11  | 1.99                     | 0.43              |
| 19:LM:50:MET:HE3   | 19:LM:50:MET:HB2   | 1.77                     | 0.43              |
| 49:S2:1099:G:H2'   | 49:S2:1100:A:O4'   | 2.19                     | 0.43              |
| 49:S2:1378:A:H4'   | 49:S2:1379:A:O5'   | 2.18                     | 0.43              |
| 51:SD:93:THR:O     | 51:SD:93:THR:OG1   | 2.36                     | 0.43              |
| 56:SI:203:LYS:HD2  | 56:SI:203:LYS:HA   | 1.74                     | 0.43              |
| 59:SL:104:LYS:CE   | 70:SX:8:ARG:HH21   | 2.32                     | 0.43              |
| 60:SN:67:THR:OG1   | 60:SN:68:GLY:N     | 2.51                     | 0.43              |
| 61:SO:97:LEU:HD21  | 61:SO:112:ALA:HB1  | 2.01                     | 0.43              |
| 70:SX:105:PHE:CE2  | 70:SX:112:VAL:HG22 | 2.53                     | 0.43              |
| 80:SM:59:PRO:HA    | 80:SM:62:VAL:HG22  | 2.00                     | 0.43              |
| 2:SA:205:ARG:NH2   | 2:SA:210:ILE:HG12  | 2.34                     | 0.43              |
| 8:L5:266:C:H2'     | 8:L5:267:G:C8      | 2.54                     | 0.43              |
| 8:L5:1733:G:N3     | 8:L5:4214:A:H2'    | 2.33                     | 0.43              |
| 8:L5:3611:A:H2     | 8:L5:5016:A:H8     | 1.67                     | 0.43              |
| 8:L5:4085:A:OP1    | 30:LX:45:THR:HG22  | 2.18                     | 0.43              |
| 8:L5:4136:G:H2'    | 8:L5:4137:C:C6     | 2.54                     | 0.43              |
| 8:L5:4342:C:H2'    | 8:L5:4343:U:H6     | 1.84                     | 0.43              |
| 8:L5:4372:U:O2     | 8:L5:4377:G:O2'    | 2.23                     | 0.43              |
| 8:L5:4749:C:H2'    | 8:L5:4750:G:O4'    | 2.18                     | 0.43              |
| 10:L8:3:A:O2'      | 22:LP:61:ARG:HD2   | 2.18                     | 0.43              |
| 13:LE:264:ILE:HD12 | 13:LE:267:LEU:HD22 | 2.01                     | 0.43              |
| 14:LF:247:MET:HE2  | 14:LF:247:MET:HB3  | 1.96                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LL:80:GLU:OE2   | 18:LL:102:ARG:NH2  | 2.51                     | 0.43              |
| 19:LM:6:PHE:O      | 19:LM:11:ARG:HD3   | 2.18                     | 0.43              |
| 26:LT:46:GLY:O     | 26:LT:49:GLN:NE2   | 2.51                     | 0.43              |
| 30:LX:145:ASP:C    | 30:LX:145:ASP:OD2  | 2.61                     | 0.43              |
| 31:LY:108:ARG:HB3  | 31:LY:108:ARG:CZ   | 2.48                     | 0.43              |
| 32:LZ:126:LYS:HD3  | 32:LZ:126:LYS:N    | 2.34                     | 0.43              |
| 33:La:100:ILE:HG12 | 33:La:123:ILE:HB   | 2.00                     | 0.43              |
| 42:Lk:26:LYS:HB2   | 42:Lk:69:LEU:HD12  | 2.01                     | 0.43              |
| 49:S2:106:C:H2'    | 49:S2:107:A:C8     | 2.51                     | 0.43              |
| 49:S2:604:A:O2'    | 49:S2:605:A:OP1    | 2.34                     | 0.43              |
| 49:S2:1387:G:H2'   | 49:S2:1388:A:O4'   | 2.19                     | 0.43              |
| 52:SE:115:THR:HG22 | 52:SE:117:GLU:N    | 2.32                     | 0.43              |
| 54:SG:176:ILE:HB   | 54:SG:179:LEU:HD12 | 2.01                     | 0.43              |
| 79:Sg:107:ASP:OD2  | 79:Sg:125:ARG:NH1  | 2.52                     | 0.43              |
| 80:SM:29:ASP:C     | 80:SM:29:ASP:OD1   | 2.62                     | 0.43              |
| 80:SM:93:LYS:HB3   | 80:SM:102:LYS:H    | 1.83                     | 0.43              |
| 1:LA:28:ARG:HB2    | 1:LA:123:ARG:HB2   | 2.01                     | 0.43              |
| 3:LB:307:TYR:HD2   | 3:LB:366:LYS:HA    | 1.84                     | 0.43              |
| 8:L5:418:A:H4'     | 8:L5:2311:C:H5'    | 2.01                     | 0.43              |
| 8:L5:952:G:H2'     | 8:L5:953:C:C6      | 2.54                     | 0.43              |
| 8:L5:1251:C:H2'    | 8:L5:1252:C:C6     | 2.54                     | 0.43              |
| 8:L5:1576:G:OP2    | 8:L5:1576:G:H8     | 2.02                     | 0.43              |
| 8:L5:4220:A:OP2    | 26:LT:2:THR:HG23   | 2.18                     | 0.43              |
| 8:L5:4538:G:H2'    | 8:L5:4539:U:H6     | 1.84                     | 0.43              |
| 8:L5:4586:G:O6     | 8:L5:4717:A:N6     | 2.52                     | 0.43              |
| 8:L5:4700:A:C2     | 16:LH:69:THR:HG22  | 2.52                     | 0.43              |
| 8:L5:4891:G:H21    | 19:LM:118:MET:HE1  | 1.84                     | 0.43              |
| 9:L7:23:A:C2       | 9:L7:118:C:H1'     | 2.53                     | 0.43              |
| 14:LF:30:ILE:O     | 14:LF:34:ARG:HG3   | 2.18                     | 0.43              |
| 14:LF:228:VAL:HA   | 25:LS:39:VAL:HG22  | 2.00                     | 0.43              |
| 31:LY:98:GLY:C     | 31:LY:99:ILE:HD12  | 2.44                     | 0.43              |
| 37:Lf:106:TYR:HB2  | 37:Lf:107:PRO:HD3  | 2.01                     | 0.43              |
| 49:S2:1101:U:H2'   | 49:S2:1102:G:H8    | 1.83                     | 0.43              |
| 51:SD:72:VAL:HG21  | 58:SK:70:TYR:CE1   | 2.54                     | 0.43              |
| 59:SL:135:SER:HB3  | 59:SL:138:VAL:HG22 | 2.00                     | 0.43              |
| 60:SN:88:LEU:HD12  | 60:SN:88:LEU:HA    | 1.86                     | 0.43              |
| 66:ST:14:PHE:HZ    | 66:ST:131:LEU:HG   | 1.84                     | 0.43              |
| 66:ST:73:GLY:H     | 66:ST:76:THR:HG23  | 1.83                     | 0.43              |
| 69:SW:3:ARG:HH22   | 69:SW:28:ARG:HH21  | 1.66                     | 0.43              |
| 3:LB:103:LYS:HB2   | 3:LB:103:LYS:HE2   | 1.78                     | 0.43              |
| 3:LB:285:TYR:CE1   | 3:LB:334:LYS:HB2   | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:SB:198:GLU:O     | 4:SB:202:GLN:NE2   | 2.49                     | 0.43              |
| 8:L5:1431:C:H2'    | 8:L5:1432:G:O4'    | 2.19                     | 0.43              |
| 8:L5:1969:G:OP2    | 8:L5:1970:A:N6     | 2.48                     | 0.43              |
| 8:L5:2309:G:O2'    | 10:L8:18:U:O2      | 2.36                     | 0.43              |
| 8:L5:2465:C:H2'    | 8:L5:2466:G:O4'    | 2.19                     | 0.43              |
| 8:L5:2782:U:OP2    | 43:L1:10:LYS:NZ    | 2.43                     | 0.43              |
| 8:L5:4139:G:N2     | 8:L5:4140:C:H41    | 2.17                     | 0.43              |
| 8:L5:4417:C:H2'    | 8:L5:4418:G:O4'    | 2.19                     | 0.43              |
| 8:L5:4577:U:H2'    | 8:L5:4578:G:C8     | 2.54                     | 0.43              |
| 10:L8:93:C:OP1     | 41:Lj:76:HIS:NE2   | 2.42                     | 0.43              |
| 11:LC:138:MET:HB3  | 11:LC:144:ILE:HG12 | 2.00                     | 0.43              |
| 18:LL:7:GLY:O      | 33:La:49:HIS:NE2   | 2.46                     | 0.43              |
| 32:LZ:22:LYS:NZ    | 32:LZ:132:GLN:O    | 2.34                     | 0.43              |
| 32:LZ:25:ILE:HA    | 32:LZ:43:VAL:HG12  | 2.01                     | 0.43              |
| 37:Lf:29:LYS:HB2   | 37:Lf:83:MET:SD    | 2.59                     | 0.43              |
| 47:Lp:45:THR:O     | 47:Lp:45:THR:OG1   | 2.32                     | 0.43              |
| 49:S2:484:A:H8     | 49:S2:484:A:OP2    | 2.02                     | 0.43              |
| 49:S2:1713:C:H2'   | 49:S2:1714:U:H6    | 1.83                     | 0.43              |
| 50:SC:232:THR:HG22 | 50:SC:234:GLY:H    | 1.84                     | 0.43              |
| 51:SD:220:THR:OG1  | 51:SD:221:THR:N    | 2.52                     | 0.43              |
| 56:SI:193:LYS:HD3  | 56:SI:193:LYS:HA   | 1.83                     | 0.43              |
| 63:SQ:42:ILE:HD13  | 63:SQ:42:ILE:HA    | 1.85                     | 0.43              |
| 66:ST:88:MET:HE2   | 66:ST:88:MET:HB3   | 1.88                     | 0.43              |
| 69:SW:26:LEU:HB2   | 74:Sb:7:LEU:HD12   | 2.00                     | 0.43              |
| 4:SB:123:ALA:HB2   | 4:SB:165:ARG:HG3   | 2.00                     | 0.42              |
| 8:L5:223:G:H4'     | 8:L5:225:G:C8      | 2.54                     | 0.42              |
| 8:L5:1295:C:H4'    | 8:L5:1296:G:C8     | 2.54                     | 0.42              |
| 8:L5:3588:C:H3'    | 8:L5:3589:G:H8     | 1.84                     | 0.42              |
| 8:L5:4685:U:OP1    | 44:Lm:112:LYS:HD2  | 2.19                     | 0.42              |
| 10:L8:52:A:O2'     | 43:Ll:19:GLN:O     | 2.37                     | 0.42              |
| 15:LG:106:THR:HG22 | 15:LG:195:HIS:CE1  | 2.54                     | 0.42              |
| 15:LG:228:ASP:OD1  | 15:LG:228:ASP:N    | 2.52                     | 0.42              |
| 18:LL:129:ARG:HE   | 18:LL:129:ARG:HB3  | 1.60                     | 0.42              |
| 19:LM:95:ILE:C     | 19:LM:97:ALA:H     | 2.27                     | 0.42              |
| 35:Lc:38:ILE:HG21  | 35:Lc:63:TYR:HB3   | 2.00                     | 0.42              |
| 38:Lg:76:ARG:HG2   | 38:Lg:77:ALA:N     | 2.34                     | 0.42              |
| 49:S2:1665:G:C8    | 66:ST:88:MET:HE3   | 2.53                     | 0.42              |
| 49:S2:1700:C:O2    | 49:S2:1834:A:N6    | 2.52                     | 0.42              |
| 59:SL:55:TYR:CD2   | 59:SL:115:PRO:HG2  | 2.54                     | 0.42              |
| 61:SO:82:ALA:HB2   | 61:SO:119:LEU:HD23 | 2.01                     | 0.42              |
| 68:SV:2:GLN:NE2    | 68:SV:8:PHE:HE1    | 2.17                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 79:Sg:223:GLU:OE1   | 79:Sg:225:LYS:HG2  | 2.19                     | 0.42              |
| 80:SM:68:LEU:HD23   | 80:SM:68:LEU:HA    | 1.87                     | 0.42              |
| 8:L5:270:U:H2'      | 8:L5:271:C:H6      | 1.84                     | 0.42              |
| 8:L5:1187:G:H2'     | 8:L5:1188:C:O4'    | 2.19                     | 0.42              |
| 8:L5:1504:G:H2'     | 8:L5:1505:C:H6     | 1.84                     | 0.42              |
| 8:L5:3744:OMG:HM23  | 8:L5:3744:OMG:H1'  | 1.84                     | 0.42              |
| 8:L5:4460:U:H2'     | 8:L5:4461:C:H6     | 1.84                     | 0.42              |
| 8:L5:4642:U:H2'     | 8:L5:4643:G:H8     | 1.82                     | 0.42              |
| 12:LD:234:ASP:O     | 12:LD:235:MET:HG2  | 2.19                     | 0.42              |
| 23:LQ:85:THR:HA     | 23:LQ:104:ARG:O    | 2.19                     | 0.42              |
| 28:LV:74:LYS:HE2    | 28:LV:74:LYS:HB3   | 1.71                     | 0.42              |
| 28:LV:96:LEU:HD13   | 29:LW:20:ARG:HG2   | 2.01                     | 0.42              |
| 32:LZ:36:ARG:HG2    | 32:LZ:38:TYR:CZ    | 2.54                     | 0.42              |
| 36:Ld:37:GLY:O      | 36:Ld:41:ARG:HG2   | 2.19                     | 0.42              |
| 40:Li:79:THR:OG1    | 40:Li:82:ARG:HG3   | 2.19                     | 0.42              |
| 48:Lr:97:ILE:HG21   | 48:Lr:107:ARG:HB2  | 2.01                     | 0.42              |
| 49:S2:553:U:H5      | 49:S2:554:A:C4     | 2.38                     | 0.42              |
| 49:S2:560:A:H5'     | 57:SJ:174:LYS:HB2  | 2.01                     | 0.42              |
| 49:S2:1227:G:C2     | 49:S2:1228:A:C8    | 3.06                     | 0.42              |
| 49:S2:1383:A2M:HM'3 | 49:S2:1383:A2M:H1' | 1.78                     | 0.42              |
| 49:S2:1544:C:O2'    | 63:SQ:75:GLY:O     | 2.13                     | 0.42              |
| 49:S2:1633:A:H2'    | 49:S2:1634:A:C8    | 2.54                     | 0.42              |
| 50:SC:165:VAL:HG21  | 50:SC:217:ALA:HB1  | 2.01                     | 0.42              |
| 54:SG:153:VAL:HG23  | 54:SG:176:ILE:HD13 | 2.00                     | 0.42              |
| 58:SK:15:LEU:HD23   | 58:SK:79:LEU:HD11  | 2.00                     | 0.42              |
| 61:SO:31:CYS:HA     | 61:SO:43:HIS:O     | 2.19                     | 0.42              |
| 62:SP:41:GLN:HG3    | 62:SP:84:ILE:HG21  | 2.01                     | 0.42              |
| 69:SW:30:CYS:SG     | 69:SW:31:SER:N     | 2.91                     | 0.42              |
| 71:SY:92:ALA:HB2    | 71:SY:97:TYR:HB3   | 2.01                     | 0.42              |
| 8:L5:40:G:N2        | 8:L5:4380:A:H62    | 2.17                     | 0.42              |
| 8:L5:1346:C:H2'     | 8:L5:1347:G:H8     | 1.84                     | 0.42              |
| 12:LD:242:LYS:HB2   | 12:LD:242:LYS:HE3  | 1.83                     | 0.42              |
| 13:LE:190:HIS:ND1   | 13:LE:192:LYS:HB2  | 2.34                     | 0.42              |
| 15:LG:63:LEU:HD22   | 20:LN:33:LEU:HD21  | 2.02                     | 0.42              |
| 23:LQ:65:ARG:HH12   | 23:LQ:142:PRO:HB3  | 1.85                     | 0.42              |
| 25:LS:147:ASP:N     | 25:LS:147:ASP:OD1  | 2.47                     | 0.42              |
| 26:LT:71:ALA:HA     | 26:LT:92:ARG:HA    | 2.00                     | 0.42              |
| 29:LW:4:GLU:OE2     | 29:LW:20:ARG:NH2   | 2.52                     | 0.42              |
| 32:LZ:115:LYS:NZ    | 32:LZ:119:GLU:OE2  | 2.38                     | 0.42              |
| 36:Ld:68:LEU:CB     | 36:Ld:108:TYR:HB2  | 2.48                     | 0.42              |
| 51:SD:162:ASP:N     | 51:SD:163:PRO:HD2  | 2.34                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:SI:75:LYS:HB3  | 56:SI:75:LYS:HE2   | 1.86                     | 0.42              |
| 71:SY:4:THR:HB    | 71:SY:5:VAL:H      | 1.70                     | 0.42              |
| 8:L5:153:G:H2'    | 8:L5:154:G:H8      | 1.84                     | 0.42              |
| 8:L5:500:G:H1'    | 8:L5:504:G:H3'     | 2.01                     | 0.42              |
| 8:L5:654:C:H2'    | 8:L5:655:C:C6      | 2.54                     | 0.42              |
| 8:L5:1246:G:H2'   | 8:L5:1247:U:H6     | 1.85                     | 0.42              |
| 8:L5:1248:C:H2'   | 8:L5:1249:C:H6     | 1.83                     | 0.42              |
| 8:L5:1518:A:N6    | 18:LL:19:GLN:OE1   | 2.53                     | 0.42              |
| 8:L5:2411:C:H2'   | 8:L5:2412:A:C8     | 2.53                     | 0.42              |
| 8:L5:2844:A:N6    | 8:L5:3839:G:O2'    | 2.53                     | 0.42              |
| 8:L5:4112:C:H2'   | 8:L5:4113:U:H5'    | 2.00                     | 0.42              |
| 13:LE:276:ALA:HB1 | 37:Lf:3:GLY:HA3    | 2.00                     | 0.42              |
| 24:LR:157:ASP:OD1 | 24:LR:157:ASP:C    | 2.61                     | 0.42              |
| 35:Lc:19:GLN:OE1  | 35:Lc:20:LEU:N     | 2.52                     | 0.42              |
| 37:Lf:57:THR:HG21 | 37:Lf:68:ARG:HG2   | 2.02                     | 0.42              |
| 49:S2:5:U:H2'     | 49:S2:6:G:C8       | 2.55                     | 0.42              |
| 49:S2:388:U:H2'   | 49:S2:389:A:C8     | 2.54                     | 0.42              |
| 52:SE:60:GLU:OE1  | 71:SY:20:ARG:NH2   | 2.49                     | 0.42              |
| 52:SE:89:VAL:HG13 | 52:SE:114:ILE:HD11 | 2.02                     | 0.42              |
| 53:SF:142:SER:OG  | 75:Sc:49:PRO:O     | 2.26                     | 0.42              |
| 54:SG:61:PHE:CD2  | 54:SG:72:ARG:HD3   | 2.54                     | 0.42              |
| 57:SJ:174:LYS:HB2 | 57:SJ:174:LYS:HE3  | 1.71                     | 0.42              |
| 65:SS:40:TYR:HA   | 65:SS:83:PHE:HE2   | 1.85                     | 0.42              |
| 67:SU:55:ARG:HG2  | 67:SU:87:ARG:CD    | 2.50                     | 0.42              |
| 71:SY:16:ARG:CZ   | 71:SY:16:ARG:HB2   | 2.49                     | 0.42              |
| 71:SY:23:MET:HE1  | 71:SY:44:LEU:HD11  | 2.00                     | 0.42              |
| 75:Sc:23:SER:O    | 75:Sc:26:GLN:NE2   | 2.53                     | 0.42              |
| 79:Sg:129:ILE:HB  | 79:Sg:142:VAL:HG23 | 2.01                     | 0.42              |
| 82:LI:87:ILE:HG12 | 82:LI:138:ILE:HG12 | 2.00                     | 0.42              |
| 3:LB:108:GLU:OE2  | 3:LB:138:GLN:NE2   | 2.52                     | 0.42              |
| 3:LB:161:ARG:HG2  | 3:LB:184:GLN:HA    | 2.02                     | 0.42              |
| 8:L5:754:U:H2'    | 8:L5:755:C:C6      | 2.55                     | 0.42              |
| 8:L5:958:G:H21    | 13:LE:125:LEU:H    | 1.68                     | 0.42              |
| 8:L5:2055:G:H4'   | 8:L5:2056:G:OP2    | 2.20                     | 0.42              |
| 8:L5:3635:A:C8    | 8:L5:3692:A:C8     | 3.08                     | 0.42              |
| 8:L5:4578:G:H2'   | 8:L5:4579:U:H6     | 1.83                     | 0.42              |
| 8:L5:4699:U:H4'   | 8:L5:4700:A:OP1    | 2.20                     | 0.42              |
| 8:L5:4868:G:O2'   | 8:L5:4872:G:OP1    | 2.38                     | 0.42              |
| 9:L7:58:A:H2'     | 9:L7:59:G:H8       | 1.84                     | 0.42              |
| 10:L8:66:A:H2'    | 10:L8:67:U:H6      | 1.83                     | 0.42              |
| 11:LC:25:PRO:HG2  | 11:LC:28:PHE:CE2   | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:LF:75:ALA:HB2   | 26:LT:140:PHE:HE2  | 1.83                     | 0.42              |
| 18:LL:55:ILE:HG23  | 18:LL:76:PHE:HE1   | 1.84                     | 0.42              |
| 21:LO:121:PRO:HD2  | 25:LS:166:ARG:O    | 2.19                     | 0.42              |
| 24:LR:19:LYS:HB2   | 24:LR:19:LYS:HE3   | 1.84                     | 0.42              |
| 24:LR:149:LYS:HB3  | 24:LR:149:LYS:HE2  | 1.70                     | 0.42              |
| 31:LY:54:GLU:HB2   | 31:LY:108:ARG:HB2  | 2.01                     | 0.42              |
| 49:S2:96:C:H2'     | 49:S2:97:U:H6      | 1.84                     | 0.42              |
| 49:S2:496:C:P      | 52:SE:49:ARG:HH12  | 2.42                     | 0.42              |
| 49:S2:677:G:P      | 60:SN:5:HIS:HE2    | 2.42                     | 0.42              |
| 49:S2:1015:U:OP2   | 74:Sb:20:LYS:NZ    | 2.40                     | 0.42              |
| 49:S2:1208:A:O2'   | 49:S2:1209:A:H8    | 2.01                     | 0.42              |
| 49:S2:1542:C:O2'   | 49:S2:1543:U:O5'   | 2.35                     | 0.42              |
| 71:SY:102:THR:CG2  | 71:SY:107:ARG:HE   | 2.31                     | 0.42              |
| 79:Sg:32:LEU:HD11  | 79:Sg:92:LEU:HD11  | 2.02                     | 0.42              |
| 79:Sg:218:LEU:HD23 | 79:Sg:218:LEU:H    | 1.85                     | 0.42              |
| 81:Le:23:HIS:HA    | 81:Le:53:ILE:HD12  | 2.02                     | 0.42              |
| 82:LI:145:LYS:HA   | 82:LI:148:VAL:HG12 | 2.00                     | 0.42              |
| 8:L5:980:U:H2'     | 8:L5:981:C:C6      | 2.54                     | 0.42              |
| 8:L5:1095:A:N1     | 8:L5:1200:G:C6     | 2.87                     | 0.42              |
| 8:L5:1221:G:H4'    | 8:L5:1222:A:H5'    | 2.01                     | 0.42              |
| 8:L5:1655:C:O2     | 8:L5:4390:A:O2'    | 2.37                     | 0.42              |
| 8:L5:1685:G:H5'    | 8:L5:1686:C:OP2    | 2.19                     | 0.42              |
| 8:L5:2374:A:H2'    | 8:L5:2375:A:H8     | 1.85                     | 0.42              |
| 8:L5:2434:G:O2'    | 8:L5:2527:A:N1     | 2.48                     | 0.42              |
| 8:L5:2542:G:H2'    | 8:L5:2543:A:C8     | 2.54                     | 0.42              |
| 8:L5:4232:U:H4'    | 8:L5:4233:A:O4'    | 2.20                     | 0.42              |
| 8:L5:4729:A:H5''   | 8:L5:4965:U:H1'    | 2.01                     | 0.42              |
| 8:L5:4934:A:H2'    | 8:L5:4935:C:C6     | 2.55                     | 0.42              |
| 9:L7:38:U:N3       | 9:L7:41:G:OP2      | 2.39                     | 0.42              |
| 11:LC:80:ARG:HA    | 11:LC:80:ARG:HD2   | 1.82                     | 0.42              |
| 15:LG:190:LEU:HD23 | 15:LG:190:LEU:HA   | 1.86                     | 0.42              |
| 16:LH:63:ASN:O     | 16:LH:67:LEU:HG    | 2.19                     | 0.42              |
| 18:LL:140:SER:C    | 18:LL:142:GLU:H    | 2.26                     | 0.42              |
| 26:LT:91:VAL:HG23  | 26:LT:96:ILE:HD11  | 2.02                     | 0.42              |
| 51:SD:99:ILE:HG23  | 51:SD:173:ARG:HH21 | 1.84                     | 0.42              |
| 54:SG:138:ALA:HB1  | 54:SG:153:VAL:HG11 | 2.00                     | 0.42              |
| 57:SJ:104:ASP:OD1  | 57:SJ:104:ASP:C    | 2.62                     | 0.42              |
| 63:SQ:73:LYS:HE2   | 63:SQ:73:LYS:HB2   | 1.88                     | 0.42              |
| 8:L5:908:G:H2'     | 8:L5:909:A:C8      | 2.54                     | 0.42              |
| 8:L5:2505:C:H4'    | 8:L5:2506:G:O4'    | 2.19                     | 0.42              |
| 8:L5:2727:C:H2'    | 8:L5:2728:U:C6     | 2.55                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:L5:3684:G:H2'   | 8:L5:3685:C:C6     | 2.55                     | 0.42              |
| 8:L5:4080:C:H2'   | 8:L5:4081:G:H8     | 1.85                     | 0.42              |
| 8:L5:4233:A:C5    | 8:L5:4235:G:C8     | 3.08                     | 0.42              |
| 8:L5:4905:C:H2'   | 8:L5:4906:C:H6     | 1.85                     | 0.42              |
| 9:L7:82:G:H2'     | 9:L7:83:A:C8       | 2.53                     | 0.42              |
| 10:L8:45:C:P      | 43:L1:15:LYS:HD3   | 2.60                     | 0.42              |
| 12:LD:255:LYS:O   | 12:LD:257:PRO:HG2  | 2.19                     | 0.42              |
| 27:LU:40:GLU:HG2  | 27:LU:63:ILE:HG22  | 2.02                     | 0.42              |
| 32:LZ:113:GLU:OE2 | 32:LZ:117:LYS:HG2  | 2.19                     | 0.42              |
| 46:Lo:26:TYR:HB2  | 46:Lo:82:MET:HE1   | 2.01                     | 0.42              |
| 49:S2:1628:C:OP1  | 66:ST:38:LYS:NZ    | 2.45                     | 0.42              |
| 49:S2:1839:U:H1'  | 49:S2:1863:A:H2    | 1.84                     | 0.42              |
| 51:SD:71:ALA:O    | 51:SD:74:GLN:HG3   | 2.20                     | 0.42              |
| 52:SE:117:GLU:HA  | 52:SE:120:LYS:HD2  | 2.01                     | 0.42              |
| 55:SH:10:LYS:HE3  | 55:SH:16:PRO:HA    | 2.02                     | 0.42              |
| 57:SJ:104:ASP:O   | 57:SJ:107:GLU:HG2  | 2.19                     | 0.42              |
| 71:SY:91:LEU:HD22 | 71:SY:96:LEU:HD12  | 2.02                     | 0.42              |
| 79:Sg:188:HIS:HD2 | 79:Sg:219:TRP:CG   | 2.38                     | 0.42              |
| 81:Le:85:LEU:HD22 | 81:Le:111:ILE:HG23 | 2.01                     | 0.42              |
| 3:LB:56:ILE:HD12  | 3:LB:368:ILE:HG12  | 2.02                     | 0.42              |
| 6:B4:21:G:N7      | 6:B4:45:G:O6       | 2.53                     | 0.42              |
| 8:L5:182:G:H22    | 8:L5:255:C:H2'     | 1.84                     | 0.42              |
| 8:L5:1246:G:H2'   | 8:L5:1247:U:C6     | 2.54                     | 0.42              |
| 8:L5:1460:C:H5''  | 23:LQ:144:LYS:HG3  | 2.01                     | 0.42              |
| 8:L5:1502:G:OP2   | 23:LQ:62:SER:OG    | 2.32                     | 0.42              |
| 8:L5:1590:C:H4'   | 8:L5:2857:A:H5'    | 2.01                     | 0.42              |
| 8:L5:1907:A:H4'   | 14:LF:220:MET:HE1  | 2.01                     | 0.42              |
| 8:L5:2730:U:H2'   | 8:L5:2731:C:C6     | 2.54                     | 0.42              |
| 8:L5:4892:A:H2'   | 8:L5:4893:A:O4'    | 2.20                     | 0.42              |
| 9:L7:111:C:H2'    | 9:L7:112:U:O4'     | 2.20                     | 0.42              |
| 12:LD:41:LYS:HB2  | 26:LT:68:THR:O     | 2.19                     | 0.42              |
| 12:LD:256:LYS:CA  | 12:LD:257:PRO:HG2  | 2.49                     | 0.42              |
| 16:LH:120:GLU:CD  | 16:LH:124:ARG:HH21 | 2.28                     | 0.42              |
| 16:LH:168:LYS:HB3 | 16:LH:168:LYS:HE2  | 1.80                     | 0.42              |
| 19:LM:74:ARG:O    | 19:LM:78:GLN:HG3   | 2.20                     | 0.42              |
| 20:LN:75:VAL:HG11 | 20:LN:80:THR:HG22  | 2.00                     | 0.42              |
| 28:LV:90:ARG:NE   | 28:LV:124:GLU:OE1  | 2.52                     | 0.42              |
| 49:S2:39:A:OP2    | 57:SJ:5:ARG:NH1    | 2.52                     | 0.42              |
| 49:S2:443:U:O4    | 49:S2:447:A:N7     | 2.53                     | 0.42              |
| 49:S2:959:G:O2'   | 49:S2:1065:G:H4'   | 2.19                     | 0.42              |
| 49:S2:1101:U:OP1  | 64:SR:132:ARG:NH1  | 2.53                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1520:G:H2'   | 49:S2:1520:G:N3    | 2.35                     | 0.42              |
| 56:SI:36:THR:HG22  | 56:SI:57:ALA:O     | 2.20                     | 0.42              |
| 62:SP:34:MET:CE    | 62:SP:46:ASN:OD1   | 2.59                     | 0.42              |
| 8:L5:731:G:C6      | 8:L5:932:A:C4      | 3.07                     | 0.42              |
| 8:L5:1099:C:H2'    | 8:L5:1100:U:O4'    | 2.20                     | 0.42              |
| 8:L5:1715:C:H2'    | 8:L5:1716:G:C4     | 2.55                     | 0.42              |
| 8:L5:2562:G:C2     | 8:L5:2566:G:C6     | 3.08                     | 0.42              |
| 8:L5:2676:A:C4     | 8:L5:2677:G:C8     | 3.07                     | 0.42              |
| 8:L5:3588:C:H2'    | 8:L5:3589:G:O4'    | 2.20                     | 0.42              |
| 8:L5:3756:A:C2'    | 8:L5:3757:G:H5'    | 2.50                     | 0.42              |
| 8:L5:4208:U:OP2    | 26:LT:4:THR:OG1    | 2.30                     | 0.42              |
| 8:L5:5003:U:H2'    | 8:L5:5004:C:C6     | 2.54                     | 0.42              |
| 12:LD:36:LEU:HG    | 12:LD:50:ARG:HD2   | 2.01                     | 0.42              |
| 13:LE:47:ASN:HD21  | 13:LE:57:TYR:H     | 1.67                     | 0.42              |
| 25:LS:74:ARG:NH1   | 25:LS:74:ARG:HB3   | 2.35                     | 0.42              |
| 27:LU:31:ASP:OD2   | 27:LU:114:TYR:OH   | 2.23                     | 0.42              |
| 31:LY:109:LEU:HD12 | 31:LY:109:LEU:HA   | 1.87                     | 0.42              |
| 33:La:76:ASP:OD1   | 33:La:77:LYS:N     | 2.52                     | 0.42              |
| 44:Lm:99:CYS:HB3   | 44:Lm:115:CYS:HB3  | 1.35                     | 0.42              |
| 49:S2:669:A:N3     | 49:S2:1164:G:O2'   | 2.48                     | 0.42              |
| 53:SF:43:GLU:C     | 53:SF:45:TYR:H     | 2.27                     | 0.42              |
| 54:SG:68:LEU:HD23  | 54:SG:68:LEU:HA    | 1.81                     | 0.42              |
| 55:SH:50:GLU:HG3   | 55:SH:58:LYS:HE2   | 2.01                     | 0.42              |
| 63:SQ:26:LYS:O     | 63:SQ:66:VAL:HA    | 2.19                     | 0.42              |
| 65:SS:100:ALA:C    | 65:SS:102:GLY:H    | 2.27                     | 0.42              |
| 67:SU:97:ILE:HD12  | 67:SU:97:ILE:HA    | 1.87                     | 0.42              |
| 73:Sa:60:ASP:OD1   | 73:Sa:60:ASP:N     | 2.51                     | 0.42              |
| 80:SM:18:LEU:HA    | 80:SM:21:VAL:HG12  | 2.01                     | 0.42              |
| 82:LI:52:MET:HB2   | 82:LI:152:LEU:HD22 | 2.02                     | 0.42              |
| 3:LB:213:GLN:NE2   | 3:LB:285:TYR:O     | 2.53                     | 0.42              |
| 8:L5:174:C:N3      | 8:L5:263:G:N1      | 2.68                     | 0.42              |
| 8:L5:1428:U:H5''   | 23:LQ:42:THR:HB    | 2.01                     | 0.42              |
| 8:L5:1513:U:H2'    | 8:L5:1514:U:O4'    | 2.20                     | 0.42              |
| 8:L5:2104:G:H2'    | 8:L5:2105:A:C4     | 2.54                     | 0.42              |
| 8:L5:2859:G:H2'    | 8:L5:2860:C:H6     | 1.85                     | 0.42              |
| 8:L5:3709:U:H2'    | 8:L5:3710:G:H5'    | 2.01                     | 0.42              |
| 8:L5:3799:A:N3     | 8:L5:4506:C:O2'    | 2.38                     | 0.42              |
| 8:L5:4966:A:H2'    | 8:L5:4967:A:O4'    | 2.19                     | 0.42              |
| 11:LC:187:GLN:HG2  | 11:LC:203:GLN:HG2  | 2.01                     | 0.42              |
| 14:LF:220:MET:CE   | 14:LF:223:LYS:HB3  | 2.50                     | 0.42              |
| 14:LF:220:MET:CE   | 14:LF:223:LYS:HE3  | 2.49                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:LG:97:LYS:HE2   | 15:LG:97:LYS:HB2   | 1.74                     | 0.42              |
| 20:LN:181:HIS:O    | 20:LN:195:ARG:NH2  | 2.50                     | 0.42              |
| 27:LU:94:ASN:N     | 27:LU:94:ASN:OD1   | 2.53                     | 0.42              |
| 29:LW:55:TYR:CD1   | 29:LW:55:TYR:C     | 2.97                     | 0.42              |
| 44:Lm:95:ILE:HG22  | 44:Lm:96:CYS:O     | 2.20                     | 0.42              |
| 49:S2:16:G:H2'     | 49:S2:17:C:C6      | 2.55                     | 0.42              |
| 49:S2:35:C:H5''    | 49:S2:579:C:H5''   | 2.02                     | 0.42              |
| 49:S2:174:OMC:HM23 | 49:S2:174:OMC:H1'  | 1.91                     | 0.42              |
| 49:S2:344:U:H2'    | 49:S2:345:U:H6     | 1.84                     | 0.42              |
| 49:S2:575:A:H2'    | 49:S2:576:A2M:O4'  | 2.19                     | 0.42              |
| 51:SD:54:ARG:HB2   | 51:SD:57:ASN:HB2   | 2.02                     | 0.42              |
| 53:SF:201:LYS:HG3  | 53:SF:204:ARG:NH1  | 2.34                     | 0.42              |
| 70:SX:101:LEU:HD22 | 70:SX:124:LYS:HD3  | 2.02                     | 0.42              |
| 71:SY:44:LEU:HD23  | 71:SY:44:LEU:HA    | 1.82                     | 0.42              |
| 78:Sf:118:ARG:HB2  | 78:Sf:131:PHE:CD2  | 2.55                     | 0.42              |
| 6:B4:47:C:C4       | 6:B4:58:A:C8       | 3.08                     | 0.41              |
| 8:L5:423:G:H2'     | 8:L5:424:U:H6      | 1.85                     | 0.41              |
| 8:L5:1882:U:C4     | 8:L5:2279:A:C2     | 3.08                     | 0.41              |
| 8:L5:1893:C:H1'    | 8:L5:1937:C:O2     | 2.19                     | 0.41              |
| 8:L5:2804:OMC:HM23 | 8:L5:2804:OMC:H1'  | 1.78                     | 0.41              |
| 8:L5:2808:G:O3'    | 24:LR:60:ARG:NH1   | 2.53                     | 0.41              |
| 8:L5:4088:C:H2'    | 8:L5:4089:G:C8     | 2.55                     | 0.41              |
| 8:L5:4460:U:H2'    | 8:L5:4461:C:C6     | 2.55                     | 0.41              |
| 8:L5:4880:C:OP1    | 19:LM:124:LYS:NZ   | 2.44                     | 0.41              |
| 10:L8:67:U:OP1     | 41:Lj:87:LYS:HG2   | 2.20                     | 0.41              |
| 12:LD:213:GLU:HG3  | 12:LD:214:GLU:N    | 2.35                     | 0.41              |
| 14:LF:214:SER:OG   | 14:LF:215:SER:N    | 2.53                     | 0.41              |
| 17:LJ:129:ASP:OD2  | 17:LJ:129:ASP:C    | 2.62                     | 0.41              |
| 18:LL:89:LYS:HA    | 18:LL:89:LYS:HD3   | 1.87                     | 0.41              |
| 21:LO:108:ILE:HD13 | 21:LO:117:ARG:HD3  | 2.01                     | 0.41              |
| 24:LR:37:SER:OG    | 24:LR:40:GLN:HG3   | 2.20                     | 0.41              |
| 27:LU:36:ALA:C     | 27:LU:38:ASN:N     | 2.78                     | 0.41              |
| 31:LY:112:ASP:H    | 31:LY:115:ARG:HB3  | 1.85                     | 0.41              |
| 49:S2:587:A:H2     | 57:SJ:172:ARG:HH12 | 1.67                     | 0.41              |
| 49:S2:1456:G:H2'   | 49:S2:1457:U:C6    | 2.55                     | 0.41              |
| 59:SL:65:ASN:O     | 59:SL:65:ASN:ND2   | 2.50                     | 0.41              |
| 66:ST:43:LYS:HA    | 66:ST:43:LYS:HD3   | 1.73                     | 0.41              |
| 67:SU:32:LEU:HD21  | 67:SU:87:ARG:HG2   | 2.02                     | 0.41              |
| 69:SW:55:ASP:N     | 69:SW:55:ASP:OD1   | 2.52                     | 0.41              |
| 78:Sf:140:TYR:HE1  | 78:Sf:145:CYS:HB2  | 1.85                     | 0.41              |
| 79:Sg:285:GLN:O    | 79:Sg:303:THR:HG23 | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:LB:252:ALA:HB3   | 8:L5:4457:U:H1'    | 2.01                     | 0.41              |
| 8:L5:757:G:H3'     | 8:L5:758:G:H8      | 1.85                     | 0.41              |
| 8:L5:2722:G:H2'    | 8:L5:2723:U:O4'    | 2.19                     | 0.41              |
| 8:L5:3724:A2M:HM'3 | 8:L5:3724:A2M:H1'  | 1.72                     | 0.41              |
| 9:L7:16:A:H2'      | 9:L7:17:C:C6       | 2.55                     | 0.41              |
| 9:L7:30:C:O2'      | 12:LD:221:LYS:NZ   | 2.36                     | 0.41              |
| 24:LR:82:LYS:HE2   | 24:LR:82:LYS:HB3   | 1.94                     | 0.41              |
| 27:LU:80:LYS:O     | 27:LU:110:TYR:HE2  | 2.03                     | 0.41              |
| 28:LV:126:ALA:HB2  | 28:LV:139:ILE:CD1  | 2.51                     | 0.41              |
| 30:LX:122:ALA:N    | 30:LX:139:ARG:O    | 2.52                     | 0.41              |
| 32:LZ:112:ARG:HD3  | 32:LZ:112:ARG:C    | 2.45                     | 0.41              |
| 49:S2:1265:A:O2'   | 49:S2:1266:C:H6    | 2.02                     | 0.41              |
| 55:SH:130:LEU:HD22 | 55:SH:139:ILE:HD11 | 2.03                     | 0.41              |
| 58:SK:45:VAL:O     | 58:SK:49:MET:HG2   | 2.21                     | 0.41              |
| 59:SL:56:ILE:HD13  | 59:SL:56:ILE:HA    | 1.85                     | 0.41              |
| 60:SN:63:VAL:HG11  | 60:SN:71:ILE:HG12  | 2.02                     | 0.41              |
| 78:Sf:135:HIS:CD2  | 78:Sf:140:TYR:HB3  | 2.56                     | 0.41              |
| 3:LB:122:TRP:CH2   | 3:LB:127:LYS:HG2   | 2.55                     | 0.41              |
| 8:L5:300:A:H2'     | 8:L5:301:G:H8      | 1.86                     | 0.41              |
| 8:L5:494:U:H2'     | 8:L5:495:C:C6      | 2.55                     | 0.41              |
| 8:L5:1173:G:C4     | 8:L5:1174:A:H1'    | 2.55                     | 0.41              |
| 8:L5:1563:A:H2'    | 8:L5:1564:A:O4'    | 2.20                     | 0.41              |
| 8:L5:1816:C:C4     | 8:L5:1817:U:C4     | 3.08                     | 0.41              |
| 8:L5:2362:U:OP1    | 22:LP:82:ARG:NH2   | 2.54                     | 0.41              |
| 8:L5:2380:G:N2     | 8:L5:2424:OMG:H5'  | 2.35                     | 0.41              |
| 8:L5:2664:G:H4'    | 8:L5:2677:G:H4'    | 2.02                     | 0.41              |
| 8:L5:4591:U:H2'    | 8:L5:4592:C:C6     | 2.55                     | 0.41              |
| 8:L5:4743:G:H2'    | 8:L5:4744:A:C8     | 2.55                     | 0.41              |
| 9:L7:4:U:H2'       | 9:L7:5:A:H8        | 1.84                     | 0.41              |
| 10:L8:14:OMU:H6    | 10:L8:14:OMU:HM22  | 2.03                     | 0.41              |
| 11:LC:349:LEU:HD12 | 11:LC:349:LEU:HA   | 1.89                     | 0.41              |
| 12:LD:195:HIS:O    | 12:LD:199:ILE:HG13 | 2.20                     | 0.41              |
| 18:LL:143:GLU:O    | 18:LL:147:ALA:HB2  | 2.21                     | 0.41              |
| 21:LO:179:LYS:HA   | 21:LO:179:LYS:HD2  | 1.55                     | 0.41              |
| 28:LV:20:LEU:HB2   | 28:LV:55:ALA:O     | 2.21                     | 0.41              |
| 37:Lf:45:LYS:HD2   | 37:Lf:105:LEU:HA   | 2.01                     | 0.41              |
| 49:S2:328:U:O2'    | 49:S2:329:G:O5'    | 2.36                     | 0.41              |
| 49:S2:413:G:H5'    | 49:S2:813:A:H61    | 1.85                     | 0.41              |
| 49:S2:562:U:HO2'   | 49:S2:563:G:H8     | 1.69                     | 0.41              |
| 49:S2:639:C:H2'    | 49:S2:640:A:C8     | 2.56                     | 0.41              |
| 49:S2:1285:G:C6    | 80:SM:57:ASP:OD2   | 2.73                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:SK:32:HIS:ND1   | 58:SK:33:PRO:HD2   | 2.36                     | 0.41              |
| 62:SP:23:ASP:N     | 62:SP:23:ASP:OD1   | 2.52                     | 0.41              |
| 64:SR:77:GLU:HG2   | 64:SR:80:ARG:NH2   | 2.36                     | 0.41              |
| 69:SW:117:ARG:HE   | 69:SW:117:ARG:HB2  | 1.72                     | 0.41              |
| 71:SY:105:LYS:HA   | 71:SY:105:LYS:HD3  | 1.85                     | 0.41              |
| 72:SZ:66:LYS:NZ    | 72:SZ:111:ARG:HH21 | 2.17                     | 0.41              |
| 79:Sg:110:SER:OG   | 79:Sg:153:CYS:HA   | 2.20                     | 0.41              |
| 6:B4:58:A:H3'      | 6:B4:59:A:C8       | 2.55                     | 0.41              |
| 8:L5:473:C:H2'     | 8:L5:474:C:C6      | 2.56                     | 0.41              |
| 8:L5:1350:C:H2'    | 8:L5:1351:G:C8     | 2.55                     | 0.41              |
| 8:L5:2045:G:O2'    | 8:L5:2046:G:H5''   | 2.21                     | 0.41              |
| 8:L5:2475:G:H5''   | 8:L5:2476:G:C8     | 2.55                     | 0.41              |
| 8:L5:2862:G:N3     | 8:L5:3624:A:H2'    | 2.36                     | 0.41              |
| 10:L8:75:OMG:HM23  | 10:L8:75:OMG:H1'   | 1.81                     | 0.41              |
| 11:LC:140:LYS:NZ   | 11:LC:245:HIS:HB2  | 2.36                     | 0.41              |
| 12:LD:64:ILE:HG12  | 12:LD:105:LEU:HD21 | 2.02                     | 0.41              |
| 25:LS:81:TRP:HE3   | 25:LS:128:LYS:O    | 2.04                     | 0.41              |
| 26:LT:14:MET:HE2   | 26:LT:58:HIS:CG    | 2.55                     | 0.41              |
| 28:LV:139:ILE:HD13 | 28:LV:139:ILE:HA   | 1.80                     | 0.41              |
| 33:La:134:GLU:HG3  | 33:La:135:GLU:N    | 2.34                     | 0.41              |
| 42:Lk:24:LYS:HG2   | 42:Lk:67:LYS:HZ3   | 1.83                     | 0.41              |
| 49:S2:140:C:O2     | 49:S2:143:U:O2'    | 2.38                     | 0.41              |
| 49:S2:495:U:H2'    | 49:S2:496:C:O4'    | 2.19                     | 0.41              |
| 49:S2:649:U:OP2    | 70:SX:108:LYS:NZ   | 2.53                     | 0.41              |
| 49:S2:1285:G:C3'   | 49:S2:1286:G:H5'   | 2.50                     | 0.41              |
| 49:S2:1585:U:H1'   | 49:S2:1586:U:OP1   | 2.20                     | 0.41              |
| 49:S2:1690:U:H2'   | 49:S2:1691:U:C6    | 2.55                     | 0.41              |
| 49:S2:1831:A:N6    | 49:S2:1832:6MZ:H9  | 2.35                     | 0.41              |
| 50:SC:78:LEU:HD23  | 50:SC:81:ILE:HD12  | 2.02                     | 0.41              |
| 50:SC:121:ARG:NH2  | 50:SC:123:ARG:HH21 | 2.17                     | 0.41              |
| 50:SC:196:ILE:HB   | 50:SC:223:TYR:HB2  | 2.01                     | 0.41              |
| 54:SG:142:ARG:HA   | 54:SG:147:LEU:HD12 | 2.02                     | 0.41              |
| 66:ST:6:VAL:HG12   | 66:ST:135:ALA:HB2  | 2.02                     | 0.41              |
| 74:Sb:36:LYS:HD3   | 74:Sb:36:LYS:HA    | 1.70                     | 0.41              |
| 75:Sc:36:ASP:OD1   | 75:Sc:37:ASP:N     | 2.52                     | 0.41              |
| 2:SA:142:LEU:O     | 68:SV:60:ARG:NH2   | 2.53                     | 0.41              |
| 8:L5:18:C:H2'      | 8:L5:19:G:H8       | 1.85                     | 0.41              |
| 8:L5:509:A:C2      | 33:La:101:ILE:HA   | 2.56                     | 0.41              |
| 8:L5:509:A:C6      | 33:La:105:ARG:HD3  | 2.55                     | 0.41              |
| 8:L5:1260:G:H2'    | 8:L5:1261:G:H8     | 1.85                     | 0.41              |
| 8:L5:2100:A:N7     | 8:L5:2101:C:N4     | 2.69                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:2669:C:OP2    | 24:LR:128:LYS:NZ   | 2.41                     | 0.41              |
| 8:L5:3651:A:H2'    | 8:L5:3652:A:C8     | 2.55                     | 0.41              |
| 8:L5:4342:C:H2'    | 8:L5:4343:U:C6     | 2.55                     | 0.41              |
| 8:L5:4968:A:H2'    | 8:L5:4969:C:C6     | 2.55                     | 0.41              |
| 12:LD:107:ARG:HA   | 12:LD:107:ARG:HD2  | 1.84                     | 0.41              |
| 13:LE:284:HIS:CD2  | 13:LE:285:LYS:HG2  | 2.56                     | 0.41              |
| 15:LG:87:LEU:HD22  | 15:LG:182:CYS:SG   | 2.61                     | 0.41              |
| 21:LO:177:LEU:HD23 | 21:LO:177:LEU:HA   | 1.83                     | 0.41              |
| 23:LQ:59:PRO:HG3   | 23:LQ:143:ARG:HA   | 2.03                     | 0.41              |
| 32:LZ:103:ASP:HB3  | 32:LZ:106:LEU:HD12 | 2.02                     | 0.41              |
| 35:Lc:17:ARG:NH1   | 35:Lc:108:MET:HE1  | 2.29                     | 0.41              |
| 35:Lc:17:ARG:NH1   | 35:Lc:108:MET:SD   | 2.93                     | 0.41              |
| 41:Lj:67:LEU:HD23  | 41:Lj:67:LEU:HA    | 1.82                     | 0.41              |
| 47:Lp:90:LYS:HB2   | 47:Lp:90:LYS:HE3   | 1.84                     | 0.41              |
| 49:S2:656:G:H5'    | 49:S2:662:G:N2     | 2.35                     | 0.41              |
| 49:S2:1533:A:C8    | 49:S2:1604:G:H1'   | 2.55                     | 0.41              |
| 49:S2:1549:U:OP1   | 76:Sd:34:TYR:OH    | 2.24                     | 0.41              |
| 49:S2:1567:G:C6    | 65:SS:82:TRP:CG    | 3.08                     | 0.41              |
| 49:S2:1579:A:O2'   | 49:S2:1581:C:OP2   | 2.24                     | 0.41              |
| 49:S2:1667:U:H2'   | 49:S2:1668:U:C6    | 2.55                     | 0.41              |
| 49:S2:1705:C:H2'   | 49:S2:1706:G:C8    | 2.56                     | 0.41              |
| 55:SH:145:ARG:HD2  | 69:SW:49:GLU:OE1   | 2.20                     | 0.41              |
| 57:SJ:128:VAL:O    | 57:SJ:132:GLN:HG3  | 2.20                     | 0.41              |
| 58:SK:42:ASN:HA    | 58:SK:45:VAL:HG12  | 2.02                     | 0.41              |
| 70:SX:105:PHE:HB2  | 70:SX:119:ARG:C    | 2.44                     | 0.41              |
| 71:SY:9:THR:HG23   | 71:SY:23:MET:HB3   | 2.03                     | 0.41              |
| 71:SY:26:ASP:OD1   | 71:SY:26:ASP:N     | 2.53                     | 0.41              |
| 79:Sg:44:LYS:HB2   | 79:Sg:56:GLN:HB2   | 2.03                     | 0.41              |
| 3:LB:196:TRP:O     | 3:LB:199:GLU:HG2   | 2.19                     | 0.41              |
| 3:LB:322:HIS:O     | 3:LB:342:LYS:HE3   | 2.21                     | 0.41              |
| 8:L5:4:G:H2'       | 8:L5:5:A:C8        | 2.56                     | 0.41              |
| 8:L5:7:C:H2'       | 8:L5:8:U:C6        | 2.56                     | 0.41              |
| 8:L5:2049:G:O2'    | 8:L5:3884:U:O2'    | 2.24                     | 0.41              |
| 8:L5:2756:G:H2'    | 8:L5:2757:A:C8     | 2.55                     | 0.41              |
| 8:L5:4099:G:O2'    | 8:L5:4100:C:O4'    | 2.22                     | 0.41              |
| 8:L5:4691:A:H2'    | 8:L5:4692:A:O4'    | 2.21                     | 0.41              |
| 13:LE:62:MET:O     | 13:LE:66:LYS:HG2   | 2.21                     | 0.41              |
| 22:LP:28:ASN:O     | 22:LP:32:THR:HG22  | 2.21                     | 0.41              |
| 41:Lj:20:ARG:HH21  | 41:Lj:39:TYR:HH    | 1.62                     | 0.41              |
| 42:Lk:54:GLU:HA    | 42:Lk:57:LYS:HD2   | 2.01                     | 0.41              |
| 49:S2:339:A:H2'    | 49:S2:340:C:H5     | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:389:A:H2'    | 49:S2:390:C:C6     | 2.56                     | 0.41              |
| 49:S2:921:G:C5     | 69:SW:28:ARG:HD3   | 2.56                     | 0.41              |
| 49:S2:1446:A:O2'   | 49:S2:1447:G:H5''  | 2.21                     | 0.41              |
| 49:S2:1447:G:C2'   | 49:S2:1448:A:H5'   | 2.50                     | 0.41              |
| 49:S2:1842:4AC:O5' | 49:S2:1842:4AC:H6  | 2.21                     | 0.41              |
| 53:SF:51:HIS:O     | 63:SQ:50:LYS:HE2   | 2.20                     | 0.41              |
| 54:SG:157:VAL:HG11 | 54:SG:176:ILE:HD11 | 2.02                     | 0.41              |
| 57:SJ:91:LYS:HE3   | 57:SJ:96:TYR:CD2   | 2.55                     | 0.41              |
| 65:SS:63:GLU:O     | 65:SS:67:VAL:HG13  | 2.20                     | 0.41              |
| 69:SW:111:MET:SD   | 69:SW:115:GLU:HG2  | 2.61                     | 0.41              |
| 77:Se:101:LYS:HD2  | 77:Se:105:ALA:HB1  | 2.03                     | 0.41              |
| 78:Sf:125:GLU:OE1  | 78:Sf:125:GLU:N    | 2.43                     | 0.41              |
| 79:Sg:249:CYS:HB3  | 79:Sg:258:ILE:HG12 | 2.03                     | 0.41              |
| 1:LA:70:LYS:NZ     | 8:L5:4084:G:O6     | 2.51                     | 0.41              |
| 2:SA:184:ARG:HB3   | 2:SA:191:ARG:NH1   | 2.36                     | 0.41              |
| 3:LB:57:VAL:HB     | 3:LB:367:PHE:HB3   | 2.03                     | 0.41              |
| 3:LB:224:LYS:HG3   | 8:L5:4625:C:OP1    | 2.21                     | 0.41              |
| 6:B4:62:A:C6       | 6:B4:63:U:C4       | 3.09                     | 0.41              |
| 8:L5:88:A:N7       | 23:LQ:173:LYS:NZ   | 2.68                     | 0.41              |
| 8:L5:156:G:N2      | 8:L5:157:U:O4      | 2.53                     | 0.41              |
| 8:L5:730:G:OP2     | 14:LF:76:ARG:NE    | 2.49                     | 0.41              |
| 8:L5:1721:G:H2'    | 8:L5:1722:C:C6     | 2.56                     | 0.41              |
| 8:L5:2464:C:HO2'   | 8:L5:2465:C:H6     | 1.67                     | 0.41              |
| 8:L5:2861:OMC:HM23 | 8:L5:2861:OMC:H1'  | 1.76                     | 0.41              |
| 8:L5:3799:A:C5     | 28:LV:40:ILE:HD12  | 2.56                     | 0.41              |
| 8:L5:4529:G:H2'    | 8:L5:4530:U:O4'    | 2.20                     | 0.41              |
| 8:L5:4593:C:H2'    | 8:L5:4594:U:C6     | 2.55                     | 0.41              |
| 8:L5:4680:G:H2'    | 8:L5:4681:A:C8     | 2.55                     | 0.41              |
| 12:LD:108:ARG:CZ   | 12:LD:253:TYR:HB2  | 2.51                     | 0.41              |
| 12:LD:216:GLU:HB3  | 12:LD:220:LYS:NZ   | 2.36                     | 0.41              |
| 12:LD:264:LYS:HA   | 12:LD:264:LYS:HD2  | 1.85                     | 0.41              |
| 14:LF:143:GLY:HA3  | 14:LF:240:ILE:HB   | 2.03                     | 0.41              |
| 24:LR:104:ARG:HD3  | 24:LR:108:ARG:NH2  | 2.36                     | 0.41              |
| 25:LS:80:ILE:HG23  | 25:LS:129:VAL:HG22 | 2.01                     | 0.41              |
| 31:LY:54:GLU:O     | 31:LY:107:THR:OG1  | 2.37                     | 0.41              |
| 45:Ln:15:ARG:O     | 45:Ln:19:LYS:HG3   | 2.21                     | 0.41              |
| 46:Lo:6:LYS:O      | 46:Lo:23:VAL:HG22  | 2.21                     | 0.41              |
| 49:S2:124:U:OP1    | 54:SG:201:LYS:NZ   | 2.45                     | 0.41              |
| 49:S2:639:C:H2'    | 49:S2:640:A:H8     | 1.85                     | 0.41              |
| 49:S2:644:OMG:H1'  | 49:S2:644:OMG:HM23 | 1.78                     | 0.41              |
| 49:S2:809:A:C1'    | 52:SE:221:ARG:HH21 | 2.30                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1388:A:N6    | 51:SD:161:GLY:HA3  | 2.32                     | 0.41              |
| 49:S2:1585:U:O2'   | 49:S2:1587:G:OP2   | 2.32                     | 0.41              |
| 59:SL:49:GLU:OE1   | 59:SL:49:GLU:N     | 2.40                     | 0.41              |
| 60:SN:29:THR:O     | 60:SN:33:VAL:HG22  | 2.21                     | 0.41              |
| 66:ST:126:GLN:HE21 | 66:ST:126:GLN:CA   | 2.14                     | 0.41              |
| 74:Sb:41:TYR:O     | 74:Sb:41:TYR:CG    | 2.73                     | 0.41              |
| 79:Sg:179:LEU:HD23 | 79:Sg:179:LEU:HA   | 1.84                     | 0.41              |
| 82:LI:76:MET:HG3   | 82:LI:87:ILE:HD11  | 2.02                     | 0.41              |
| 3:LB:253:CYS:SG    | 8:L5:4521:U:H1'    | 2.60                     | 0.41              |
| 8:L5:186:G:H8      | 8:L5:186:G:OP2     | 2.03                     | 0.41              |
| 8:L5:1383:G:H2'    | 8:L5:1384:C:C6     | 2.56                     | 0.41              |
| 8:L5:2408:U:OP2    | 43:Ll:42:ARG:NH2   | 2.41                     | 0.41              |
| 8:L5:2675:G:O6     | 35:Lc:30:GLY:HA3   | 2.21                     | 0.41              |
| 8:L5:3848:U:H2'    | 8:L5:3849:A:H8     | 1.85                     | 0.41              |
| 8:L5:4755:G:N7     | 13:LE:279:ASN:ND2  | 2.68                     | 0.41              |
| 9:L7:28:C:O2'      | 9:L7:54:A:N1       | 2.54                     | 0.41              |
| 11:LC:149:GLU:OE2  | 48:Lr:71:ARG:NE    | 2.51                     | 0.41              |
| 14:LF:36:LYS:N     | 14:LF:36:LYS:HD3   | 2.35                     | 0.41              |
| 14:LF:216:PRO:HB3  | 14:LF:247:MET:HG2  | 2.02                     | 0.41              |
| 18:LL:87:HIS:HB3   | 18:LL:90:VAL:HG23  | 2.02                     | 0.41              |
| 34:Lb:11:ASN:OD1   | 34:Lb:14:ARG:HD3   | 2.21                     | 0.41              |
| 39:Lh:35:LYS:HA    | 39:Lh:44:LEU:HD21  | 2.03                     | 0.41              |
| 41:Lj:44:LYS:HE2   | 41:Lj:44:LYS:HB3   | 1.98                     | 0.41              |
| 49:S2:102:A:H4'    | 49:S2:104:A:C8     | 2.56                     | 0.41              |
| 49:S2:809:A:C4'    | 52:SE:221:ARG:HH21 | 2.21                     | 0.41              |
| 49:S2:1370:A:N3    | 49:S2:1372:U:H5'   | 2.36                     | 0.41              |
| 50:SC:145:LYS:HG2  | 50:SC:146:GLU:HG3  | 2.03                     | 0.41              |
| 51:SD:16:ILE:HD11  | 76:Sd:36:LEU:HD23  | 2.03                     | 0.41              |
| 53:SF:126:THR:HG21 | 75:Sc:27:CYS:SG    | 2.61                     | 0.41              |
| 65:SS:10:GLN:H     | 65:SS:10:GLN:HG3   | 1.59                     | 0.41              |
| 67:SU:80:PHE:HB3   | 76:Sd:52:PHE:HB3   | 2.03                     | 0.41              |
| 71:SY:55:ILE:HG12  | 71:SY:75:ILE:HG12  | 2.03                     | 0.41              |
| 79:Sg:152:SER:H    | 79:Sg:169:GLY:HA2  | 1.86                     | 0.41              |
| 80:SM:27:ILE:HD13  | 80:SM:27:ILE:HA    | 1.89                     | 0.41              |
| 2:SA:12:GLU:HG2    | 64:SR:114:LEU:HD21 | 2.02                     | 0.41              |
| 2:SA:94:THR:HG23   | 2:SA:186:ARG:HH12  | 1.84                     | 0.41              |
| 3:LB:121:ASN:ND2   | 3:LB:124:LYS:HB2   | 2.35                     | 0.41              |
| 3:LB:285:TYR:N     | 3:LB:332:MET:O     | 2.53                     | 0.41              |
| 6:B4:49:A:H2'      | 6:B4:50:U:C6       | 2.56                     | 0.41              |
| 8:L5:468:U:C4      | 8:L5:686:A:N3      | 2.89                     | 0.41              |
| 8:L5:1305:C:OP1    | 10:L8:7:U:O2'      | 2.39                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:1443:A:C6     | 8:L5:1444:G:N7     | 2.89                     | 0.41              |
| 8:L5:1662:C:H2'    | 8:L5:1663:C:H6     | 1.86                     | 0.41              |
| 8:L5:2052:G:O2'    | 8:L5:2057:A:N1     | 2.51                     | 0.41              |
| 8:L5:2376:A:H2'    | 8:L5:2377:C:C6     | 2.56                     | 0.41              |
| 8:L5:2381:A:H1'    | 8:L5:2383:C:OP2    | 2.21                     | 0.41              |
| 8:L5:2407:G:O6     | 43:L1:2:SER:N      | 2.53                     | 0.41              |
| 8:L5:2693:G:H2'    | 8:L5:2694:G:N2     | 2.35                     | 0.41              |
| 8:L5:2870:A:H2'    | 8:L5:2871:A:C8     | 2.56                     | 0.41              |
| 8:L5:2876:OMG:OP1  | 47:Lp:8:VAL:HG22   | 2.21                     | 0.41              |
| 8:L5:2876:OMG:HM22 | 8:L5:2877:G:H5'    | 2.03                     | 0.41              |
| 8:L5:3654:G:O2'    | 8:L5:3693:U:OP1    | 2.38                     | 0.41              |
| 8:L5:4154:G:H2'    | 8:L5:4155:C:H6     | 1.86                     | 0.41              |
| 8:L5:4192:A:H2'    | 8:L5:4193:C:H6     | 1.85                     | 0.41              |
| 8:L5:4228:OMG:H5'' | 8:L5:4229:U:O4'    | 2.20                     | 0.41              |
| 8:L5:4385:A:H61    | 8:L5:4531:U:H5'    | 1.86                     | 0.41              |
| 8:L5:4565:C:OP1    | 21:LO:65:ASN:ND2   | 2.54                     | 0.41              |
| 9:L7:58:A:H2'      | 9:L7:59:G:C8       | 2.56                     | 0.41              |
| 12:LD:99:TYR:CE2   | 12:LD:199:ILE:HD13 | 2.56                     | 0.41              |
| 14:LF:220:MET:HE2  | 14:LF:223:LYS:HB3  | 2.02                     | 0.41              |
| 15:LG:73:ARG:HD3   | 15:LG:73:ARG:HA    | 1.69                     | 0.41              |
| 18:LL:81:LEU:HD11  | 18:LL:98:VAL:HG22  | 2.02                     | 0.41              |
| 25:LS:173:ASN:OD1  | 25:LS:174:THR:N    | 2.54                     | 0.41              |
| 30:LX:147:LEU:HD23 | 30:LX:147:LEU:HA   | 1.82                     | 0.41              |
| 49:S2:355:G:OP1    | 59:SL:105:ARG:NH1  | 2.48                     | 0.41              |
| 49:S2:367:U:OP1    | 56:SI:11:ARG:NH1   | 2.54                     | 0.41              |
| 49:S2:432:G:H2'    | 49:S2:433:A:C8     | 2.56                     | 0.41              |
| 49:S2:576:A2M:HM'2 | 49:S2:577:U:H5'    | 2.03                     | 0.41              |
| 49:S2:1217:A:H2'   | 49:S2:1218:C:H6    | 1.85                     | 0.41              |
| 49:S2:1309:C:OP1   | 78:Sf:133:ALA:HA   | 2.21                     | 0.41              |
| 49:S2:1445:U:O2'   | 49:S2:1446:A:H5'   | 2.21                     | 0.41              |
| 49:S2:1493:C:O2'   | 49:S2:1499:U:O4    | 2.39                     | 0.41              |
| 49:S2:1562:C:H2'   | 49:S2:1563:G:H8    | 1.86                     | 0.41              |
| 49:S2:1599:U:OP2   | 72:SZ:46:ASN:ND2   | 2.53                     | 0.41              |
| 49:S2:1616:U:O2    | 49:S2:1661:A:H2    | 2.04                     | 0.41              |
| 49:S2:1678:A2M:OP2 | 53:SF:63:LYS:NZ    | 2.41                     | 0.41              |
| 50:SC:120:GLN:H    | 50:SC:120:GLN:HG2  | 1.66                     | 0.41              |
| 50:SC:160:LEU:HD23 | 50:SC:160:LEU:HA   | 1.94                     | 0.41              |
| 51:SD:103:GLU:OE2  | 51:SD:173:ARG:NE   | 2.39                     | 0.41              |
| 54:SG:154:ARG:C    | 54:SG:156:TYR:H    | 2.29                     | 0.41              |
| 55:SH:61:ILE:HD11  | 55:SH:95:ILE:HG13  | 2.03                     | 0.41              |
| 57:SJ:37:LEU:HB3   | 57:SJ:42:GLU:OE1   | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:SJ:113:GLN:HG3  | 57:SJ:149:VAL:HG21 | 2.03                     | 0.41              |
| 58:SK:60:GLU:HB2   | 58:SK:69:TRP:NE1   | 2.36                     | 0.41              |
| 59:SL:50:ALA:HA    | 59:SL:55:TYR:HE1   | 1.86                     | 0.41              |
| 63:SQ:50:LYS:NZ    | 63:SQ:53:GLU:OE2   | 2.54                     | 0.41              |
| 64:SR:20:TYR:CD1   | 64:SR:38:ILE:HD12  | 2.55                     | 0.41              |
| 65:SS:91:LYS:HB3   | 65:SS:91:LYS:HE3   | 1.76                     | 0.41              |
| 67:SU:26:SER:OG    | 67:SU:32:LEU:HB2   | 2.21                     | 0.41              |
| 68:SV:81:LYS:HA    | 68:SV:81:LYS:HD3   | 1.87                     | 0.41              |
| 69:SW:66:THR:OG1   | 69:SW:68:ARG:HG3   | 2.21                     | 0.41              |
| 70:SX:96:GLU:OE1   | 70:SX:96:GLU:HA    | 2.21                     | 0.41              |
| 71:SY:35:VAL:HG23  | 71:SY:40:ILE:HD11  | 2.03                     | 0.41              |
| 72:SZ:48:VAL:HG13  | 72:SZ:49:LEU:HG    | 2.03                     | 0.41              |
| 74:Sb:32:PHE:O     | 74:Sb:82:LYS:HB3   | 2.20                     | 0.41              |
| 80:SM:35:ILE:HD13  | 80:SM:35:ILE:HA    | 1.85                     | 0.41              |
| 2:SA:16:LEU:HD21   | 64:SR:114:LEU:HD22 | 2.03                     | 0.41              |
| 4:SB:83:LYS:HB2    | 4:SB:83:LYS:HE3    | 1.79                     | 0.41              |
| 4:SB:140:VAL:HG12  | 4:SB:213:ARG:HB2   | 2.03                     | 0.41              |
| 8:L5:198:A:O2'     | 8:L5:221:C:O2      | 2.36                     | 0.41              |
| 8:L5:757:G:C4      | 8:L5:758:G:C8      | 3.09                     | 0.41              |
| 8:L5:758:G:N3      | 8:L5:758:G:H2'     | 2.35                     | 0.41              |
| 8:L5:1340:OMC:HM23 | 8:L5:1340:OMC:H1'  | 1.85                     | 0.41              |
| 8:L5:1693:U:H2'    | 8:L5:1694:C:O4'    | 2.21                     | 0.41              |
| 8:L5:1947:U:C5     | 44:Lm:108:VAL:HG11 | 2.56                     | 0.41              |
| 8:L5:2347:A:C4     | 81:Le:31:ILE:HD11  | 2.57                     | 0.41              |
| 8:L5:2366:A:N3     | 8:L5:3850:C:O2'    | 2.51                     | 0.41              |
| 8:L5:2480:G:H2'    | 8:L5:2481:G:H8     | 1.85                     | 0.41              |
| 8:L5:2538:U:H2'    | 8:L5:2539:C:C6     | 2.56                     | 0.41              |
| 8:L5:3816:A:OP1    | 8:L5:3818:U:H5     | 2.03                     | 0.41              |
| 8:L5:4968:A:H2'    | 8:L5:4969:C:H6     | 1.86                     | 0.41              |
| 10:L8:67:U:H2'     | 10:L8:68:G:H8      | 1.84                     | 0.41              |
| 11:LC:289:LEU:HD13 | 23:LQ:27:LEU:HD22  | 2.03                     | 0.41              |
| 16:LH:76:HIS:O     | 16:LH:80:MET:HG3   | 2.20                     | 0.41              |
| 17:LJ:19:LYS:HG3   | 17:LJ:133:VAL:CG1  | 2.51                     | 0.41              |
| 27:LU:105:ASN:OD1  | 27:LU:109:SER:OG   | 2.21                     | 0.41              |
| 28:LV:45:ILE:HD13  | 28:LV:45:ILE:HA    | 1.99                     | 0.41              |
| 34:Lb:5:LYS:HE3    | 34:Lb:8:THR:HB     | 2.03                     | 0.41              |
| 37:Lf:4:ARG:HG2    | 37:Lf:6:TRP:O      | 2.21                     | 0.41              |
| 39:Lh:105:LYS:HE2  | 39:Lh:105:LYS:HB2  | 1.89                     | 0.41              |
| 46:Lo:100:LYS:HB3  | 46:Lo:102:GLN:NE2  | 2.36                     | 0.41              |
| 49:S2:67:C:O2'     | 54:SG:164:LYS:HD2  | 2.21                     | 0.41              |
| 49:S2:1148:A:H4'   | 49:S2:1149:A:O4'   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1619:A:OP2   | 62:SP:47:ARG:NH1   | 2.53                     | 0.41              |
| 58:SK:52:LEU:HD12  | 58:SK:55:ARG:HH21  | 1.85                     | 0.41              |
| 64:SR:58:MET:HE3   | 64:SR:58:MET:HB3   | 1.83                     | 0.41              |
| 71:SY:29:HIS:O     | 71:SY:29:HIS:ND1   | 2.54                     | 0.41              |
| 8:L5:1563:A:H8     | 8:L5:1563:A:O5'    | 2.03                     | 0.40              |
| 8:L5:1601:A:N7     | 8:L5:3643:A:C4     | 2.89                     | 0.40              |
| 8:L5:1715:C:H3'    | 8:L5:1716:G:C8     | 2.56                     | 0.40              |
| 8:L5:2296:G:O4'    | 11:LC:45:ARG:NH1   | 2.54                     | 0.40              |
| 8:L5:2815:A2M:H2'  | 8:L5:2816:G:C8     | 2.56                     | 0.40              |
| 10:L8:87:G:H8      | 10:L8:87:G:OP2     | 2.04                     | 0.40              |
| 31:LY:89:LYS:HE3   | 31:LY:89:LYS:HB3   | 1.86                     | 0.40              |
| 33:La:26:ARG:HD3   | 33:La:26:ARG:HA    | 1.78                     | 0.40              |
| 35:Lc:17:ARG:NE    | 35:Lc:17:ARG:CA    | 2.81                     | 0.40              |
| 39:Lh:116:LEU:H    | 39:Lh:116:LEU:HD12 | 1.86                     | 0.40              |
| 49:S2:441:C:H2'    | 49:S2:442:C:C6     | 2.56                     | 0.40              |
| 49:S2:909:G:H2'    | 49:S2:910:G:C8     | 2.57                     | 0.40              |
| 49:S2:940:U:H2'    | 49:S2:941:C:C6     | 2.56                     | 0.40              |
| 50:SC:221:ASP:N    | 50:SC:221:ASP:OD1  | 2.54                     | 0.40              |
| 57:SJ:65:GLU:OE1   | 57:SJ:66:LYS:N     | 2.36                     | 0.40              |
| 60:SN:46:THR:OG1   | 60:SN:49:GLN:HB2   | 2.21                     | 0.40              |
| 60:SN:94:LYS:HG2   | 60:SN:118:ILE:HD13 | 2.03                     | 0.40              |
| 75:Sc:20:ARG:HD2   | 75:Sc:28:THR:HG23  | 2.02                     | 0.40              |
| 79:Sg:224:GLY:O    | 79:Sg:225:LYS:HD3  | 2.21                     | 0.40              |
| 1:LA:171:GLY:O     | 47:Lp:68:ALA:HB2   | 2.21                     | 0.40              |
| 3:LB:11:HIS:NE2    | 8:L5:4458:C:OP1    | 2.55                     | 0.40              |
| 3:LB:324:GLY:HA2   | 8:L5:5051:C:H4'    | 2.03                     | 0.40              |
| 5:A4:47:A:H4'      | 49:S2:1830:U:C4    | 2.56                     | 0.40              |
| 6:B4:50:U:C4       | 6:B4:51:G:N7       | 2.89                     | 0.40              |
| 6:B4:63:U:H2'      | 6:B4:64:C:C6       | 2.57                     | 0.40              |
| 8:L5:267:G:H2'     | 8:L5:268:G:C8      | 2.55                     | 0.40              |
| 8:L5:652:G:H2'     | 8:L5:653:U:C6      | 2.57                     | 0.40              |
| 8:L5:1720:C:H2'    | 8:L5:1721:G:O4'    | 2.20                     | 0.40              |
| 8:L5:1888:A:C8     | 8:L5:2049:G:O4'    | 2.74                     | 0.40              |
| 8:L5:1961:G:N2     | 8:L5:2025:A:H62    | 2.19                     | 0.40              |
| 8:L5:2385:U:OP1    | 24:LR:5:ARG:NH1    | 2.55                     | 0.40              |
| 8:L5:2408:U:P      | 43:Ll:42:ARG:HH22  | 2.42                     | 0.40              |
| 8:L5:2689:C:H2'    | 8:L5:2690:C:C6     | 2.57                     | 0.40              |
| 8:L5:2690:C:H2'    | 8:L5:2691:U:O4'    | 2.21                     | 0.40              |
| 8:L5:2758:G:H2'    | 8:L5:2759:G:N7     | 2.36                     | 0.40              |
| 8:L5:3841:OMC:HM23 | 8:L5:3841:OMC:H1'  | 1.70                     | 0.40              |
| 8:L5:3848:U:H2'    | 8:L5:3849:A:C8     | 2.56                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:L5:3925:OMU:H2'  | 8:L5:3926:C:O4'   | 2.21                     | 0.40              |
| 8:L5:4872:G:O6     | 19:LM:98:ARG:NH1  | 2.54                     | 0.40              |
| 8:L5:4897:G:H2'    | 8:L5:4898:G:H8    | 1.87                     | 0.40              |
| 8:L5:4905:C:H2'    | 8:L5:4906:C:C6    | 2.56                     | 0.40              |
| 17:LJ:112:HIS:CE1  | 17:LJ:125:ILE:HA  | 2.56                     | 0.40              |
| 30:LX:148:ASP:HB3  | 30:LX:152:LYS:HZ3 | 1.85                     | 0.40              |
| 31:LY:14:ASN:HD22  | 31:LY:14:ASN:HA   | 1.65                     | 0.40              |
| 32:LZ:92:ASP:OD1   | 32:LZ:94:THR:N    | 2.54                     | 0.40              |
| 37:Lf:47:CYS:SG    | 37:Lf:74:VAL:HG23 | 2.62                     | 0.40              |
| 46:Lo:32:SER:O     | 46:Lo:33:LEU:HB3  | 2.22                     | 0.40              |
| 49:S2:126:G:H5'    | 49:S2:127:C:OP2   | 2.21                     | 0.40              |
| 49:S2:382:C:H2'    | 49:S2:383:G:H8    | 1.86                     | 0.40              |
| 49:S2:496:C:H2'    | 49:S2:497:C:C6    | 2.55                     | 0.40              |
| 49:S2:499:G:H2'    | 49:S2:501:C:O2    | 2.21                     | 0.40              |
| 49:S2:566:U:H3     | 49:S2:584:G:H1    | 1.68                     | 0.40              |
| 49:S2:943:U:H2'    | 49:S2:944:A:H8    | 1.85                     | 0.40              |
| 49:S2:1829:G:H1'   | 49:S2:1850:MA6:C2 | 2.49                     | 0.40              |
| 54:SG:221:LYS:HD2  | 54:SG:221:LYS:HA  | 1.83                     | 0.40              |
| 55:SH:143:ARG:HB3  | 69:SW:51:GLU:OE2  | 2.21                     | 0.40              |
| 60:SN:54:LEU:HB3   | 60:SN:60:VAL:CG2  | 2.51                     | 0.40              |
| 61:SO:45:THR:OG1   | 61:SO:49:GLY:HA2  | 2.21                     | 0.40              |
| 66:ST:27:LYS:HB2   | 66:ST:110:LEU:CD1 | 2.51                     | 0.40              |
| 79:Sg:194:TYR:CZ   | 79:Sg:212:LYS:HB2 | 2.56                     | 0.40              |
| 81:Le:9:LYS:HE3    | 81:Le:9:LYS:HB2   | 1.81                     | 0.40              |
| 8:L5:50:C:C2       | 8:L5:51:A:C8      | 3.09                     | 0.40              |
| 8:L5:410:A:O2'     | 8:L5:414:C:O2'    | 2.29                     | 0.40              |
| 8:L5:1241:C:H2'    | 8:L5:1242:G:O4'   | 2.21                     | 0.40              |
| 8:L5:1669:A:OP1    | 34:Lb:18:ARG:NH1  | 2.53                     | 0.40              |
| 8:L5:1819:G:O2'    | 12:LD:115:MET:HE1 | 2.20                     | 0.40              |
| 8:L5:3587:C:H2'    | 8:L5:3588:C:C6    | 2.57                     | 0.40              |
| 8:L5:3877:A:O2'    | 8:L5:4400:G:N2    | 2.45                     | 0.40              |
| 8:L5:4188:U:H2'    | 8:L5:4189:U:C6    | 2.55                     | 0.40              |
| 8:L5:4371:G:O2'    | 8:L5:4372:U:OP2   | 2.34                     | 0.40              |
| 8:L5:4424:A:C4     | 8:L5:4425:G:C8    | 3.10                     | 0.40              |
| 12:LD:94:ASN:OD1   | 12:LD:94:ASN:N    | 2.55                     | 0.40              |
| 13:LE:125:LEU:HD12 | 13:LE:125:LEU:HA  | 1.89                     | 0.40              |
| 21:LO:113:ASP:OD1  | 21:LO:113:ASP:C   | 2.64                     | 0.40              |
| 30:LX:47:ARG:HE    | 30:LX:47:ARG:HB3  | 1.58                     | 0.40              |
| 33:La:134:GLU:O    | 33:La:138:LYS:HG3 | 2.21                     | 0.40              |
| 35:Lc:17:ARG:O     | 35:Lc:19:GLN:N    | 2.52                     | 0.40              |
| 49:S2:28:U:H2'     | 49:S2:29:G:C8     | 2.54                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:616:A:OP1    | 70:SX:68:LYS:NZ    | 2.53                     | 0.40              |
| 49:S2:650:A:OP2    | 70:SX:108:LYS:HG2  | 2.21                     | 0.40              |
| 49:S2:1252:C:N4    | 63:SQ:146:ARG:OXT  | 2.45                     | 0.40              |
| 50:SC:180:VAL:HG13 | 50:SC:219:ILE:HD13 | 2.03                     | 0.40              |
| 54:SG:28:TYR:O     | 54:SG:30:LYS:HG2   | 2.21                     | 0.40              |
| 57:SJ:81:LEU:HD13  | 57:SJ:97:ILE:HD12  | 2.02                     | 0.40              |
| 79:Sg:35:SER:OG    | 79:Sg:37:ASP:OD1   | 2.39                     | 0.40              |
| 1:LA:199:VAL:HG21  | 8:L5:1631:A:N7     | 2.37                     | 0.40              |
| 3:LB:254:ILE:HG12  | 8:L5:3897:G:H4'    | 2.03                     | 0.40              |
| 3:LB:305:THR:C     | 3:LB:307:TYR:H     | 2.29                     | 0.40              |
| 4:SB:97:LEU:HG     | 4:SB:232:HIS:CE1   | 2.57                     | 0.40              |
| 8:L5:35:U:H4'      | 8:L5:1525:A:C2     | 2.57                     | 0.40              |
| 8:L5:1084:C:H2'    | 8:L5:1085:C:H6     | 1.85                     | 0.40              |
| 8:L5:1257:A:H3'    | 8:L5:1258:G:H8     | 1.86                     | 0.40              |
| 8:L5:2296:G:O2'    | 11:LC:242:PRO:O    | 2.34                     | 0.40              |
| 8:L5:3702:A:C6     | 8:L5:3703:G:C8     | 3.09                     | 0.40              |
| 8:L5:3860:A:N3     | 22:LP:131:ARG:NH1  | 2.68                     | 0.40              |
| 17:LJ:99:PHE:CD2   | 17:LJ:105:PHE:HB3  | 2.56                     | 0.40              |
| 23:LQ:128:LEU:HD23 | 23:LQ:128:LEU:HA   | 1.88                     | 0.40              |
| 27:LU:62:THR:O     | 27:LU:72:VAL:HA    | 2.22                     | 0.40              |
| 32:LZ:92:ASP:OD1   | 32:LZ:92:ASP:C     | 2.64                     | 0.40              |
| 33:La:75:LEU:HD22  | 33:La:117:LEU:HD11 | 2.03                     | 0.40              |
| 38:Lg:83:CYS:O     | 38:Lg:87:VAL:HG13  | 2.21                     | 0.40              |
| 45:Ln:11:ARG:O     | 45:Ln:15:ARG:HG3   | 2.22                     | 0.40              |
| 49:S2:389:A:H1'    | 56:SI:87:ASN:H     | 1.86                     | 0.40              |
| 49:S2:1365:G:H2'   | 49:S2:1366:G:H8    | 1.85                     | 0.40              |
| 52:SE:95:THR:HG23  | 71:SY:16:ARG:NH1   | 2.35                     | 0.40              |
| 52:SE:140:VAL:HA   | 52:SE:145:ARG:O    | 2.21                     | 0.40              |
| 54:SG:20:ASP:OD2   | 54:SG:23:LYS:N     | 2.48                     | 0.40              |
| 65:SS:121:ARG:HG3  | 65:SS:131:VAL:HG13 | 2.03                     | 0.40              |
| 66:ST:5:THR:HG22   | 66:ST:7:LYS:H      | 1.87                     | 0.40              |
| 69:SW:5:ASN:HB3    | 69:SW:8:ALA:HB3    | 2.04                     | 0.40              |
| 79:Sg:140:TYR:HE1  | 79:Sg:142:VAL:HG13 | 1.86                     | 0.40              |
| 81:Le:46:ARG:HG3   | 81:Le:47:ARG:N     | 2.36                     | 0.40              |
| 1:LA:141:PRO:O     | 1:LA:144:LYS:HD3   | 2.22                     | 0.40              |
| 3:LB:201:LEU:HD12  | 3:LB:201:LEU:HA    | 1.98                     | 0.40              |
| 3:LB:357:ARG:CD    | 8:L5:4615:C:H5''   | 2.52                     | 0.40              |
| 8:L5:90:G:OP2      | 46:Lo:40:ARG:NH1   | 2.54                     | 0.40              |
| 8:L5:302:C:H2'     | 8:L5:303:C:H6      | 1.87                     | 0.40              |
| 8:L5:1446:C:N3     | 8:L5:2100:A:H2     | 2.19                     | 0.40              |
| 8:L5:2475:G:N1     | 30:LX:51:THR:O     | 2.39                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:2608:G:H2'    | 8:L5:2609:G:H8     | 1.86                     | 0.40              |
| 8:L5:2745:A:H2'    | 8:L5:2746:A:C8     | 2.57                     | 0.40              |
| 8:L5:4753:U:OP1    | 37:Lf:100:ARG:NH2  | 2.48                     | 0.40              |
| 24:LR:153:LYS:HE3  | 24:LR:153:LYS:HB3  | 1.80                     | 0.40              |
| 26:LT:103:ASP:OD1  | 26:LT:103:ASP:C    | 2.64                     | 0.40              |
| 30:LX:60:TYR:O     | 30:LX:62:ARG:NH1   | 2.54                     | 0.40              |
| 33:La:119:LYS:H    | 33:La:119:LYS:HG2  | 1.68                     | 0.40              |
| 42:Lk:51:GLU:C     | 42:Lk:55:LYS:HE3   | 2.47                     | 0.40              |
| 49:S2:1016:U:H5''  | 60:SN:15:ALA:O     | 2.22                     | 0.40              |
| 49:S2:1446:A:N3    | 67:SU:55:ARG:NE    | 2.69                     | 0.40              |
| 54:SG:69:THR:O     | 54:SG:99:GLY:HA3   | 2.22                     | 0.40              |
| 55:SH:100:ILE:HD11 | 55:SH:122:LEU:HD12 | 2.04                     | 0.40              |
| 57:SJ:35:TYR:HD1   | 57:SJ:112:THR:HG21 | 1.87                     | 0.40              |
| 61:SO:40:THR:HG21  | 61:SO:74:ALA:HB2   | 2.03                     | 0.40              |
| 61:SO:96:LYS:HB3   | 61:SO:132:VAL:HG21 | 2.02                     | 0.40              |
| 64:SR:37:GLU:CD    | 79:Sg:150:TRP:HE1  | 2.30                     | 0.40              |
| 78:Sf:138:ARG:HD2  | 78:Sf:147:THR:HG21 | 2.03                     | 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    | 246/257 (96%) | 225 (92%) | 21 (8%) | 0        | 100         | 100 |
| 2   | SA    | 215/295 (73%) | 206 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 3   | LB    | 396/403 (98%) | 367 (93%) | 29 (7%) | 0        | 100         | 100 |
| 4   | SB    | 211/264 (80%) | 207 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 11  | LC    | 360/427 (84%) | 342 (95%) | 18 (5%) | 0        | 100         | 100 |
| 12  | LD    | 292/297 (98%) | 285 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 13  | LE    | 197/288 (68%) | 181 (92%) | 16 (8%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14  | LF    | 220/248 (89%) | 214 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 15  | LG    | 220/266 (83%) | 211 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 16  | LH    | 189/192 (98%) | 181 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 17  | LJ    | 163/178 (92%) | 153 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 18  | LL    | 192/211 (91%) | 171 (89%) | 21 (11%) | 0        | 100         | 100 |
| 19  | LM    | 135/215 (63%) | 126 (93%) | 8 (6%)   | 1 (1%)   | 18          | 49  |
| 20  | LN    | 201/204 (98%) | 196 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 21  | LO    | 199/203 (98%) | 196 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 22  | LP    | 155/184 (84%) | 150 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 23  | LQ    | 185/188 (98%) | 177 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 24  | LR    | 173/196 (88%) | 171 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 25  | LS    | 169/176 (96%) | 158 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 26  | LT    | 151/160 (94%) | 146 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 27  | LU    | 97/128 (76%)  | 89 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 28  | LV    | 129/140 (92%) | 119 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 29  | LW    | 83/157 (53%)  | 81 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 30  | LX    | 116/156 (74%) | 110 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 31  | LY    | 132/145 (91%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 32  | LZ    | 134/136 (98%) | 130 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 33  | La    | 145/148 (98%) | 135 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 34  | Lb    | 88/159 (55%)  | 86 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 35  | Lc    | 91/115 (79%)  | 83 (91%)  | 7 (8%)   | 1 (1%)   | 11          | 40  |
| 36  | Ld    | 104/125 (83%) | 100 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 37  | Lf    | 107/110 (97%) | 104 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 38  | Lg    | 108/117 (92%) | 104 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 39  | Lh    | 120/123 (98%) | 115 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | Li    | 98/105 (93%)  | 93 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 41  | Lj    | 85/97 (88%)   | 82 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 42  | Lk    | 67/70 (96%)   | 64 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 43  | Ll    | 47/51 (92%)   | 43 (92%)  | 4 (8%)   | 0        | 100         | 100 |
| 44  | Lm    | 49/128 (38%)  | 48 (98%)  | 1 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 45  | Ln    | 23/25 (92%)   | 23 (100%) | 0       | 0        | 100         | 100 |
| 46  | Lo    | 100/106 (94%) | 92 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 47  | Lp    | 89/92 (97%)   | 85 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 48  | Lr    | 123/137 (90%) | 116 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 50  | SC    | 218/293 (74%) | 208 (95%) | 10 (5%) | 0        | 100         | 100 |
| 51  | SD    | 219/243 (90%) | 211 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 52  | SE    | 256/263 (97%) | 242 (94%) | 14 (6%) | 0        | 100         | 100 |
| 53  | SF    | 183/204 (90%) | 173 (94%) | 10 (6%) | 0        | 100         | 100 |
| 54  | SG    | 219/249 (88%) | 204 (93%) | 15 (7%) | 0        | 100         | 100 |
| 55  | SH    | 169/194 (87%) | 160 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 56  | SI    | 193/208 (93%) | 182 (94%) | 11 (6%) | 0        | 100         | 100 |
| 57  | SJ    | 176/194 (91%) | 170 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 58  | SK    | 94/165 (57%)  | 88 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 59  | SL    | 136/158 (86%) | 127 (93%) | 9 (7%)  | 0        | 100         | 100 |
| 60  | SN    | 148/151 (98%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 61  | SO    | 127/151 (84%) | 117 (92%) | 10 (8%) | 0        | 100         | 100 |
| 62  | SP    | 127/145 (88%) | 123 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 63  | SQ    | 139/146 (95%) | 135 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 64  | SR    | 128/135 (95%) | 122 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 65  | SS    | 140/152 (92%) | 130 (93%) | 10 (7%) | 0        | 100         | 100 |
| 66  | ST    | 139/145 (96%) | 135 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 67  | SU    | 99/119 (83%)  | 90 (91%)  | 9 (9%)  | 0        | 100         | 100 |
| 68  | SV    | 81/83 (98%)   | 77 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 69  | SW    | 127/130 (98%) | 120 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 70  | SX    | 139/143 (97%) | 128 (92%) | 11 (8%) | 0        | 100         | 100 |
| 71  | SY    | 121/133 (91%) | 118 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 72  | SZ    | 70/125 (56%)  | 63 (90%)  | 7 (10%) | 0        | 100         | 100 |
| 73  | Sa    | 97/115 (84%)  | 95 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 74  | Sb    | 81/84 (96%)   | 74 (91%)  | 7 (9%)  | 0        | 100         | 100 |
| 75  | Sc    | 61/69 (88%)   | 53 (87%)  | 8 (13%) | 0        | 100         | 100 |
| 76  | Sd    | 50/56 (89%)   | 48 (96%)  | 2 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 77  | Se    | 46/59 (78%)       | 45 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 78  | Sf    | 59/156 (38%)      | 46 (78%)    | 13 (22%) | 0        | 100         | 100 |
| 79  | Sg    | 302/317 (95%)     | 279 (92%)   | 23 (8%)  | 0        | 100         | 100 |
| 80  | SM    | 94/132 (71%)      | 86 (92%)    | 8 (8%)   | 0        | 100         | 100 |
| 81  | Le    | 125/135 (93%)     | 121 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 82  | LI    | 199/214 (93%)     | 194 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| All | All   | 10966/12688 (86%) | 10396 (95%) | 568 (5%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | LM    | 32  | ASP  |
| 35  | Lc    | 99  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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    | 187/199 (94%) | 187 (100%) | 0        | 100         | 100 |
| 2   | SA    | 178/243 (73%) | 177 (99%)  | 1 (1%)   | 78          | 81  |
| 3   | LB    | 330/349 (95%) | 328 (99%)  | 2 (1%)   | 78          | 81  |
| 4   | SB    | 193/231 (84%) | 192 (100%) | 1 (0%)   | 81          | 82  |
| 11  | LC    | 299/348 (86%) | 299 (100%) | 0        | 100         | 100 |
| 12  | LD    | 247/250 (99%) | 247 (100%) | 0        | 100         | 100 |
| 13  | LE    | 175/252 (69%) | 175 (100%) | 0        | 100         | 100 |
| 14  | LF    | 192/215 (89%) | 192 (100%) | 0        | 100         | 100 |
| 15  | LG    | 189/223 (85%) | 189 (100%) | 0        | 100         | 100 |
| 16  | LH    | 170/171 (99%) | 170 (100%) | 0        | 100         | 100 |
| 17  | LJ    | 138/149 (93%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 18  | LL    | 161/177 (91%) | 161 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 19  | LM    | 115/161 (71%)  | 115 (100%) | 0        | 100         | 100 |
| 20  | LN    | 171/172 (99%)  | 170 (99%)  | 1 (1%)   | 78          | 81  |
| 21  | LO    | 172/174 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 22  | LP    | 137/163 (84%)  | 137 (100%) | 0        | 100         | 100 |
| 23  | LQ    | 164/165 (99%)  | 164 (100%) | 0        | 100         | 100 |
| 24  | LR    | 153/175 (87%)  | 153 (100%) | 0        | 100         | 100 |
| 25  | LS    | 152/157 (97%)  | 152 (100%) | 0        | 100         | 100 |
| 26  | LT    | 132/140 (94%)  | 132 (100%) | 0        | 100         | 100 |
| 27  | LU    | 89/115 (77%)   | 89 (100%)  | 0        | 100         | 100 |
| 28  | LV    | 101/107 (94%)  | 99 (98%)   | 2 (2%)   | 48          | 67  |
| 29  | LW    | 57/126 (45%)   | 57 (100%)  | 0        | 100         | 100 |
| 30  | LX    | 105/133 (79%)  | 105 (100%) | 0        | 100         | 100 |
| 31  | LY    | 121/135 (90%)  | 121 (100%) | 0        | 100         | 100 |
| 32  | LZ    | 118/118 (100%) | 118 (100%) | 0        | 100         | 100 |
| 33  | La    | 119/121 (98%)  | 119 (100%) | 0        | 100         | 100 |
| 34  | Lb    | 75/126 (60%)   | 75 (100%)  | 0        | 100         | 100 |
| 35  | Lc    | 78/97 (80%)    | 78 (100%)  | 0        | 100         | 100 |
| 36  | Ld    | 94/110 (86%)   | 93 (99%)   | 1 (1%)   | 65          | 75  |
| 37  | Lf    | 86/89 (97%)    | 86 (100%)  | 0        | 100         | 100 |
| 38  | Lg    | 91/100 (91%)   | 91 (100%)  | 0        | 100         | 100 |
| 39  | Lh    | 108/110 (98%)  | 108 (100%) | 0        | 100         | 100 |
| 40  | Li    | 85/89 (96%)    | 84 (99%)   | 1 (1%)   | 63          | 74  |
| 41  | Lj    | 74/80 (92%)    | 74 (100%)  | 0        | 100         | 100 |
| 42  | Lk    | 60/65 (92%)    | 60 (100%)  | 0        | 100         | 100 |
| 43  | Ll    | 46/48 (96%)    | 46 (100%)  | 0        | 100         | 100 |
| 44  | Lm    | 45/116 (39%)   | 45 (100%)  | 0        | 100         | 100 |
| 45  | Ln    | 24/24 (100%)   | 24 (100%)  | 0        | 100         | 100 |
| 46  | Lo    | 90/94 (96%)    | 89 (99%)   | 1 (1%)   | 65          | 75  |
| 47  | Lp    | 74/75 (99%)    | 73 (99%)   | 1 (1%)   | 59          | 72  |
| 48  | Lr    | 105/121 (87%)  | 104 (99%)  | 1 (1%)   | 68          | 75  |
| 50  | SC    | 185/225 (82%)  | 185 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 51  | SD    | 174/202 (86%) | 174 (100%) | 0        | 100         | 100 |
| 52  | SE    | 221/225 (98%) | 221 (100%) | 0        | 100         | 100 |
| 53  | SF    | 159/170 (94%) | 158 (99%)  | 1 (1%)   | 78          | 81  |
| 54  | SG    | 183/218 (84%) | 183 (100%) | 0        | 100         | 100 |
| 55  | SH    | 139/174 (80%) | 138 (99%)  | 1 (1%)   | 76          | 79  |
| 56  | SI    | 162/180 (90%) | 161 (99%)  | 1 (1%)   | 78          | 81  |
| 57  | SJ    | 158/168 (94%) | 157 (99%)  | 1 (1%)   | 78          | 81  |
| 58  | SK    | 86/136 (63%)  | 85 (99%)   | 1 (1%)   | 63          | 74  |
| 59  | SL    | 126/142 (89%) | 126 (100%) | 0        | 100         | 100 |
| 60  | SN    | 129/131 (98%) | 129 (100%) | 0        | 100         | 100 |
| 61  | SO    | 98/119 (82%)  | 96 (98%)   | 2 (2%)   | 48          | 67  |
| 62  | SP    | 114/130 (88%) | 114 (100%) | 0        | 100         | 100 |
| 63  | SQ    | 116/121 (96%) | 115 (99%)  | 1 (1%)   | 70          | 77  |
| 64  | SR    | 117/122 (96%) | 117 (100%) | 0        | 100         | 100 |
| 65  | SS    | 121/132 (92%) | 121 (100%) | 0        | 100         | 100 |
| 66  | ST    | 111/115 (96%) | 111 (100%) | 0        | 100         | 100 |
| 67  | SU    | 89/107 (83%)  | 89 (100%)  | 0        | 100         | 100 |
| 68  | SV    | 67/67 (100%)  | 66 (98%)   | 1 (2%)   | 57          | 71  |
| 69  | SW    | 112/113 (99%) | 110 (98%)  | 2 (2%)   | 51          | 69  |
| 70  | SX    | 110/115 (96%) | 110 (100%) | 0        | 100         | 100 |
| 71  | SY    | 103/115 (90%) | 102 (99%)  | 1 (1%)   | 68          | 75  |
| 72  | SZ    | 64/103 (62%)  | 63 (98%)   | 1 (2%)   | 55          | 71  |
| 73  | Sa    | 85/98 (87%)   | 84 (99%)   | 1 (1%)   | 63          | 74  |
| 74  | Sb    | 69/76 (91%)   | 69 (100%)  | 0        | 100         | 100 |
| 75  | Sc    | 54/62 (87%)   | 51 (94%)   | 3 (6%)   | 19          | 47  |
| 76  | Sd    | 46/49 (94%)   | 45 (98%)   | 1 (2%)   | 45          | 65  |
| 77  | Se    | 40/48 (83%)   | 40 (100%)  | 0        | 100         | 100 |
| 78  | Sf    | 52/140 (37%)  | 52 (100%)  | 0        | 100         | 100 |
| 79  | Sg    | 265/275 (96%) | 264 (100%) | 1 (0%)   | 84          | 83  |
| 80  | SM    | 74/108 (68%)  | 73 (99%)   | 1 (1%)   | 59          | 72  |
| 81  | Le    | 113/121 (93%) | 113 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 82  | LI    | 172/181 (95%)    | 172 (100%)  | 0        | 100         | 100 |
| All | All   | 9414/10801 (87%) | 9381 (100%) | 33 (0%)  | 81          | 83  |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | SA    | 145 | ILE  |
| 3   | LB    | 214 | ASP  |
| 3   | LB    | 345 | LEU  |
| 4   | SB    | 139 | CYS  |
| 17  | LJ    | 125 | ILE  |
| 20  | LN    | 87  | HIS  |
| 28  | LV    | 22  | VAL  |
| 28  | LV    | 117 | ILE  |
| 36  | Ld    | 68  | LEU  |
| 40  | Li    | 41  | ARG  |
| 46  | Lo    | 24  | THR  |
| 47  | Lp    | 78  | THR  |
| 48  | Lr    | 63  | VAL  |
| 53  | SF    | 55  | ARG  |
| 55  | SH    | 45  | ILE  |
| 56  | SI    | 7   | ASN  |
| 57  | SJ    | 161 | LEU  |
| 58  | SK    | 90  | VAL  |
| 61  | SO    | 66  | ARG  |
| 61  | SO    | 75  | MET  |
| 63  | SQ    | 67  | ASP  |
| 68  | SV    | 39  | VAL  |
| 69  | SW    | 26  | LEU  |
| 69  | SW    | 80  | ASP  |
| 71  | SY    | 26  | ASP  |
| 72  | SZ    | 97  | ILE  |
| 73  | Sa    | 94  | ASP  |
| 75  | Sc    | 18  | LEU  |
| 75  | Sc    | 57  | THR  |
| 75  | Sc    | 58  | LEU  |
| 76  | Sd    | 16  | GLN  |
| 79  | Sg    | 113 | PHE  |
| 80  | SM    | 69  | CYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | LA    | 83  | HIS  |
| 1   | LA    | 205 | ASN  |
| 2   | SA    | 113 | GLN  |
| 2   | SA    | 132 | GLN  |
| 3   | LB    | 184 | GLN  |
| 3   | LB    | 186 | ASN  |
| 3   | LB    | 289 | GLN  |
| 3   | LB    | 322 | HIS  |
| 11  | LC    | 21  | ASN  |
| 11  | LC    | 187 | GLN  |
| 11  | LC    | 198 | ASN  |
| 11  | LC    | 203 | GLN  |
| 11  | LC    | 329 | ASN  |
| 12  | LD    | 122 | GLN  |
| 12  | LD    | 267 | ASN  |
| 12  | LD    | 275 | GLN  |
| 13  | LE    | 47  | ASN  |
| 13  | LE    | 256 | GLN  |
| 13  | LE    | 268 | GLN  |
| 14  | LF    | 80  | ASN  |
| 14  | LF    | 116 | GLN  |
| 14  | LF    | 119 | ASN  |
| 14  | LF    | 126 | ASN  |
| 14  | LF    | 241 | ASN  |
| 15  | LG    | 38  | ASN  |
| 15  | LG    | 46  | GLN  |
| 15  | LG    | 141 | ASN  |
| 15  | LG    | 153 | GLN  |
| 15  | LG    | 236 | HIS  |
| 16  | LH    | 98  | HIS  |
| 16  | LH    | 102 | ASN  |
| 17  | LJ    | 10  | ASN  |
| 17  | LJ    | 65  | ASN  |
| 17  | LJ    | 98  | ASN  |
| 17  | LJ    | 112 | HIS  |
| 19  | LM    | 56  | GLN  |
| 20  | LN    | 87  | HIS  |
| 20  | LN    | 158 | HIS  |
| 21  | LO    | 26  | GLN  |
| 22  | LP    | 10  | ASN  |
| 22  | LP    | 21  | ASN  |
| 22  | LP    | 72  | GLN  |
| 22  | LP    | 80  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | LP    | 137 | ASN  |
| 23  | LQ    | 44  | ASN  |
| 23  | LQ    | 125 | GLN  |
| 24  | LR    | 34  | ASN  |
| 26  | LT    | 49  | GLN  |
| 26  | LT    | 66  | ASN  |
| 28  | LV    | 50  | ASN  |
| 29  | LW    | 63  | GLN  |
| 30  | LX    | 73  | HIS  |
| 31  | LY    | 43  | ASN  |
| 31  | LY    | 61  | HIS  |
| 31  | LY    | 127 | GLN  |
| 33  | La    | 39  | HIS  |
| 33  | La    | 62  | HIS  |
| 34  | Lb    | 6   | ASN  |
| 35  | Lc    | 72  | HIS  |
| 36  | Ld    | 79  | ASN  |
| 36  | Ld    | 121 | ASN  |
| 37  | Lf    | 21  | GLN  |
| 38  | Lg    | 28  | ASN  |
| 39  | Lh    | 98  | HIS  |
| 40  | Li    | 15  | HIS  |
| 40  | Li    | 20  | ASN  |
| 41  | Lj    | 30  | GLN  |
| 43  | Ll    | 17  | GLN  |
| 44  | Lm    | 87  | GLN  |
| 44  | Lm    | 120 | ASN  |
| 46  | Lo    | 3   | ASN  |
| 48  | Lr    | 21  | ASN  |
| 48  | Lr    | 30  | ASN  |
| 51  | SD    | 101 | GLN  |
| 53  | SF    | 83  | ASN  |
| 53  | SF    | 118 | ASN  |
| 54  | SG    | 155 | GLN  |
| 54  | SG    | 177 | GLN  |
| 55  | SH    | 68  | GLN  |
| 56  | SI    | 64  | ASN  |
| 57  | SJ    | 132 | GLN  |
| 59  | SL    | 11  | GLN  |
| 59  | SL    | 13  | GLN  |
| 61  | SO    | 103 | ASN  |
| 64  | SR    | 93  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | ST    | 126 | GLN  |
| 68  | SV    | 2   | GLN  |
| 69  | SW    | 5   | ASN  |
| 69  | SW    | 91  | ASN  |
| 75  | Sc    | 26  | GLN  |
| 76  | Sd    | 26  | ASN  |
| 77  | Se    | 95  | GLN  |
| 78  | Sf    | 139 | HIS  |
| 79  | Sg    | 64  | HIS  |
| 79  | Sg    | 188 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | L8    | 144/156 (92%)   | 27 (18%)          | 0               |
| 49  | S2    | 1561/1869 (83%) | 347 (22%)         | 6 (0%)          |
| 5   | A4    | 10/13 (76%)     | 0                 | 0               |
| 6   | B4    | 74/75 (98%)     | 18 (24%)          | 0               |
| 7   | D4    | 60/76 (78%)     | 23 (38%)          | 0               |
| 8   | L5    | 3436/5070 (67%) | 666 (19%)         | 16 (0%)         |
| 9   | L7    | 118/120 (98%)   | 11 (9%)           | 0               |
| All | All   | 5403/7379 (73%) | 1092 (20%)        | 22 (0%)         |

All (1092) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | B4    | 8   | U    |
| 6   | B4    | 10  | G    |
| 6   | B4    | 11  | C    |
| 6   | B4    | 12  | G    |
| 6   | B4    | 17  | G    |
| 6   | B4    | 18  | G    |
| 6   | B4    | 19  | A    |
| 6   | B4    | 20  | A    |
| 6   | B4    | 21  | G    |
| 6   | B4    | 46  | U    |
| 6   | B4    | 48  | G    |
| 6   | B4    | 51  | G    |
| 6   | B4    | 52  | G    |
| 6   | B4    | 55  | C    |
| 6   | B4    | 56  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | B4    | 60  | C    |
| 6   | B4    | 74  | C    |
| 6   | B4    | 75  | A    |
| 7   | D4    | 6   | G    |
| 7   | D4    | 7   | A    |
| 7   | D4    | 8   | U    |
| 7   | D4    | 9   | A    |
| 7   | D4    | 12  | U    |
| 7   | D4    | 14  | A    |
| 7   | D4    | 15  | G    |
| 7   | D4    | 19  | G    |
| 7   | D4    | 22  | G    |
| 7   | D4    | 26  | A    |
| 7   | D4    | 27  | G    |
| 7   | D4    | 29  | G    |
| 7   | D4    | 30  | G    |
| 7   | D4    | 46  | G    |
| 7   | D4    | 47  | U    |
| 7   | D4    | 49  | C    |
| 7   | D4    | 52  | G    |
| 7   | D4    | 54  | U    |
| 7   | D4    | 60  | U    |
| 7   | D4    | 61  | C    |
| 7   | D4    | 62  | C    |
| 7   | D4    | 63  | G    |
| 7   | D4    | 68  | C    |
| 8   | L5    | 13  | U    |
| 8   | L5    | 21  | G    |
| 8   | L5    | 25  | A    |
| 8   | L5    | 26  | C    |
| 8   | L5    | 39  | A    |
| 8   | L5    | 42  | A    |
| 8   | L5    | 48  | G    |
| 8   | L5    | 59  | A    |
| 8   | L5    | 64  | A    |
| 8   | L5    | 65  | A    |
| 8   | L5    | 73  | A    |
| 8   | L5    | 91  | G    |
| 8   | L5    | 98  | A    |
| 8   | L5    | 104 | G    |
| 8   | L5    | 106 | A    |
| 8   | L5    | 108 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | L5    | 109 | G    |
| 8   | L5    | 110 | C    |
| 8   | L5    | 116 | G    |
| 8   | L5    | 117 | C    |
| 8   | L5    | 119 | G    |
| 8   | L5    | 124 | C    |
| 8   | L5    | 133 | C    |
| 8   | L5    | 134 | G    |
| 8   | L5    | 135 | G    |
| 8   | L5    | 136 | C    |
| 8   | L5    | 139 | G    |
| 8   | L5    | 144 | G    |
| 8   | L5    | 152 | U    |
| 8   | L5    | 159 | C    |
| 8   | L5    | 165 | A    |
| 8   | L5    | 166 | C    |
| 8   | L5    | 183 | C    |
| 8   | L5    | 184 | U    |
| 8   | L5    | 185 | C    |
| 8   | L5    | 197 | A    |
| 8   | L5    | 200 | U    |
| 8   | L5    | 209 | U    |
| 8   | L5    | 216 | C    |
| 8   | L5    | 217 | C    |
| 8   | L5    | 218 | A    |
| 8   | L5    | 233 | U    |
| 8   | L5    | 234 | G    |
| 8   | L5    | 265 | C    |
| 8   | L5    | 266 | C    |
| 8   | L5    | 269 | G    |
| 8   | L5    | 275 | C    |
| 8   | L5    | 276 | C    |
| 8   | L5    | 280 | G    |
| 8   | L5    | 297 | U    |
| 8   | L5    | 306 | A    |
| 8   | L5    | 309 | C    |
| 8   | L5    | 310 | G    |
| 8   | L5    | 315 | G    |
| 8   | L5    | 316 | U    |
| 8   | L5    | 340 | C    |
| 8   | L5    | 341 | G    |
| 8   | L5    | 350 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | L5    | 387 | G    |
| 8   | L5    | 388 | A    |
| 8   | L5    | 396 | A    |
| 8   | L5    | 407 | A    |
| 8   | L5    | 409 | G    |
| 8   | L5    | 411 | G    |
| 8   | L5    | 412 | G    |
| 8   | L5    | 414 | C    |
| 8   | L5    | 415 | G    |
| 8   | L5    | 449 | C    |
| 8   | L5    | 450 | G    |
| 8   | L5    | 452 | A    |
| 8   | L5    | 454 | U    |
| 8   | L5    | 456 | C    |
| 8   | L5    | 457 | G    |
| 8   | L5    | 465 | G    |
| 8   | L5    | 468 | U    |
| 8   | L5    | 473 | C    |
| 8   | L5    | 483 | G    |
| 8   | L5    | 484 | U    |
| 8   | L5    | 485 | C    |
| 8   | L5    | 486 | C    |
| 8   | L5    | 489 | C    |
| 8   | L5    | 497 | G    |
| 8   | L5    | 498 | C    |
| 8   | L5    | 500 | G    |
| 8   | L5    | 502 | C    |
| 8   | L5    | 503 | C    |
| 8   | L5    | 504 | G    |
| 8   | L5    | 505 | G    |
| 8   | L5    | 506 | C    |
| 8   | L5    | 509 | A    |
| 8   | L5    | 510 | U    |
| 8   | L5    | 512 | U    |
| 8   | L5    | 513 | U    |
| 8   | L5    | 514 | U    |
| 8   | L5    | 515 | C    |
| 8   | L5    | 516 | C    |
| 8   | L5    | 517 | C    |
| 8   | L5    | 519 | C    |
| 8   | L5    | 643 | C    |
| 8   | L5    | 644 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | L5    | 646 | G    |
| 8   | L5    | 654 | C    |
| 8   | L5    | 655 | C    |
| 8   | L5    | 656 | C    |
| 8   | L5    | 657 | C    |
| 8   | L5    | 659 | G    |
| 8   | L5    | 665 | C    |
| 8   | L5    | 666 | G    |
| 8   | L5    | 667 | A    |
| 8   | L5    | 668 | C    |
| 8   | L5    | 674 | G    |
| 8   | L5    | 686 | A    |
| 8   | L5    | 687 | U    |
| 8   | L5    | 696 | C    |
| 8   | L5    | 703 | G    |
| 8   | L5    | 704 | C    |
| 8   | L5    | 706 | C    |
| 8   | L5    | 731 | G    |
| 8   | L5    | 739 | G    |
| 8   | L5    | 740 | G    |
| 8   | L5    | 741 | C    |
| 8   | L5    | 742 | G    |
| 8   | L5    | 743 | G    |
| 8   | L5    | 744 | G    |
| 8   | L5    | 745 | G    |
| 8   | L5    | 758 | G    |
| 8   | L5    | 759 | G    |
| 8   | L5    | 904 | C    |
| 8   | L5    | 905 | C    |
| 8   | L5    | 914 | U    |
| 8   | L5    | 915 | A    |
| 8   | L5    | 917 | A    |
| 8   | L5    | 932 | A    |
| 8   | L5    | 933 | G    |
| 8   | L5    | 934 | C    |
| 8   | L5    | 935 | A    |
| 8   | L5    | 944 | A    |
| 8   | L5    | 945 | U    |
| 8   | L5    | 956 | A    |
| 8   | L5    | 959 | G    |
| 8   | L5    | 960 | A    |
| 8   | L5    | 961 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 982  | U    |
| 8   | L5    | 1075 | G    |
| 8   | L5    | 1082 | C    |
| 8   | L5    | 1083 | U    |
| 8   | L5    | 1169 | G    |
| 8   | L5    | 1171 | G    |
| 8   | L5    | 1172 | C    |
| 8   | L5    | 1173 | G    |
| 8   | L5    | 1174 | A    |
| 8   | L5    | 1176 | C    |
| 8   | L5    | 1182 | C    |
| 8   | L5    | 1183 | C    |
| 8   | L5    | 1200 | G    |
| 8   | L5    | 1202 | C    |
| 8   | L5    | 1203 | G    |
| 8   | L5    | 1210 | C    |
| 8   | L5    | 1211 | G    |
| 8   | L5    | 1214 | C    |
| 8   | L5    | 1215 | C    |
| 8   | L5    | 1218 | G    |
| 8   | L5    | 1220 | G    |
| 8   | L5    | 1221 | G    |
| 8   | L5    | 1235 | G    |
| 8   | L5    | 1241 | C    |
| 8   | L5    | 1243 | C    |
| 8   | L5    | 1244 | G    |
| 8   | L5    | 1258 | G    |
| 8   | L5    | 1259 | G    |
| 8   | L5    | 1266 | G    |
| 8   | L5    | 1271 | G    |
| 8   | L5    | 1272 | C    |
| 8   | L5    | 1273 | G    |
| 8   | L5    | 1280 | C    |
| 8   | L5    | 1284 | G    |
| 8   | L5    | 1287 | G    |
| 8   | L5    | 1293 | G    |
| 8   | L5    | 1294 | A    |
| 8   | L5    | 1301 | C    |
| 8   | L5    | 1326 | A2M  |
| 8   | L5    | 1339 | U    |
| 8   | L5    | 1354 | A    |
| 8   | L5    | 1358 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 1359 | G    |
| 8   | L5    | 1365 | C    |
| 8   | L5    | 1366 | G    |
| 8   | L5    | 1377 | G    |
| 8   | L5    | 1381 | U    |
| 8   | L5    | 1387 | A    |
| 8   | L5    | 1393 | G    |
| 8   | L5    | 1394 | G    |
| 8   | L5    | 1397 | A    |
| 8   | L5    | 1398 | A    |
| 8   | L5    | 1399 | G    |
| 8   | L5    | 1402 | C    |
| 8   | L5    | 1403 | G    |
| 8   | L5    | 1404 | G    |
| 8   | L5    | 1405 | C    |
| 8   | L5    | 1407 | C    |
| 8   | L5    | 1408 | G    |
| 8   | L5    | 1409 | C    |
| 8   | L5    | 1410 | U    |
| 8   | L5    | 1414 | C    |
| 8   | L5    | 1420 | A    |
| 8   | L5    | 1421 | G    |
| 8   | L5    | 1439 | C    |
| 8   | L5    | 1447 | C    |
| 8   | L5    | 1448 | G    |
| 8   | L5    | 1482 | G    |
| 8   | L5    | 1483 | C    |
| 8   | L5    | 1497 | A    |
| 8   | L5    | 1498 | G    |
| 8   | L5    | 1502 | G    |
| 8   | L5    | 1518 | A    |
| 8   | L5    | 1525 | A    |
| 8   | L5    | 1534 | A    |
| 8   | L5    | 1547 | A    |
| 8   | L5    | 1566 | C    |
| 8   | L5    | 1576 | G    |
| 8   | L5    | 1578 | U    |
| 8   | L5    | 1591 | U    |
| 8   | L5    | 1596 | U    |
| 8   | L5    | 1612 | G    |
| 8   | L5    | 1624 | G    |
| 8   | L5    | 1625 | OMG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 1631 | A    |
| 8   | L5    | 1633 | G    |
| 8   | L5    | 1634 | A    |
| 8   | L5    | 1638 | A    |
| 8   | L5    | 1640 | C    |
| 8   | L5    | 1641 | G    |
| 8   | L5    | 1642 | A    |
| 8   | L5    | 1654 | G    |
| 8   | L5    | 1661 | C    |
| 8   | L5    | 1663 | C    |
| 8   | L5    | 1676 | C    |
| 8   | L5    | 1677 | U    |
| 8   | L5    | 1681 | G    |
| 8   | L5    | 1684 | A    |
| 8   | L5    | 1685 | G    |
| 8   | L5    | 1691 | G    |
| 8   | L5    | 1694 | C    |
| 8   | L5    | 1717 | C    |
| 8   | L5    | 1718 | C    |
| 8   | L5    | 1719 | A    |
| 8   | L5    | 1731 | C    |
| 8   | L5    | 1734 | G    |
| 8   | L5    | 1740 | C    |
| 8   | L5    | 1742 | A    |
| 8   | L5    | 1750 | G    |
| 8   | L5    | 1783 | C    |
| 8   | L5    | 1787 | A    |
| 8   | L5    | 1803 | G    |
| 8   | L5    | 1804 | A    |
| 8   | L5    | 1810 | G    |
| 8   | L5    | 1815 | G    |
| 8   | L5    | 1820 | C    |
| 8   | L5    | 1821 | G    |
| 8   | L5    | 1822 | U    |
| 8   | L5    | 1836 | G    |
| 8   | L5    | 1837 | A    |
| 8   | L5    | 1842 | G    |
| 8   | L5    | 1855 | G    |
| 8   | L5    | 1869 | G    |
| 8   | L5    | 1897 | A    |
| 8   | L5    | 1918 | U    |
| 8   | L5    | 1919 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 1920 | C    |
| 8   | L5    | 1921 | C    |
| 8   | L5    | 1922 | G    |
| 8   | L5    | 1931 | C    |
| 8   | L5    | 1932 | A    |
| 8   | L5    | 1936 | C    |
| 8   | L5    | 1940 | G    |
| 8   | L5    | 1948 | G    |
| 8   | L5    | 1955 | G    |
| 8   | L5    | 1959 | U    |
| 8   | L5    | 1960 | A    |
| 8   | L5    | 1961 | G    |
| 8   | L5    | 1962 | A    |
| 8   | L5    | 1966 | C    |
| 8   | L5    | 1968 | G    |
| 8   | L5    | 1970 | A    |
| 8   | L5    | 1971 | C    |
| 8   | L5    | 1998 | A    |
| 8   | L5    | 1999 | A    |
| 8   | L5    | 2000 | G    |
| 8   | L5    | 2018 | C    |
| 8   | L5    | 2020 | U    |
| 8   | L5    | 2022 | C    |
| 8   | L5    | 2024 | G    |
| 8   | L5    | 2025 | A    |
| 8   | L5    | 2026 | A    |
| 8   | L5    | 2033 | A    |
| 8   | L5    | 2046 | G    |
| 8   | L5    | 2048 | U    |
| 8   | L5    | 2055 | G    |
| 8   | L5    | 2056 | G    |
| 8   | L5    | 2069 | A    |
| 8   | L5    | 2070 | U    |
| 8   | L5    | 2084 | C    |
| 8   | L5    | 2085 | G    |
| 8   | L5    | 2101 | C    |
| 8   | L5    | 2102 | G    |
| 8   | L5    | 2104 | G    |
| 8   | L5    | 2106 | G    |
| 8   | L5    | 2107 | C    |
| 8   | L5    | 2289 | C    |
| 8   | L5    | 2300 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 2301 | G    |
| 8   | L5    | 2313 | A    |
| 8   | L5    | 2333 | G    |
| 8   | L5    | 2348 | G    |
| 8   | L5    | 2351 | OMC  |
| 8   | L5    | 2366 | A    |
| 8   | L5    | 2370 | A    |
| 8   | L5    | 2389 | A    |
| 8   | L5    | 2395 | A    |
| 8   | L5    | 2396 | A    |
| 8   | L5    | 2397 | G    |
| 8   | L5    | 2401 | A2M  |
| 8   | L5    | 2410 | C    |
| 8   | L5    | 2417 | A    |
| 8   | L5    | 2421 | G    |
| 8   | L5    | 2422 | OMC  |
| 8   | L5    | 2424 | OMG  |
| 8   | L5    | 2425 | U    |
| 8   | L5    | 2441 | C    |
| 8   | L5    | 2450 | G    |
| 8   | L5    | 2464 | C    |
| 8   | L5    | 2465 | C    |
| 8   | L5    | 2471 | G    |
| 8   | L5    | 2474 | G    |
| 8   | L5    | 2475 | G    |
| 8   | L5    | 2483 | G    |
| 8   | L5    | 2484 | A    |
| 8   | L5    | 2492 | C    |
| 8   | L5    | 2493 | G    |
| 8   | L5    | 2494 | U    |
| 8   | L5    | 2496 | G    |
| 8   | L5    | 2504 | C    |
| 8   | L5    | 2506 | G    |
| 8   | L5    | 2513 | A    |
| 8   | L5    | 2514 | G    |
| 8   | L5    | 2519 | U    |
| 8   | L5    | 2520 | C    |
| 8   | L5    | 2529 | A    |
| 8   | L5    | 2537 | A    |
| 8   | L5    | 2544 | G    |
| 8   | L5    | 2546 | G    |
| 8   | L5    | 2547 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 2554 | U    |
| 8   | L5    | 2555 | G    |
| 8   | L5    | 2556 | G    |
| 8   | L5    | 2560 | C    |
| 8   | L5    | 2567 | G    |
| 8   | L5    | 2568 | C    |
| 8   | L5    | 2573 | A    |
| 8   | L5    | 2583 | C    |
| 8   | L5    | 2586 | G    |
| 8   | L5    | 2587 | A    |
| 8   | L5    | 2589 | C    |
| 8   | L5    | 2618 | G    |
| 8   | L5    | 2627 | C    |
| 8   | L5    | 2653 | C    |
| 8   | L5    | 2662 | G    |
| 8   | L5    | 2669 | C    |
| 8   | L5    | 2675 | G    |
| 8   | L5    | 2676 | A    |
| 8   | L5    | 2687 | U    |
| 8   | L5    | 2694 | G    |
| 8   | L5    | 2695 | A    |
| 8   | L5    | 2696 | A    |
| 8   | L5    | 2703 | G    |
| 8   | L5    | 2711 | G    |
| 8   | L5    | 2712 | G    |
| 8   | L5    | 2714 | G    |
| 8   | L5    | 2717 | G    |
| 8   | L5    | 2724 | G    |
| 8   | L5    | 2726 | G    |
| 8   | L5    | 2728 | U    |
| 8   | L5    | 2732 | G    |
| 8   | L5    | 2739 | C    |
| 8   | L5    | 2742 | G    |
| 8   | L5    | 2743 | A    |
| 8   | L5    | 2754 | G    |
| 8   | L5    | 2759 | G    |
| 8   | L5    | 2761 | U    |
| 8   | L5    | 2763 | U    |
| 8   | L5    | 2764 | A    |
| 8   | L5    | 2769 | U    |
| 8   | L5    | 2770 | C    |
| 8   | L5    | 2788 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 2790 | U    |
| 8   | L5    | 2804 | OMC  |
| 8   | L5    | 2814 | C    |
| 8   | L5    | 2826 | U    |
| 8   | L5    | 2827 | G    |
| 8   | L5    | 2829 | U    |
| 8   | L5    | 2842 | G    |
| 8   | L5    | 2855 | G    |
| 8   | L5    | 2856 | C    |
| 8   | L5    | 2876 | OMG  |
| 8   | L5    | 2877 | G    |
| 8   | L5    | 2892 | C    |
| 8   | L5    | 2897 | G    |
| 8   | L5    | 2900 | U    |
| 8   | L5    | 2902 | G    |
| 8   | L5    | 2903 | G    |
| 8   | L5    | 2904 | U    |
| 8   | L5    | 2905 | C    |
| 8   | L5    | 3585 | G    |
| 8   | L5    | 3587 | C    |
| 8   | L5    | 3588 | C    |
| 8   | L5    | 3590 | G    |
| 8   | L5    | 3591 | C    |
| 8   | L5    | 3592 | G    |
| 8   | L5    | 3594 | C    |
| 8   | L5    | 3595 | U    |
| 8   | L5    | 3596 | A    |
| 8   | L5    | 3597 | G    |
| 8   | L5    | 3599 | A    |
| 8   | L5    | 3604 | A    |
| 8   | L5    | 3605 | C    |
| 8   | L5    | 3606 | U    |
| 8   | L5    | 3615 | G    |
| 8   | L5    | 3618 | C    |
| 8   | L5    | 3619 | G    |
| 8   | L5    | 3620 | G    |
| 8   | L5    | 3626 | G    |
| 8   | L5    | 3630 | A    |
| 8   | L5    | 3635 | A    |
| 8   | L5    | 3644 | U    |
| 8   | L5    | 3646 | A    |
| 8   | L5    | 3662 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 3663 | A    |
| 8   | L5    | 3673 | C    |
| 8   | L5    | 3674 | G    |
| 8   | L5    | 3701 | OMC  |
| 8   | L5    | 3702 | A    |
| 8   | L5    | 3710 | G    |
| 8   | L5    | 3711 | A    |
| 8   | L5    | 3717 | A    |
| 8   | L5    | 3735 | G    |
| 8   | L5    | 3736 | A    |
| 8   | L5    | 3737 | A    |
| 8   | L5    | 3748 | A    |
| 8   | L5    | 3750 | G    |
| 8   | L5    | 3757 | G    |
| 8   | L5    | 3761 | C    |
| 8   | L5    | 3769 | C    |
| 8   | L5    | 3771 | C    |
| 8   | L5    | 3773 | U    |
| 8   | L5    | 3774 | A    |
| 8   | L5    | 3776 | G    |
| 8   | L5    | 3777 | G    |
| 8   | L5    | 3784 | A    |
| 8   | L5    | 3785 | A    |
| 8   | L5    | 3786 | U    |
| 8   | L5    | 3801 | U    |
| 8   | L5    | 3802 | U    |
| 8   | L5    | 3811 | G    |
| 8   | L5    | 3813 | A    |
| 8   | L5    | 3814 | U    |
| 8   | L5    | 3817 | A    |
| 8   | L5    | 3818 | U    |
| 8   | L5    | 3819 | G    |
| 8   | L5    | 3838 | U    |
| 8   | L5    | 3839 | G    |
| 8   | L5    | 3840 | U    |
| 8   | L5    | 3851 | U    |
| 8   | L5    | 3867 | A    |
| 8   | L5    | 3877 | A    |
| 8   | L5    | 3878 | C    |
| 8   | L5    | 3879 | G    |
| 8   | L5    | 3892 | U    |
| 8   | L5    | 3897 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 3901 | A    |
| 8   | L5    | 3906 | A    |
| 8   | L5    | 3907 | G    |
| 8   | L5    | 3908 | A    |
| 8   | L5    | 3915 | U    |
| 8   | L5    | 3926 | C    |
| 8   | L5    | 3927 | U    |
| 8   | L5    | 3933 | G    |
| 8   | L5    | 3938 | G    |
| 8   | L5    | 3939 | G    |
| 8   | L5    | 3942 | C    |
| 8   | L5    | 4076 | G    |
| 8   | L5    | 4084 | G    |
| 8   | L5    | 4085 | A    |
| 8   | L5    | 4086 | G    |
| 8   | L5    | 4091 | G    |
| 8   | L5    | 4097 | G    |
| 8   | L5    | 4099 | G    |
| 8   | L5    | 4100 | C    |
| 8   | L5    | 4113 | U    |
| 8   | L5    | 4114 | C    |
| 8   | L5    | 4115 | G    |
| 8   | L5    | 4116 | C    |
| 8   | L5    | 4117 | U    |
| 8   | L5    | 4119 | C    |
| 8   | L5    | 4121 | G    |
| 8   | L5    | 4122 | G    |
| 8   | L5    | 4127 | A    |
| 8   | L5    | 4141 | G    |
| 8   | L5    | 4142 | C    |
| 8   | L5    | 4143 | G    |
| 8   | L5    | 4144 | C    |
| 8   | L5    | 4146 | G    |
| 8   | L5    | 4149 | C    |
| 8   | L5    | 4150 | G    |
| 8   | L5    | 4160 | C    |
| 8   | L5    | 4162 | C    |
| 8   | L5    | 4163 | U    |
| 8   | L5    | 4170 | A    |
| 8   | L5    | 4183 | G    |
| 8   | L5    | 4184 | G    |
| 8   | L5    | 4191 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 4201 | G    |
| 8   | L5    | 4203 | A    |
| 8   | L5    | 4205 | A    |
| 8   | L5    | 4212 | A    |
| 8   | L5    | 4222 | G    |
| 8   | L5    | 4229 | U    |
| 8   | L5    | 4233 | A    |
| 8   | L5    | 4234 | A    |
| 8   | L5    | 4251 | A    |
| 8   | L5    | 4254 | G    |
| 8   | L5    | 4256 | A    |
| 8   | L5    | 4257 | A    |
| 8   | L5    | 4265 | U    |
| 8   | L5    | 4273 | A    |
| 8   | L5    | 4284 | C    |
| 8   | L5    | 4291 | G    |
| 8   | L5    | 4297 | G    |
| 8   | L5    | 4304 | A    |
| 8   | L5    | 4305 | G    |
| 8   | L5    | 4306 | U    |
| 8   | L5    | 4314 | C    |
| 8   | L5    | 4330 | G    |
| 8   | L5    | 4332 | C    |
| 8   | L5    | 4339 | A    |
| 8   | L5    | 4349 | C    |
| 8   | L5    | 4354 | U    |
| 8   | L5    | 4373 | G    |
| 8   | L5    | 4377 | G    |
| 8   | L5    | 4378 | A    |
| 8   | L5    | 4379 | A    |
| 8   | L5    | 4381 | A    |
| 8   | L5    | 4387 | C    |
| 8   | L5    | 4394 | A    |
| 8   | L5    | 4421 | C    |
| 8   | L5    | 4422 | A    |
| 8   | L5    | 4444 | C    |
| 8   | L5    | 4448 | G    |
| 8   | L5    | 4449 | A    |
| 8   | L5    | 4453 | C    |
| 8   | L5    | 4464 | A    |
| 8   | L5    | 4466 | C    |
| 8   | L5    | 4475 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 4500 | U    |
| 8   | L5    | 4512 | U    |
| 8   | L5    | 4513 | A    |
| 8   | L5    | 4515 | G    |
| 8   | L5    | 4519 | C    |
| 8   | L5    | 4524 | G    |
| 8   | L5    | 4525 | C    |
| 8   | L5    | 4532 | U    |
| 8   | L5    | 4545 | G    |
| 8   | L5    | 4548 | A    |
| 8   | L5    | 4549 | G    |
| 8   | L5    | 4554 | G    |
| 8   | L5    | 4560 | C    |
| 8   | L5    | 4567 | G    |
| 8   | L5    | 4573 | G    |
| 8   | L5    | 4575 | G    |
| 8   | L5    | 4584 | A    |
| 8   | L5    | 4589 | A    |
| 8   | L5    | 4590 | A2M  |
| 8   | L5    | 4619 | U    |
| 8   | L5    | 4620 | OMU  |
| 8   | L5    | 4623 | OMG  |
| 8   | L5    | 4624 | A    |
| 8   | L5    | 4635 | A    |
| 8   | L5    | 4636 | U    |
| 8   | L5    | 4637 | OMG  |
| 8   | L5    | 4648 | A    |
| 8   | L5    | 4652 | G    |
| 8   | L5    | 4656 | A    |
| 8   | L5    | 4658 | G    |
| 8   | L5    | 4670 | C    |
| 8   | L5    | 4672 | A    |
| 8   | L5    | 4687 | A    |
| 8   | L5    | 4700 | A    |
| 8   | L5    | 4708 | A    |
| 8   | L5    | 4709 | U    |
| 8   | L5    | 4719 | G    |
| 8   | L5    | 4730 | C    |
| 8   | L5    | 4731 | G    |
| 8   | L5    | 4733 | C    |
| 8   | L5    | 4734 | A    |
| 8   | L5    | 4740 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 4741 | C    |
| 8   | L5    | 4742 | G    |
| 8   | L5    | 4745 | G    |
| 8   | L5    | 4747 | C    |
| 8   | L5    | 4751 | G    |
| 8   | L5    | 4754 | G    |
| 8   | L5    | 4757 | C    |
| 8   | L5    | 4759 | C    |
| 8   | L5    | 4761 | G    |
| 8   | L5    | 4765 | G    |
| 8   | L5    | 4772 | C    |
| 8   | L5    | 4773 | C    |
| 8   | L5    | 4775 | C    |
| 8   | L5    | 4776 | G    |
| 8   | L5    | 4859 | C    |
| 8   | L5    | 4861 | G    |
| 8   | L5    | 4864 | U    |
| 8   | L5    | 4870 | G    |
| 8   | L5    | 4871 | C    |
| 8   | L5    | 4875 | G    |
| 8   | L5    | 4877 | G    |
| 8   | L5    | 4881 | U    |
| 8   | L5    | 4882 | U    |
| 8   | L5    | 4883 | C    |
| 8   | L5    | 4886 | C    |
| 8   | L5    | 4889 | G    |
| 8   | L5    | 4895 | C    |
| 8   | L5    | 4896 | G    |
| 8   | L5    | 4897 | G    |
| 8   | L5    | 4898 | G    |
| 8   | L5    | 4900 | C    |
| 8   | L5    | 4901 | G    |
| 8   | L5    | 4910 | G    |
| 8   | L5    | 4912 | G    |
| 8   | L5    | 4914 | C    |
| 8   | L5    | 4916 | G    |
| 8   | L5    | 4917 | C    |
| 8   | L5    | 4923 | C    |
| 8   | L5    | 4934 | A    |
| 8   | L5    | 4937 | C    |
| 8   | L5    | 4938 | A    |
| 8   | L5    | 4940 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 4943 | A    |
| 8   | L5    | 4949 | G    |
| 8   | L5    | 4951 | G    |
| 8   | L5    | 4955 | A    |
| 8   | L5    | 4960 | G    |
| 8   | L5    | 4963 | G    |
| 8   | L5    | 4966 | A    |
| 8   | L5    | 4967 | A    |
| 8   | L5    | 4976 | U    |
| 8   | L5    | 4985 | U    |
| 8   | L5    | 5009 | G    |
| 8   | L5    | 5013 | C    |
| 8   | L5    | 5014 | A    |
| 8   | L5    | 5017 | G    |
| 8   | L5    | 5034 | A    |
| 8   | L5    | 5041 | G    |
| 8   | L5    | 5047 | C    |
| 8   | L5    | 5050 | C    |
| 8   | L5    | 5058 | A    |
| 8   | L5    | 5069 | U    |
| 9   | L7    | 7    | G    |
| 9   | L7    | 24   | C    |
| 9   | L7    | 27   | G    |
| 9   | L7    | 41   | G    |
| 9   | L7    | 53   | U    |
| 9   | L7    | 54   | A    |
| 9   | L7    | 63   | C    |
| 9   | L7    | 64   | G    |
| 9   | L7    | 97   | G    |
| 9   | L7    | 100  | A    |
| 9   | L7    | 111  | C    |
| 10  | L8    | 22   | U    |
| 10  | L8    | 23   | C    |
| 10  | L8    | 34   | U    |
| 10  | L8    | 35   | C    |
| 10  | L8    | 39   | G    |
| 10  | L8    | 48   | A    |
| 10  | L8    | 51   | U    |
| 10  | L8    | 52   | A    |
| 10  | L8    | 55   | PSU  |
| 10  | L8    | 59   | A    |
| 10  | L8    | 62   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | L8    | 63  | U    |
| 10  | L8    | 85  | U    |
| 10  | L8    | 86  | U    |
| 10  | L8    | 87  | G    |
| 10  | L8    | 88  | A    |
| 10  | L8    | 94  | G    |
| 10  | L8    | 103 | A    |
| 10  | L8    | 105 | C    |
| 10  | L8    | 106 | G    |
| 10  | L8    | 107 | C    |
| 10  | L8    | 110 | U    |
| 10  | L8    | 111 | U    |
| 10  | L8    | 114 | G    |
| 10  | L8    | 147 | G    |
| 10  | L8    | 153 | C    |
| 10  | L8    | 156 | U    |
| 49  | S2    | 2   | A    |
| 49  | S2    | 25  | A    |
| 49  | S2    | 33  | G    |
| 49  | S2    | 41  | G    |
| 49  | S2    | 42  | A    |
| 49  | S2    | 44  | U    |
| 49  | S2    | 45  | A    |
| 49  | S2    | 46  | A    |
| 49  | S2    | 56  | G    |
| 49  | S2    | 60  | A    |
| 49  | S2    | 61  | A    |
| 49  | S2    | 65  | C    |
| 49  | S2    | 67  | C    |
| 49  | S2    | 68  | A    |
| 49  | S2    | 71  | G    |
| 49  | S2    | 81  | U    |
| 49  | S2    | 93  | U    |
| 49  | S2    | 99  | A    |
| 49  | S2    | 103 | A    |
| 49  | S2    | 113 | G    |
| 49  | S2    | 115 | U    |
| 49  | S2    | 126 | G    |
| 49  | S2    | 130 | G    |
| 49  | S2    | 142 | C    |
| 49  | S2    | 143 | U    |
| 49  | S2    | 148 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 155 | G    |
| 49  | S2    | 159 | A2M  |
| 49  | S2    | 160 | U    |
| 49  | S2    | 162 | C    |
| 49  | S2    | 168 | C    |
| 49  | S2    | 169 | U    |
| 49  | S2    | 170 | A    |
| 49  | S2    | 173 | A    |
| 49  | S2    | 175 | A    |
| 49  | S2    | 179 | C    |
| 49  | S2    | 192 | C    |
| 49  | S2    | 215 | G    |
| 49  | S2    | 290 | U    |
| 49  | S2    | 291 | G    |
| 49  | S2    | 293 | C    |
| 49  | S2    | 294 | U    |
| 49  | S2    | 295 | C    |
| 49  | S2    | 302 | A    |
| 49  | S2    | 305 | U    |
| 49  | S2    | 306 | C    |
| 49  | S2    | 308 | G    |
| 49  | S2    | 309 | G    |
| 49  | S2    | 310 | C    |
| 49  | S2    | 311 | C    |
| 49  | S2    | 319 | C    |
| 49  | S2    | 323 | C    |
| 49  | S2    | 328 | U    |
| 49  | S2    | 329 | G    |
| 49  | S2    | 332 | G    |
| 49  | S2    | 351 | G    |
| 49  | S2    | 362 | C    |
| 49  | S2    | 364 | A    |
| 49  | S2    | 368 | U    |
| 49  | S2    | 370 | G    |
| 49  | S2    | 380 | G    |
| 49  | S2    | 381 | C    |
| 49  | S2    | 384 | U    |
| 49  | S2    | 385 | G    |
| 49  | S2    | 386 | C    |
| 49  | S2    | 398 | A    |
| 49  | S2    | 407 | G    |
| 49  | S2    | 408 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 409 | C    |
| 49  | S2    | 413 | G    |
| 49  | S2    | 421 | G    |
| 49  | S2    | 428 | OMU  |
| 49  | S2    | 429 | C    |
| 49  | S2    | 448 | A    |
| 49  | S2    | 449 | A    |
| 49  | S2    | 450 | C    |
| 49  | S2    | 452 | G    |
| 49  | S2    | 464 | A    |
| 49  | S2    | 465 | A    |
| 49  | S2    | 467 | G    |
| 49  | S2    | 471 | G    |
| 49  | S2    | 472 | C    |
| 49  | S2    | 473 | A    |
| 49  | S2    | 474 | G    |
| 49  | S2    | 482 | G    |
| 49  | S2    | 484 | A    |
| 49  | S2    | 485 | A    |
| 49  | S2    | 487 | U    |
| 49  | S2    | 488 | U    |
| 49  | S2    | 489 | A    |
| 49  | S2    | 492 | C    |
| 49  | S2    | 493 | A    |
| 49  | S2    | 501 | C    |
| 49  | S2    | 502 | C    |
| 49  | S2    | 503 | C    |
| 49  | S2    | 523 | A    |
| 49  | S2    | 525 | A    |
| 49  | S2    | 551 | U    |
| 49  | S2    | 555 | A    |
| 49  | S2    | 556 | U    |
| 49  | S2    | 557 | U    |
| 49  | S2    | 558 | G    |
| 49  | S2    | 560 | A    |
| 49  | S2    | 576 | A2M  |
| 49  | S2    | 578 | C    |
| 49  | S2    | 583 | C    |
| 49  | S2    | 587 | A    |
| 49  | S2    | 589 | G    |
| 49  | S2    | 590 | A    |
| 49  | S2    | 591 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 592 | C    |
| 49  | S2    | 593 | C    |
| 49  | S2    | 595 | U    |
| 49  | S2    | 596 | U    |
| 49  | S2    | 601 | OMG  |
| 49  | S2    | 602 | G    |
| 49  | S2    | 604 | A    |
| 49  | S2    | 605 | A    |
| 49  | S2    | 606 | G    |
| 49  | S2    | 607 | U    |
| 49  | S2    | 608 | C    |
| 49  | S2    | 614 | C    |
| 49  | S2    | 617 | G    |
| 49  | S2    | 618 | C    |
| 49  | S2    | 627 | U    |
| 49  | S2    | 628 | A    |
| 49  | S2    | 643 | A    |
| 49  | S2    | 644 | OMG  |
| 49  | S2    | 645 | C    |
| 49  | S2    | 655 | A    |
| 49  | S2    | 660 | C    |
| 49  | S2    | 668 | A2M  |
| 49  | S2    | 669 | A    |
| 49  | S2    | 671 | A    |
| 49  | S2    | 672 | A    |
| 49  | S2    | 673 | G    |
| 49  | S2    | 683 | OMG  |
| 49  | S2    | 688 | U    |
| 49  | S2    | 821 | G    |
| 49  | S2    | 822 | U    |
| 49  | S2    | 824 | C    |
| 49  | S2    | 830 | A    |
| 49  | S2    | 842 | C    |
| 49  | S2    | 847 | A    |
| 49  | S2    | 851 | C    |
| 49  | S2    | 856 | C    |
| 49  | S2    | 857 | U    |
| 49  | S2    | 869 | A    |
| 49  | S2    | 870 | A    |
| 49  | S2    | 871 | U    |
| 49  | S2    | 872 | A    |
| 49  | S2    | 874 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 877  | C    |
| 49  | S2    | 878  | G    |
| 49  | S2    | 879  | C    |
| 49  | S2    | 880  | G    |
| 49  | S2    | 881  | G    |
| 49  | S2    | 907  | G    |
| 49  | S2    | 909  | G    |
| 49  | S2    | 913  | A    |
| 49  | S2    | 919  | A    |
| 49  | S2    | 920  | A    |
| 49  | S2    | 930  | C    |
| 49  | S2    | 933  | G    |
| 49  | S2    | 950  | C    |
| 49  | S2    | 958  | G    |
| 49  | S2    | 963  | A    |
| 49  | S2    | 970  | G    |
| 49  | S2    | 971  | G    |
| 49  | S2    | 990  | A    |
| 49  | S2    | 992  | A    |
| 49  | S2    | 996  | A    |
| 49  | S2    | 999  | G    |
| 49  | S2    | 1001 | A    |
| 49  | S2    | 1008 | A    |
| 49  | S2    | 1016 | U    |
| 49  | S2    | 1017 | U    |
| 49  | S2    | 1023 | A    |
| 49  | S2    | 1027 | A    |
| 49  | S2    | 1045 | U    |
| 49  | S2    | 1049 | A    |
| 49  | S2    | 1050 | A    |
| 49  | S2    | 1055 | A    |
| 49  | S2    | 1061 | U    |
| 49  | S2    | 1062 | A    |
| 49  | S2    | 1078 | C    |
| 49  | S2    | 1083 | A    |
| 49  | S2    | 1085 | C    |
| 49  | S2    | 1086 | G    |
| 49  | S2    | 1087 | A    |
| 49  | S2    | 1088 | U    |
| 49  | S2    | 1100 | A    |
| 49  | S2    | 1110 | G    |
| 49  | S2    | 1113 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1115 | U    |
| 49  | S2    | 1116 | C    |
| 49  | S2    | 1117 | C    |
| 49  | S2    | 1118 | C    |
| 49  | S2    | 1119 | A    |
| 49  | S2    | 1126 | G    |
| 49  | S2    | 1133 | A    |
| 49  | S2    | 1153 | C    |
| 49  | S2    | 1154 | U    |
| 49  | S2    | 1155 | U    |
| 49  | S2    | 1157 | G    |
| 49  | S2    | 1183 | A    |
| 49  | S2    | 1195 | A    |
| 49  | S2    | 1207 | G    |
| 49  | S2    | 1208 | A    |
| 49  | S2    | 1209 | A    |
| 49  | S2    | 1215 | C    |
| 49  | S2    | 1217 | A    |
| 49  | S2    | 1224 | G    |
| 49  | S2    | 1238 | U    |
| 49  | S2    | 1242 | U    |
| 49  | S2    | 1243 | U    |
| 49  | S2    | 1247 | C    |
| 49  | S2    | 1248 | B8N  |
| 49  | S2    | 1251 | A    |
| 49  | S2    | 1253 | A    |
| 49  | S2    | 1256 | G    |
| 49  | S2    | 1257 | G    |
| 49  | S2    | 1259 | A    |
| 49  | S2    | 1265 | A    |
| 49  | S2    | 1269 | G    |
| 49  | S2    | 1271 | C    |
| 49  | S2    | 1274 | G    |
| 49  | S2    | 1275 | G    |
| 49  | S2    | 1277 | C    |
| 49  | S2    | 1282 | A    |
| 49  | S2    | 1286 | G    |
| 49  | S2    | 1288 | OMU  |
| 49  | S2    | 1298 | G    |
| 49  | S2    | 1299 | A    |
| 49  | S2    | 1301 | A    |
| 49  | S2    | 1302 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1303 | C    |
| 49  | S2    | 1304 | U    |
| 49  | S2    | 1308 | U    |
| 49  | S2    | 1309 | C    |
| 49  | S2    | 1327 | G    |
| 49  | S2    | 1330 | G    |
| 49  | S2    | 1331 | C    |
| 49  | S2    | 1337 | 4AC  |
| 49  | S2    | 1342 | U    |
| 49  | S2    | 1348 | G    |
| 49  | S2    | 1371 | U    |
| 49  | S2    | 1372 | U    |
| 49  | S2    | 1373 | C    |
| 49  | S2    | 1378 | A    |
| 49  | S2    | 1382 | A    |
| 49  | S2    | 1396 | A    |
| 49  | S2    | 1402 | A    |
| 49  | S2    | 1403 | C    |
| 49  | S2    | 1406 | G    |
| 49  | S2    | 1409 | A    |
| 49  | S2    | 1415 | C    |
| 49  | S2    | 1440 | C    |
| 49  | S2    | 1448 | A    |
| 49  | S2    | 1449 | G    |
| 49  | S2    | 1450 | G    |
| 49  | S2    | 1452 | A    |
| 49  | S2    | 1454 | A    |
| 49  | S2    | 1474 | A    |
| 49  | S2    | 1477 | U    |
| 49  | S2    | 1487 | A    |
| 49  | S2    | 1489 | A    |
| 49  | S2    | 1490 | G    |
| 49  | S2    | 1495 | G    |
| 49  | S2    | 1498 | A    |
| 49  | S2    | 1505 | U    |
| 49  | S2    | 1506 | A    |
| 49  | S2    | 1508 | A    |
| 49  | S2    | 1519 | U    |
| 49  | S2    | 1520 | G    |
| 49  | S2    | 1521 | C    |
| 49  | S2    | 1522 | A    |
| 49  | S2    | 1528 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1533 | A    |
| 49  | S2    | 1543 | U    |
| 49  | S2    | 1544 | C    |
| 49  | S2    | 1546 | G    |
| 49  | S2    | 1552 | G    |
| 49  | S2    | 1553 | C    |
| 49  | S2    | 1569 | A    |
| 49  | S2    | 1570 | G    |
| 49  | S2    | 1574 | C    |
| 49  | S2    | 1578 | U    |
| 49  | S2    | 1580 | A    |
| 49  | S2    | 1585 | U    |
| 49  | S2    | 1586 | U    |
| 49  | S2    | 1588 | A    |
| 49  | S2    | 1589 | A    |
| 49  | S2    | 1599 | U    |
| 49  | S2    | 1601 | A    |
| 49  | S2    | 1604 | G    |
| 49  | S2    | 1606 | G    |
| 49  | S2    | 1607 | A    |
| 49  | S2    | 1621 | U    |
| 49  | S2    | 1623 | A    |
| 49  | S2    | 1624 | U    |
| 49  | S2    | 1633 | A    |
| 49  | S2    | 1634 | A    |
| 49  | S2    | 1646 | C    |
| 49  | S2    | 1648 | G    |
| 49  | S2    | 1652 | G    |
| 49  | S2    | 1654 | G    |
| 49  | S2    | 1661 | A    |
| 49  | S2    | 1662 | U    |
| 49  | S2    | 1663 | A    |
| 49  | S2    | 1664 | A    |
| 49  | S2    | 1665 | G    |
| 49  | S2    | 1671 | G    |
| 49  | S2    | 1680 | G    |
| 49  | S2    | 1683 | C    |
| 49  | S2    | 1695 | A    |
| 49  | S2    | 1698 | C    |
| 49  | S2    | 1709 | G    |
| 49  | S2    | 1715 | A    |
| 49  | S2    | 1719 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1722 | G    |
| 49  | S2    | 1726 | G    |
| 49  | S2    | 1729 | U    |
| 49  | S2    | 1742 | C    |
| 49  | S2    | 1743 | G    |
| 49  | S2    | 1744 | G    |
| 49  | S2    | 1813 | A    |
| 49  | S2    | 1822 | A    |
| 49  | S2    | 1823 | A    |
| 49  | S2    | 1824 | A    |
| 49  | S2    | 1829 | G    |
| 49  | S2    | 1831 | A    |
| 49  | S2    | 1832 | 6MZ  |
| 49  | S2    | 1834 | A    |
| 49  | S2    | 1835 | A    |
| 49  | S2    | 1837 | G    |
| 49  | S2    | 1838 | U    |
| 49  | S2    | 1849 | G    |
| 49  | S2    | 1850 | MA6  |
| 49  | S2    | 1851 | MA6  |
| 49  | S2    | 1852 | C    |
| 49  | S2    | 1861 | G    |
| 49  | S2    | 1862 | G    |
| 49  | S2    | 1863 | A    |
| 49  | S2    | 1865 | C    |
| 49  | S2    | 1868 | U    |
| 49  | S2    | 1869 | A    |

All (22) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 233  | U    |
| 8   | L5    | 406  | C    |
| 8   | L5    | 667  | A    |
| 8   | L5    | 1082 | C    |
| 8   | L5    | 1210 | C    |
| 8   | L5    | 1271 | G    |
| 8   | L5    | 2019 | C    |
| 8   | L5    | 2416 | G    |
| 8   | L5    | 2675 | G    |
| 8   | L5    | 2760 | G    |
| 8   | L5    | 3614 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | L5    | 3673 | C    |
| 8   | L5    | 3701 | OMC  |
| 8   | L5    | 4699 | U    |
| 8   | L5    | 4740 | G    |
| 8   | L5    | 4913 | G    |
| 49  | S2    | 601  | OMG  |
| 49  | S2    | 604  | A    |
| 49  | S2    | 1395 | C    |
| 49  | S2    | 1519 | U    |
| 49  | S2    | 1585 | U    |
| 49  | S2    | 1664 | A    |

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

76 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$ |
| 49  | A2M  | S2    | 27   | 49,84 | 22,25,26     | 3.48 | 10 (45%)    | 31,36,39    | 2.40 | 10 (32%)    |
| 8   | A2M  | L5    | 4590 | 8,84  | 22,25,26     | 3.46 | 9 (40%)     | 31,36,39    | 2.47 | 11 (35%)    |
| 49  | OMG  | S2    | 644  | 49    | 23,26,27     | 2.40 | 9 (39%)     | 33,38,41    | 2.59 | 10 (30%)    |
| 10  | OMU  | L8    | 14   | 10    | 19,22,23     | 3.05 | 8 (42%)     | 26,31,34    | 1.83 | 7 (26%)     |
| 8   | OMC  | L5    | 2365 | 8     | 19,22,23     | 2.94 | 8 (42%)     | 26,31,34    | 0.76 | 0           |
| 8   | A2M  | L5    | 3825 | 8     | 22,25,26     | 3.49 | 10 (45%)    | 31,36,39    | 2.37 | 11 (35%)    |
| 8   | A2M  | L5    | 3724 | 8     | 22,25,26     | 3.46 | 10 (45%)    | 31,36,39    | 2.40 | 11 (35%)    |
| 49  | OMG  | S2    | 1328 | 49    | 23,26,27     | 2.37 | 9 (39%)     | 33,38,41    | 2.52 | 10 (30%)    |
| 8   | OMG  | L5    | 4228 | 8     | 23,26,27     | 2.35 | 9 (39%)     | 33,38,41    | 2.44 | 12 (36%)    |
| 49  | OMC  | S2    | 174  | 49    | 19,22,23     | 2.97 | 8 (42%)     | 26,31,34    | 0.75 | 0           |
| 49  | OMC  | S2    | 1703 | 49    | 19,22,23     | 2.94 | 8 (42%)     | 26,31,34    | 0.67 | 0           |
| 10  | PSU  | L8    | 55   | 10    | 18,21,22     | 4.39 | 7 (38%)     | 22,30,33    | 1.63 | 4 (18%)     |
| 8   | OMU  | L5    | 4620 | 8     | 19,22,23     | 2.91 | 8 (42%)     | 26,31,34    | 1.79 | 5 (19%)     |
| 8   | OMG  | L5    | 3744 | 8     | 23,26,27     | 2.38 | 9 (39%)     | 33,38,41    | 2.51 | 11 (33%)    |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | OMG  | L5    | 4623 | 8     | 23,26,27     | 2.36 | 9 (39%)  | 33,38,41    | 2.49 | 11 (33%) |
| 8   | OMC  | L5    | 1340 | 8     | 19,22,23     | 2.91 | 8 (42%)  | 26,31,34    | 0.74 | 0        |
| 8   | OMG  | L5    | 4494 | 8     | 23,26,27     | 2.42 | 9 (39%)  | 33,38,41    | 2.58 | 10 (30%) |
| 8   | A2M  | L5    | 2401 | 8     | 22,25,26     | 3.45 | 9 (40%)  | 31,36,39    | 2.35 | 10 (32%) |
| 8   | PSU  | L5    | 1782 | 8     | 18,21,22     | 4.43 | 7 (38%)  | 22,30,33    | 1.72 | 4 (18%)  |
| 8   | A2M  | L5    | 3723 | 8     | 22,25,26     | 3.48 | 9 (40%)  | 31,36,39    | 2.33 | 10 (32%) |
| 8   | A2M  | L5    | 3760 | 8     | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.32 | 8 (25%)  |
| 8   | PSU  | L5    | 4353 | 8     | 18,21,22     | 4.41 | 7 (38%)  | 22,30,33    | 1.82 | 5 (22%)  |
| 8   | A2M  | L5    | 1871 | 8     | 22,25,26     | 3.51 | 10 (45%) | 31,36,39    | 2.40 | 10 (32%) |
| 49  | A2M  | S2    | 1678 | 49    | 22,25,26     | 3.52 | 9 (40%)  | 31,36,39    | 2.49 | 11 (35%) |
| 49  | 6MZ  | S2    | 1832 | 49    | 22,25,26     | 2.52 | 4 (18%)  | 30,36,39    | 2.27 | 9 (30%)  |
| 8   | PSU  | L5    | 3758 | 8     | 18,21,22     | 4.37 | 7 (38%)  | 22,30,33    | 1.81 | 4 (18%)  |
| 8   | PSU  | L5    | 3729 | 8     | 18,21,22     | 4.38 | 7 (38%)  | 22,30,33    | 1.77 | 5 (22%)  |
| 49  | OMG  | S2    | 683  | 49    | 23,26,27     | 2.39 | 9 (39%)  | 33,38,41    | 2.49 | 12 (36%) |
| 8   | PSU  | L5    | 1683 | 8     | 18,21,22     | 4.37 | 7 (38%)  | 22,30,33    | 1.78 | 5 (22%)  |
| 49  | B8N  | S2    | 1248 | 49    | 24,29,30     | 3.07 | 8 (33%)  | 29,42,45    | 2.06 | 9 (31%)  |
| 8   | OMC  | L5    | 2422 | 8,84  | 19,22,23     | 2.95 | 8 (42%)  | 26,31,34    | 0.74 | 0        |
| 8   | OMG  | L5    | 4637 | 8     | 23,26,27     | 2.41 | 9 (39%)  | 33,38,41    | 2.68 | 10 (30%) |
| 8   | PSU  | L5    | 3734 | 8     | 18,21,22     | 4.53 | 7 (38%)  | 22,30,33    | 1.77 | 5 (22%)  |
| 49  | OMU  | S2    | 1288 | 49    | 19,22,23     | 2.98 | 8 (42%)  | 26,31,34    | 1.70 | 5 (19%)  |
| 8   | A2M  | L5    | 1326 | 8     | 22,25,26     | 3.46 | 10 (45%) | 31,36,39    | 2.40 | 11 (35%) |
| 8   | OMG  | L5    | 1625 | 8     | 23,26,27     | 2.40 | 9 (39%)  | 33,38,41    | 2.58 | 10 (30%) |
| 8   | OMG  | L5    | 4370 | 8     | 23,26,27     | 2.37 | 9 (39%)  | 33,38,41    | 2.52 | 10 (30%) |
| 49  | A2M  | S2    | 668  | 49,84 | 22,25,26     | 3.45 | 10 (45%) | 31,36,39    | 2.43 | 11 (35%) |
| 49  | MA6  | S2    | 1851 | 49    | 23,26,27     | 1.40 | 4 (17%)  | 34,38,41    | 3.44 | 11 (32%) |
| 8   | OMG  | L5    | 4618 | 8     | 23,26,27     | 2.37 | 9 (39%)  | 33,38,41    | 2.48 | 11 (33%) |
| 49  | A2M  | S2    | 1383 | 49    | 22,25,26     | 3.44 | 9 (40%)  | 31,36,39    | 2.40 | 10 (32%) |
| 49  | OMU  | S2    | 1442 | 49,84 | 19,22,23     | 2.94 | 8 (42%)  | 26,31,34    | 1.72 | 5 (19%)  |
| 8   | OMC  | L5    | 2351 | 8     | 19,22,23     | 2.94 | 8 (42%)  | 26,31,34    | 0.86 | 0        |
| 8   | A2M  | L5    | 398  | 8     | 22,25,26     | 3.47 | 10 (45%) | 31,36,39    | 2.39 | 10 (32%) |
| 8   | OMG  | L5    | 3627 | 8     | 23,26,27     | 2.37 | 9 (39%)  | 33,38,41    | 2.46 | 11 (33%) |
| 8   | OMC  | L5    | 2861 | 8     | 19,22,23     | 2.91 | 8 (42%)  | 26,31,34    | 0.70 | 0        |
| 8   | OMC  | L5    | 3701 | 8,84  | 19,22,23     | 2.92 | 8 (42%)  | 26,31,34    | 0.71 | 0        |
| 8   | OMG  | L5    | 4499 | 8     | 23,26,27     | 2.38 | 9 (39%)  | 33,38,41    | 2.53 | 10 (30%) |
| 8   | OMC  | L5    | 4536 | 8     | 19,22,23     | 2.88 | 8 (42%)  | 26,31,34    | 0.76 | 0        |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | OMG  | L5    | 2424 | 8     | 23,26,27     | 2.43 | 9 (39%)  | 33,38,41    | 2.56 | 10 (30%) |
| 8   | OMG  | L5    | 3792 | 8     | 23,26,27     | 2.38 | 9 (39%)  | 33,38,41    | 2.61 | 10 (30%) |
| 49  | A2M  | S2    | 159  | 49    | 22,25,26     | 3.49 | 9 (40%)  | 31,36,39    | 2.45 | 10 (32%) |
| 49  | 4AC  | S2    | 1842 | 49    | 21,24,25     | 3.37 | 9 (42%)  | 29,34,37    | 1.02 | 4 (13%)  |
| 8   | A2M  | L5    | 3718 | 8     | 22,25,26     | 3.46 | 9 (40%)  | 31,36,39    | 2.40 | 12 (38%) |
| 8   | A2M  | L5    | 1524 | 8     | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.28 | 10 (32%) |
| 49  | A2M  | S2    | 576  | 49    | 22,25,26     | 3.46 | 9 (40%)  | 31,36,39    | 2.39 | 12 (38%) |
| 8   | OMG  | L5    | 1522 | 8     | 23,26,27     | 2.35 | 9 (39%)  | 33,38,41    | 2.52 | 11 (33%) |
| 49  | OMU  | S2    | 428  | 49    | 19,22,23     | 3.01 | 8 (42%)  | 26,31,34    | 1.68 | 5 (19%)  |
| 8   | OMC  | L5    | 1881 | 8,84  | 19,22,23     | 2.90 | 8 (42%)  | 26,31,34    | 0.79 | 0        |
| 49  | OMC  | S2    | 1391 | 49    | 19,22,23     | 2.94 | 8 (42%)  | 26,31,34    | 0.76 | 0        |
| 49  | G7M  | S2    | 1639 | 49,6  | 23,26,27     | 2.60 | 9 (39%)  | 35,39,42    | 2.50 | 11 (31%) |
| 49  | A2M  | S2    | 1031 | 49,83 | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.41 | 10 (32%) |
| 49  | UY1  | S2    | 1326 | 49,84 | 19,22,23     | 4.02 | 7 (36%)  | 22,31,34    | 1.82 | 5 (22%)  |
| 49  | 4AC  | S2    | 1337 | 49    | 21,24,25     | 3.37 | 9 (42%)  | 29,34,37    | 1.20 | 4 (13%)  |
| 8   | OMG  | L5    | 1316 | 8     | 23,26,27     | 2.39 | 9 (39%)  | 33,38,41    | 2.61 | 10 (30%) |
| 49  | MA6  | S2    | 1850 | 49    | 23,26,27     | 1.44 | 4 (17%)  | 34,38,41    | 3.10 | 11 (32%) |
| 8   | OMC  | L5    | 3841 | 8     | 19,22,23     | 2.87 | 8 (42%)  | 26,31,34    | 0.65 | 0        |
| 8   | OMG  | L5    | 2364 | 8     | 23,26,27     | 2.37 | 9 (39%)  | 33,38,41    | 2.52 | 11 (33%) |
| 8   | OMG  | L5    | 2876 | 8     | 23,26,27     | 2.35 | 9 (39%)  | 33,38,41    | 2.66 | 10 (30%) |
| 8   | OMC  | L5    | 2804 | 8     | 19,22,23     | 2.87 | 8 (42%)  | 26,31,34    | 0.71 | 0        |
| 8   | A2M  | L5    | 2787 | 8,84  | 22,25,26     | 3.43 | 9 (40%)  | 31,36,39    | 2.36 | 11 (35%) |
| 49  | OMG  | S2    | 601  | 49    | 23,26,27     | 2.40 | 9 (39%)  | 33,38,41    | 2.72 | 9 (27%)  |
| 8   | OMU  | L5    | 3925 | 8     | 19,22,23     | 2.85 | 8 (42%)  | 26,31,34    | 1.66 | 5 (19%)  |
| 8   | A2M  | L5    | 2815 | 8     | 22,25,26     | 3.43 | 9 (40%)  | 31,36,39    | 2.44 | 10 (32%) |
| 8   | A2M  | L5    | 2363 | 8,84  | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.38 | 10 (32%) |
| 10  | OMG  | L8    | 75   | 10    | 23,26,27     | 2.39 | 9 (39%)  | 33,38,41    | 2.53 | 10 (30%) |

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   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 49  | A2M  | S2    | 27   | 49,84 | -       | 1/9/27/28 | 0/3/3/3 |
| 8   | A2M  | L5    | 4590 | 8,84  | -       | 2/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 49  | OMG  | S2    | 644  | 49    | -       | 4/9/27/28  | 0/3/3/3 |
| 10  | OMU  | L8    | 14   | 10    | -       | 5/9/27/28  | 0/2/2/2 |
| 8   | OMC  | L5    | 2365 | 8     | -       | 0/9/27/28  | 0/2/2/2 |
| 8   | A2M  | L5    | 3825 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | A2M  | L5    | 3724 | 8     | -       | 1/9/27/28  | 0/3/3/3 |
| 49  | OMG  | S2    | 1328 | 49    | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 4228 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 49  | OMC  | S2    | 174  | 49    | -       | 0/9/27/28  | 0/2/2/2 |
| 49  | OMC  | S2    | 1703 | 49    | -       | 2/9/27/28  | 0/2/2/2 |
| 10  | PSU  | L8    | 55   | 10    | -       | 2/7/25/26  | 0/2/2/2 |
| 8   | OMU  | L5    | 4620 | 8     | -       | 2/9/27/28  | 0/2/2/2 |
| 8   | OMG  | L5    | 3744 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 4623 | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMC  | L5    | 1340 | 8     | -       | 0/9/27/28  | 0/2/2/2 |
| 8   | OMG  | L5    | 4494 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | A2M  | L5    | 2401 | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | PSU  | L5    | 1782 | 8     | -       | 0/7/25/26  | 0/2/2/2 |
| 8   | A2M  | L5    | 3723 | 8     | -       | 1/9/27/28  | 0/3/3/3 |
| 8   | A2M  | L5    | 3760 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | PSU  | L5    | 4353 | 8     | -       | 0/7/25/26  | 0/2/2/2 |
| 8   | A2M  | L5    | 1871 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 49  | A2M  | S2    | 1678 | 49    | -       | 1/9/27/28  | 0/3/3/3 |
| 49  | 6MZ  | S2    | 1832 | 49    | -       | 3/9/27/28  | 0/3/3/3 |
| 8   | PSU  | L5    | 3758 | 8     | -       | 0/7/25/26  | 0/2/2/2 |
| 8   | PSU  | L5    | 3729 | 8     | -       | 2/7/25/26  | 0/2/2/2 |
| 49  | OMG  | S2    | 683  | 49    | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | PSU  | L5    | 1683 | 8     | -       | 0/7/25/26  | 0/2/2/2 |
| 49  | B8N  | S2    | 1248 | 49    | -       | 7/16/34/35 | 0/2/2/2 |
| 8   | OMC  | L5    | 2422 | 8,84  | -       | 2/9/27/28  | 0/2/2/2 |
| 8   | OMG  | L5    | 4637 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | PSU  | L5    | 3734 | 8     | -       | 2/7/25/26  | 0/2/2/2 |
| 49  | OMU  | S2    | 1288 | 49    | -       | 2/9/27/28  | 0/2/2/2 |
| 8   | A2M  | L5    | 1326 | 8     | -       | 1/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 1625 | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 4370 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 49  | A2M  | S2    | 668  | 49,84 | -       | 3/9/27/28  | 0/3/3/3 |
| 49  | MA6  | S2    | 1851 | 49    | -       | 3/11/29/30 | 0/3/3/3 |
| 8   | OMG  | L5    | 4618 | 8     | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 49  | A2M  | S2    | 1383 | 49    | -       | 1/9/27/28  | 0/3/3/3 |
| 49  | OMU  | S2    | 1442 | 49,84 | -       | 1/9/27/28  | 0/2/2/2 |
| 8   | OMC  | L5    | 2351 | 8     | -       | 5/9/27/28  | 0/2/2/2 |
| 8   | A2M  | L5    | 398  | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 3627 | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMC  | L5    | 2861 | 8     | -       | 1/9/27/28  | 0/2/2/2 |
| 8   | OMC  | L5    | 3701 | 8,84  | -       | 5/9/27/28  | 0/2/2/2 |
| 8   | OMG  | L5    | 4499 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | OMC  | L5    | 4536 | 8     | -       | 0/9/27/28  | 0/2/2/2 |
| 8   | OMG  | L5    | 2424 | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 3792 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 49  | A2M  | S2    | 159  | 49    | -       | 2/9/27/28  | 0/3/3/3 |
| 49  | 4AC  | S2    | 1842 | 49    | -       | 0/11/29/30 | 0/2/2/2 |
| 8   | A2M  | L5    | 3718 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | A2M  | L5    | 1524 | 8     | -       | 1/9/27/28  | 0/3/3/3 |
| 49  | A2M  | S2    | 576  | 49    | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 1522 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 49  | OMU  | S2    | 428  | 49    | -       | 6/9/27/28  | 0/2/2/2 |
| 8   | OMC  | L5    | 1881 | 8,84  | -       | 0/9/27/28  | 0/2/2/2 |
| 49  | OMC  | S2    | 1391 | 49    | -       | 0/9/27/28  | 0/2/2/2 |
| 49  | G7M  | S2    | 1639 | 49,6  | -       | 1/7/25/26  | 0/3/3/3 |
| 49  | A2M  | S2    | 1031 | 49,83 | -       | 0/9/27/28  | 0/3/3/3 |
| 49  | UY1  | S2    | 1326 | 49,84 | -       | 2/9/27/28  | 0/2/2/2 |
| 49  | 4AC  | S2    | 1337 | 49    | -       | 0/11/29/30 | 0/2/2/2 |
| 8   | OMG  | L5    | 1316 | 8     | -       | 1/9/27/28  | 0/3/3/3 |
| 49  | MA6  | S2    | 1850 | 49    | -       | 1/11/29/30 | 0/3/3/3 |
| 8   | OMC  | L5    | 3841 | 8     | -       | 1/9/27/28  | 0/2/2/2 |
| 8   | OMG  | L5    | 2364 | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMG  | L5    | 2876 | 8     | -       | 2/9/27/28  | 0/3/3/3 |
| 8   | OMC  | L5    | 2804 | 8     | -       | 1/9/27/28  | 0/2/2/2 |
| 8   | A2M  | L5    | 2787 | 8,84  | -       | 3/9/27/28  | 0/3/3/3 |
| 49  | OMG  | S2    | 601  | 49    | -       | 5/9/27/28  | 0/3/3/3 |
| 8   | OMU  | L5    | 3925 | 8     | -       | 1/9/27/28  | 0/2/2/2 |
| 8   | A2M  | L5    | 2815 | 8     | -       | 0/9/27/28  | 0/3/3/3 |
| 8   | A2M  | L5    | 2363 | 8,84  | -       | 0/9/27/28  | 0/3/3/3 |
| 10  | OMG  | L8    | 75   | 10    | -       | 0/9/27/28  | 0/3/3/3 |

All (644) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 3734 | PSU  | C6-C5   | 11.80 | 1.49        | 1.35     |
| 8   | L5    | 1782 | PSU  | C6-C5   | 11.44 | 1.48        | 1.35     |
| 10  | L8    | 55   | PSU  | C6-C5   | 11.40 | 1.48        | 1.35     |
| 8   | L5    | 1683 | PSU  | C6-C5   | 11.32 | 1.48        | 1.35     |
| 8   | L5    | 4353 | PSU  | C6-C5   | 11.30 | 1.48        | 1.35     |
| 8   | L5    | 3729 | PSU  | C6-C5   | 11.23 | 1.48        | 1.35     |
| 8   | L5    | 3758 | PSU  | C6-C5   | 11.13 | 1.48        | 1.35     |
| 49  | S2    | 1326 | UY1  | C6-C5   | 10.71 | 1.47        | 1.35     |
| 49  | S2    | 1832 | 6MZ  | C6-N6   | 10.40 | 1.45        | 1.34     |
| 8   | L5    | 3734 | PSU  | C2-N1   | 9.67  | 1.49        | 1.36     |
| 8   | L5    | 4353 | PSU  | C2-N1   | 9.54  | 1.49        | 1.36     |
| 8   | L5    | 1782 | PSU  | C2-N1   | 9.46  | 1.49        | 1.36     |
| 8   | L5    | 3758 | PSU  | C2-N1   | 9.38  | 1.49        | 1.36     |
| 49  | S2    | 1326 | UY1  | C2-N1   | 9.38  | 1.49        | 1.36     |
| 8   | L5    | 1683 | PSU  | C2-N1   | 9.30  | 1.49        | 1.36     |
| 8   | L5    | 3729 | PSU  | C2-N1   | 9.29  | 1.49        | 1.36     |
| 49  | S2    | 1248 | B8N  | C4-N3   | -9.24 | 1.23        | 1.40     |
| 10  | L8    | 55   | PSU  | C2-N1   | 9.16  | 1.49        | 1.36     |
| 49  | S2    | 27   | A2M  | C2'-C1' | -8.99 | 1.29        | 1.53     |
| 8   | L5    | 2363 | A2M  | C2'-C1' | -8.97 | 1.30        | 1.53     |
| 49  | S2    | 1678 | A2M  | C2'-C1' | -8.96 | 1.30        | 1.53     |
| 8   | L5    | 3760 | A2M  | C2'-C1' | -8.96 | 1.30        | 1.53     |
| 8   | L5    | 3825 | A2M  | C2'-C1' | -8.94 | 1.30        | 1.53     |
| 8   | L5    | 1871 | A2M  | C2'-C1' | -8.88 | 1.30        | 1.53     |
| 49  | S2    | 1031 | A2M  | C2'-C1' | -8.82 | 1.30        | 1.53     |
| 8   | L5    | 2401 | A2M  | C2'-C1' | -8.82 | 1.30        | 1.53     |
| 8   | L5    | 2787 | A2M  | C2'-C1' | -8.81 | 1.30        | 1.53     |
| 49  | S2    | 576  | A2M  | C2'-C1' | -8.81 | 1.30        | 1.53     |
| 8   | L5    | 1326 | A2M  | C2'-C1' | -8.80 | 1.30        | 1.53     |
| 8   | L5    | 398  | A2M  | C2'-C1' | -8.77 | 1.30        | 1.53     |
| 8   | L5    | 1524 | A2M  | C2'-C1' | -8.76 | 1.30        | 1.53     |
| 8   | L5    | 2815 | A2M  | C2'-C1' | -8.75 | 1.30        | 1.53     |
| 8   | L5    | 3723 | A2M  | C2'-C1' | -8.75 | 1.30        | 1.53     |
| 49  | S2    | 159  | A2M  | C2'-C1' | -8.75 | 1.30        | 1.53     |
| 8   | L5    | 3718 | A2M  | C2'-C1' | -8.70 | 1.30        | 1.53     |
| 8   | L5    | 3724 | A2M  | C2'-C1' | -8.67 | 1.30        | 1.53     |
| 8   | L5    | 398  | A2M  | O4'-C1' | 8.67  | 1.62        | 1.42     |
| 8   | L5    | 4590 | A2M  | C2'-C1' | -8.66 | 1.30        | 1.53     |
| 49  | S2    | 1383 | A2M  | C2'-C1' | -8.65 | 1.30        | 1.53     |
| 8   | L5    | 3718 | A2M  | O4'-C1' | 8.65  | 1.62        | 1.42     |
| 49  | S2    | 668  | A2M  | C2'-C1' | -8.63 | 1.30        | 1.53     |
| 8   | L5    | 4590 | A2M  | O4'-C1' | 8.61  | 1.62        | 1.42     |
| 8   | L5    | 3723 | A2M  | O4'-C1' | 8.61  | 1.62        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 1871 | A2M  | O4'-C1' | 8.61  | 1.62        | 1.42     |
| 49  | S2    | 1383 | A2M  | O4'-C1' | 8.61  | 1.62        | 1.42     |
| 8   | L5    | 3724 | A2M  | O4'-C1' | 8.60  | 1.62        | 1.42     |
| 49  | S2    | 1678 | A2M  | O4'-C1' | 8.59  | 1.62        | 1.42     |
| 49  | S2    | 576  | A2M  | O4'-C1' | 8.55  | 1.62        | 1.42     |
| 49  | S2    | 159  | A2M  | O4'-C1' | 8.55  | 1.62        | 1.42     |
| 8   | L5    | 3825 | A2M  | O4'-C1' | 8.47  | 1.62        | 1.42     |
| 8   | L5    | 2787 | A2M  | O4'-C1' | 8.47  | 1.62        | 1.42     |
| 8   | L5    | 2815 | A2M  | O4'-C1' | 8.45  | 1.62        | 1.42     |
| 8   | L5    | 1524 | A2M  | O4'-C1' | 8.42  | 1.61        | 1.42     |
| 8   | L5    | 2401 | A2M  | O4'-C1' | 8.40  | 1.61        | 1.42     |
| 49  | S2    | 27   | A2M  | O4'-C1' | 8.36  | 1.61        | 1.42     |
| 49  | S2    | 1031 | A2M  | O4'-C1' | 8.36  | 1.61        | 1.42     |
| 8   | L5    | 2363 | A2M  | O4'-C1' | 8.34  | 1.61        | 1.42     |
| 8   | L5    | 1326 | A2M  | O4'-C1' | 8.32  | 1.61        | 1.42     |
| 8   | L5    | 3760 | A2M  | O4'-C1' | 8.22  | 1.61        | 1.42     |
| 49  | S2    | 668  | A2M  | O4'-C1' | 8.19  | 1.61        | 1.42     |
| 8   | L5    | 3734 | PSU  | C2-N3   | 7.52  | 1.50        | 1.37     |
| 8   | L5    | 3729 | PSU  | C2-N3   | 7.46  | 1.50        | 1.37     |
| 8   | L5    | 1782 | PSU  | C2-N3   | 7.41  | 1.50        | 1.37     |
| 10  | L8    | 55   | PSU  | C2-N3   | 7.41  | 1.50        | 1.37     |
| 8   | L5    | 1683 | PSU  | C2-N3   | 7.33  | 1.50        | 1.37     |
| 8   | L5    | 3758 | PSU  | C2-N3   | 7.31  | 1.50        | 1.37     |
| 8   | L5    | 4353 | PSU  | C2-N3   | 7.30  | 1.50        | 1.37     |
| 10  | L8    | 14   | OMU  | C2-N1   | 7.28  | 1.50        | 1.38     |
| 49  | S2    | 1326 | UY1  | C2-N3   | 7.04  | 1.49        | 1.37     |
| 49  | S2    | 428  | OMU  | C2-N1   | 6.97  | 1.49        | 1.38     |
| 49  | S2    | 668  | A2M  | O4'-C4' | -6.84 | 1.29        | 1.45     |
| 49  | S2    | 1337 | 4AC  | C4-N3   | 6.80  | 1.44        | 1.32     |
| 49  | S2    | 1031 | A2M  | O4'-C4' | -6.78 | 1.29        | 1.45     |
| 49  | S2    | 1248 | B8N  | C6-N1   | 6.78  | 1.53        | 1.36     |
| 49  | S2    | 1288 | OMU  | C2-N3   | 6.76  | 1.50        | 1.38     |
| 49  | S2    | 1288 | OMU  | C2-N1   | 6.76  | 1.49        | 1.38     |
| 49  | S2    | 1842 | 4AC  | C4-N3   | 6.72  | 1.44        | 1.32     |
| 49  | S2    | 1442 | OMU  | C2-N1   | 6.71  | 1.49        | 1.38     |
| 49  | S2    | 428  | OMU  | C2-N3   | 6.71  | 1.49        | 1.38     |
| 10  | L8    | 14   | OMU  | C2-N3   | 6.67  | 1.49        | 1.38     |
| 49  | S2    | 1442 | OMU  | C2-N3   | 6.65  | 1.49        | 1.38     |
| 49  | S2    | 1678 | A2M  | O4'-C4' | -6.62 | 1.30        | 1.45     |
| 8   | L5    | 2363 | A2M  | O4'-C4' | -6.61 | 1.30        | 1.45     |
| 8   | L5    | 4620 | OMU  | C2-N1   | 6.58  | 1.49        | 1.38     |
| 8   | L5    | 1524 | A2M  | O4'-C4' | -6.57 | 1.30        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 4620 | OMU  | C2-N3   | 6.53  | 1.49        | 1.38     |
| 8   | L5    | 3825 | A2M  | O4'-C4' | -6.52 | 1.30        | 1.45     |
| 8   | L5    | 3723 | A2M  | O4'-C4' | -6.49 | 1.30        | 1.45     |
| 8   | L5    | 1326 | A2M  | O4'-C4' | -6.49 | 1.30        | 1.45     |
| 8   | L5    | 4590 | A2M  | O4'-C4' | -6.48 | 1.30        | 1.45     |
| 8   | L5    | 3925 | OMU  | C2-N1   | 6.46  | 1.48        | 1.38     |
| 49  | S2    | 1842 | 4AC  | C6-C5   | 6.43  | 1.50        | 1.35     |
| 8   | L5    | 1871 | A2M  | O4'-C4' | -6.42 | 1.30        | 1.45     |
| 49  | S2    | 159  | A2M  | O4'-C4' | -6.42 | 1.30        | 1.45     |
| 8   | L5    | 3760 | A2M  | O4'-C4' | -6.42 | 1.30        | 1.45     |
| 8   | L5    | 3724 | A2M  | O4'-C4' | -6.40 | 1.30        | 1.45     |
| 49  | S2    | 27   | A2M  | O4'-C4' | -6.39 | 1.30        | 1.45     |
| 8   | L5    | 3925 | OMU  | C2-N3   | 6.39  | 1.49        | 1.38     |
| 49  | S2    | 1383 | A2M  | O4'-C4' | -6.38 | 1.30        | 1.45     |
| 8   | L5    | 4494 | OMG  | C4-N3   | 6.37  | 1.49        | 1.34     |
| 8   | L5    | 4637 | OMG  | C4-N3   | 6.35  | 1.49        | 1.34     |
| 8   | L5    | 2424 | OMG  | C4-N3   | 6.35  | 1.49        | 1.34     |
| 8   | L5    | 3718 | A2M  | O4'-C4' | -6.34 | 1.30        | 1.45     |
| 8   | L5    | 2815 | A2M  | O4'-C4' | -6.33 | 1.30        | 1.45     |
| 8   | L5    | 398  | A2M  | O4'-C4' | -6.32 | 1.30        | 1.45     |
| 8   | L5    | 2401 | A2M  | O4'-C4' | -6.29 | 1.30        | 1.45     |
| 8   | L5    | 2787 | A2M  | O4'-C4' | -6.29 | 1.30        | 1.45     |
| 49  | S2    | 576  | A2M  | O4'-C4' | -6.28 | 1.31        | 1.45     |
| 49  | S2    | 644  | OMG  | C4-N3   | 6.28  | 1.49        | 1.34     |
| 8   | L5    | 3792 | OMG  | C4-N3   | 6.27  | 1.49        | 1.34     |
| 49  | S2    | 174  | OMC  | C2-N3   | 6.26  | 1.49        | 1.36     |
| 8   | L5    | 4370 | OMG  | C4-N3   | 6.26  | 1.49        | 1.34     |
| 8   | L5    | 1625 | OMG  | C4-N3   | 6.24  | 1.49        | 1.34     |
| 8   | L5    | 2351 | OMC  | C2-N3   | 6.23  | 1.49        | 1.36     |
| 8   | L5    | 1340 | OMC  | C2-N3   | 6.21  | 1.48        | 1.36     |
| 49  | S2    | 1328 | OMG  | C4-N3   | 6.21  | 1.49        | 1.34     |
| 8   | L5    | 4499 | OMG  | C4-N3   | 6.20  | 1.49        | 1.34     |
| 8   | L5    | 3744 | OMG  | C4-N3   | 6.19  | 1.49        | 1.34     |
| 10  | L8    | 75   | OMG  | C4-N3   | 6.19  | 1.49        | 1.34     |
| 49  | S2    | 1337 | 4AC  | C6-C5   | 6.18  | 1.49        | 1.35     |
| 8   | L5    | 2876 | OMG  | C4-N3   | 6.18  | 1.48        | 1.34     |
| 8   | L5    | 1316 | OMG  | C4-N3   | 6.17  | 1.48        | 1.34     |
| 8   | L5    | 3701 | OMC  | C2-N3   | 6.16  | 1.48        | 1.36     |
| 49  | S2    | 683  | OMG  | C4-N3   | 6.16  | 1.48        | 1.34     |
| 8   | L5    | 2422 | OMC  | C2-N3   | 6.16  | 1.48        | 1.36     |
| 49  | S2    | 1639 | G7M  | C4-N3   | 6.15  | 1.48        | 1.34     |
| 8   | L5    | 2365 | OMC  | C2-N3   | 6.13  | 1.48        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 49  | S2    | 1391 | OMC  | C2-N3 | 6.12 | 1.48        | 1.36     |
| 8   | L5    | 3627 | OMG  | C4-N3 | 6.12 | 1.48        | 1.34     |
| 8   | L5    | 4618 | OMG  | C4-N3 | 6.12 | 1.48        | 1.34     |
| 8   | L5    | 1522 | OMG  | C4-N3 | 6.11 | 1.48        | 1.34     |
| 8   | L5    | 4536 | OMC  | C2-N3 | 6.10 | 1.48        | 1.36     |
| 8   | L5    | 2861 | OMC  | C2-N3 | 6.10 | 1.48        | 1.36     |
| 8   | L5    | 2364 | OMG  | C4-N3 | 6.09 | 1.48        | 1.34     |
| 8   | L5    | 1881 | OMC  | C2-N3 | 6.08 | 1.48        | 1.36     |
| 8   | L5    | 2804 | OMC  | C2-N3 | 6.04 | 1.48        | 1.36     |
| 8   | L5    | 4623 | OMG  | C4-N3 | 6.04 | 1.48        | 1.34     |
| 8   | L5    | 3841 | OMC  | C2-N3 | 6.03 | 1.48        | 1.36     |
| 49  | S2    | 601  | OMG  | C4-N3 | 6.03 | 1.48        | 1.34     |
| 49  | S2    | 1337 | 4AC  | C7-N4 | 6.03 | 1.48        | 1.37     |
| 49  | S2    | 1703 | OMC  | C2-N3 | 6.02 | 1.48        | 1.36     |
| 8   | L5    | 4228 | OMG  | C4-N3 | 5.99 | 1.48        | 1.34     |
| 49  | S2    | 174  | OMC  | C6-C5 | 5.96 | 1.48        | 1.35     |
| 49  | S2    | 1337 | 4AC  | C2-N3 | 5.94 | 1.48        | 1.36     |
| 49  | S2    | 1703 | OMC  | C6-C5 | 5.93 | 1.48        | 1.35     |
| 8   | L5    | 1340 | OMC  | C6-C5 | 5.90 | 1.48        | 1.35     |
| 8   | L5    | 2365 | OMC  | C6-C5 | 5.89 | 1.48        | 1.35     |
| 8   | L5    | 2422 | OMC  | C6-C5 | 5.89 | 1.48        | 1.35     |
| 8   | L5    | 2861 | OMC  | C6-C5 | 5.88 | 1.48        | 1.35     |
| 8   | L5    | 3701 | OMC  | C6-C5 | 5.87 | 1.48        | 1.35     |
| 8   | L5    | 4536 | OMC  | C6-C5 | 5.87 | 1.48        | 1.35     |
| 49  | S2    | 1391 | OMC  | C6-C5 | 5.87 | 1.48        | 1.35     |
| 8   | L5    | 2351 | OMC  | C6-C5 | 5.83 | 1.48        | 1.35     |
| 8   | L5    | 3841 | OMC  | C6-C5 | 5.83 | 1.48        | 1.35     |
| 49  | S2    | 1842 | 4AC  | C7-N4 | 5.83 | 1.48        | 1.37     |
| 8   | L5    | 1881 | OMC  | C6-C5 | 5.79 | 1.48        | 1.35     |
| 49  | S2    | 428  | OMU  | C6-C5 | 5.68 | 1.48        | 1.35     |
| 49  | S2    | 1842 | 4AC  | C2-N3 | 5.67 | 1.47        | 1.36     |
| 8   | L5    | 2804 | OMC  | C6-C5 | 5.66 | 1.48        | 1.35     |
| 49  | S2    | 1288 | OMU  | C6-C5 | 5.63 | 1.48        | 1.35     |
| 8   | L5    | 4620 | OMU  | C6-C5 | 5.60 | 1.48        | 1.35     |
| 49  | S2    | 1248 | B8N  | C6-C5 | 5.59 | 1.42        | 1.34     |
| 10  | L8    | 14   | OMU  | C6-C5 | 5.57 | 1.48        | 1.35     |
| 49  | S2    | 1442 | OMU  | C6-C5 | 5.56 | 1.48        | 1.35     |
| 49  | S2    | 1248 | B8N  | C2-N1 | 5.44 | 1.55        | 1.39     |
| 8   | L5    | 3925 | OMU  | C6-C5 | 5.41 | 1.47        | 1.35     |
| 8   | L5    | 4637 | OMG  | C2-N3 | 5.40 | 1.46        | 1.33     |
| 8   | L5    | 3734 | PSU  | C6-N1 | 5.39 | 1.45        | 1.36     |
| 49  | S2    | 601  | OMG  | C2-N3 | 5.38 | 1.46        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 8   | L5    | 2424 | OMG  | C2-N3 | 5.37  | 1.46        | 1.33     |
| 8   | L5    | 4494 | OMG  | C2-N3 | 5.31  | 1.46        | 1.33     |
| 8   | L5    | 3758 | PSU  | C6-N1 | 5.28  | 1.45        | 1.36     |
| 49  | S2    | 644  | OMG  | C2-N3 | 5.28  | 1.45        | 1.33     |
| 8   | L5    | 1782 | PSU  | C6-N1 | 5.26  | 1.45        | 1.36     |
| 8   | L5    | 1625 | OMG  | C2-N3 | 5.25  | 1.45        | 1.33     |
| 10  | L8    | 55   | PSU  | C6-N1 | 5.25  | 1.44        | 1.36     |
| 49  | S2    | 1639 | G7M  | C2-N3 | 5.24  | 1.45        | 1.33     |
| 8   | L5    | 4353 | PSU  | C6-N1 | 5.24  | 1.44        | 1.36     |
| 10  | L8    | 75   | OMG  | C2-N3 | 5.22  | 1.45        | 1.33     |
| 8   | L5    | 4370 | OMG  | C2-N3 | 5.21  | 1.45        | 1.33     |
| 8   | L5    | 4499 | OMG  | C2-N3 | 5.20  | 1.45        | 1.33     |
| 8   | L5    | 3729 | PSU  | C6-N1 | 5.17  | 1.44        | 1.36     |
| 49  | S2    | 1639 | G7M  | C5-N7 | -5.16 | 1.33        | 1.39     |
| 8   | L5    | 1316 | OMG  | C2-N3 | 5.16  | 1.45        | 1.33     |
| 8   | L5    | 3792 | OMG  | C2-N3 | 5.14  | 1.45        | 1.33     |
| 49  | S2    | 1328 | OMG  | C2-N3 | 5.12  | 1.45        | 1.33     |
| 49  | S2    | 683  | OMG  | C2-N3 | 5.12  | 1.45        | 1.33     |
| 8   | L5    | 4618 | OMG  | C2-N3 | 5.10  | 1.45        | 1.33     |
| 8   | L5    | 1683 | PSU  | C6-N1 | 5.07  | 1.44        | 1.36     |
| 49  | S2    | 1703 | OMC  | C4-N4 | 5.07  | 1.45        | 1.33     |
| 8   | L5    | 2876 | OMG  | C2-N3 | 5.07  | 1.45        | 1.33     |
| 8   | L5    | 2364 | OMG  | C2-N3 | 5.06  | 1.45        | 1.33     |
| 8   | L5    | 3701 | OMC  | C4-N3 | 5.06  | 1.44        | 1.34     |
| 49  | S2    | 1391 | OMC  | C4-N3 | 5.03  | 1.44        | 1.34     |
| 8   | L5    | 3744 | OMG  | C2-N3 | 5.03  | 1.45        | 1.33     |
| 49  | S2    | 174  | OMC  | C4-N3 | 5.03  | 1.44        | 1.34     |
| 49  | S2    | 174  | OMC  | C4-N4 | 5.03  | 1.45        | 1.33     |
| 8   | L5    | 2365 | OMC  | C4-N3 | 5.02  | 1.44        | 1.34     |
| 49  | S2    | 1326 | UY1  | C6-N1 | 5.00  | 1.44        | 1.36     |
| 8   | L5    | 2422 | OMC  | C4-N3 | 5.00  | 1.44        | 1.34     |
| 8   | L5    | 2365 | OMC  | C4-N4 | 5.00  | 1.45        | 1.33     |
| 8   | L5    | 4623 | OMG  | C2-N3 | 4.99  | 1.45        | 1.33     |
| 8   | L5    | 2804 | OMC  | C4-N4 | 4.98  | 1.45        | 1.33     |
| 49  | S2    | 1703 | OMC  | C4-N3 | 4.98  | 1.44        | 1.34     |
| 49  | S2    | 1391 | OMC  | C4-N4 | 4.97  | 1.45        | 1.33     |
| 8   | L5    | 2422 | OMC  | C4-N4 | 4.96  | 1.45        | 1.33     |
| 8   | L5    | 1522 | OMG  | C2-N3 | 4.95  | 1.45        | 1.33     |
| 8   | L5    | 2351 | OMC  | C4-N3 | 4.93  | 1.44        | 1.34     |
| 8   | L5    | 2804 | OMC  | C4-N3 | 4.92  | 1.44        | 1.34     |
| 8   | L5    | 1340 | OMC  | C4-N3 | 4.92  | 1.44        | 1.34     |
| 8   | L5    | 2861 | OMC  | C4-N4 | 4.91  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8   | L5    | 1340 | OMC  | C4-N4  | 4.89  | 1.45        | 1.33     |
| 8   | L5    | 4536 | OMC  | C4-N4  | 4.89  | 1.45        | 1.33     |
| 8   | L5    | 3627 | OMG  | C2-N3  | 4.88  | 1.44        | 1.33     |
| 8   | L5    | 4228 | OMG  | C2-N3  | 4.88  | 1.44        | 1.33     |
| 8   | L5    | 2861 | OMC  | C4-N3  | 4.87  | 1.44        | 1.34     |
| 8   | L5    | 2351 | OMC  | C4-N4  | 4.85  | 1.45        | 1.33     |
| 8   | L5    | 1881 | OMC  | C4-N4  | 4.84  | 1.45        | 1.33     |
| 8   | L5    | 1881 | OMC  | C4-N3  | 4.84  | 1.44        | 1.34     |
| 8   | L5    | 3841 | OMC  | C4-N3  | 4.84  | 1.44        | 1.34     |
| 8   | L5    | 3701 | OMC  | C4-N4  | 4.83  | 1.45        | 1.33     |
| 8   | L5    | 4536 | OMC  | C4-N3  | 4.83  | 1.44        | 1.34     |
| 49  | S2    | 601  | OMG  | C2-N2  | 4.82  | 1.45        | 1.34     |
| 8   | L5    | 3841 | OMC  | C4-N4  | 4.81  | 1.45        | 1.33     |
| 8   | L5    | 2424 | OMG  | C2-N2  | 4.70  | 1.45        | 1.34     |
| 8   | L5    | 1625 | OMG  | C2-N2  | 4.65  | 1.45        | 1.34     |
| 8   | L5    | 1316 | OMG  | C2-N2  | 4.64  | 1.45        | 1.34     |
| 10  | L8    | 75   | OMG  | C2-N2  | 4.64  | 1.45        | 1.34     |
| 8   | L5    | 3792 | OMG  | C2-N2  | 4.63  | 1.45        | 1.34     |
| 49  | S2    | 1639 | G7M  | C2-N2  | 4.63  | 1.45        | 1.34     |
| 49  | S2    | 683  | OMG  | C2-N2  | 4.62  | 1.45        | 1.34     |
| 8   | L5    | 4499 | OMG  | C2-N2  | 4.61  | 1.45        | 1.34     |
| 49  | S2    | 27   | A2M  | C6-N6  | 4.56  | 1.45        | 1.34     |
| 49  | S2    | 644  | OMG  | C2-N2  | 4.56  | 1.45        | 1.34     |
| 8   | L5    | 2876 | OMG  | C2-N2  | 4.53  | 1.45        | 1.34     |
| 8   | L5    | 4623 | OMG  | C2-N2  | 4.53  | 1.45        | 1.34     |
| 8   | L5    | 2364 | OMG  | C2-N2  | 4.53  | 1.45        | 1.34     |
| 49  | S2    | 576  | A2M  | C6-N6  | 4.52  | 1.45        | 1.34     |
| 8   | L5    | 4494 | OMG  | C2-N2  | 4.52  | 1.44        | 1.34     |
| 8   | L5    | 4618 | OMG  | C2-N2  | 4.52  | 1.44        | 1.34     |
| 8   | L5    | 4637 | OMG  | C2-N2  | 4.52  | 1.44        | 1.34     |
| 49  | S2    | 1328 | OMG  | C2-N2  | 4.51  | 1.44        | 1.34     |
| 8   | L5    | 3758 | PSU  | C1'-C5 | -4.51 | 1.39        | 1.50     |
| 8   | L5    | 3723 | A2M  | C6-N6  | 4.50  | 1.45        | 1.34     |
| 8   | L5    | 1326 | A2M  | C6-N6  | 4.50  | 1.45        | 1.34     |
| 8   | L5    | 3744 | OMG  | C2-N2  | 4.49  | 1.44        | 1.34     |
| 8   | L5    | 4370 | OMG  | C2-N2  | 4.48  | 1.44        | 1.34     |
| 8   | L5    | 3724 | A2M  | C6-N6  | 4.48  | 1.45        | 1.34     |
| 8   | L5    | 398  | A2M  | C6-N6  | 4.47  | 1.45        | 1.34     |
| 8   | L5    | 3627 | OMG  | C2-N2  | 4.47  | 1.44        | 1.34     |
| 8   | L5    | 4353 | PSU  | C1'-C5 | -4.46 | 1.40        | 1.50     |
| 8   | L5    | 1524 | A2M  | C6-N6  | 4.46  | 1.45        | 1.34     |
| 8   | L5    | 4590 | A2M  | C6-N6  | 4.46  | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8   | L5    | 2787 | A2M  | C6-N6  | 4.45  | 1.45        | 1.34     |
| 8   | L5    | 3718 | A2M  | C6-N6  | 4.45  | 1.45        | 1.34     |
| 8   | L5    | 3729 | PSU  | C1'-C5 | -4.45 | 1.40        | 1.50     |
| 8   | L5    | 1871 | A2M  | C6-N6  | 4.45  | 1.45        | 1.34     |
| 49  | S2    | 668  | A2M  | C6-N6  | 4.44  | 1.45        | 1.34     |
| 8   | L5    | 1522 | OMG  | C2-N2  | 4.44  | 1.44        | 1.34     |
| 8   | L5    | 1683 | PSU  | C1'-C5 | -4.44 | 1.40        | 1.50     |
| 8   | L5    | 2815 | A2M  | C6-N6  | 4.44  | 1.45        | 1.34     |
| 10  | L8    | 55   | PSU  | C1'-C5 | -4.44 | 1.40        | 1.50     |
| 8   | L5    | 2401 | A2M  | C6-N6  | 4.43  | 1.45        | 1.34     |
| 8   | L5    | 3825 | A2M  | C6-N6  | 4.42  | 1.45        | 1.34     |
| 49  | S2    | 1031 | A2M  | C6-N6  | 4.41  | 1.45        | 1.34     |
| 8   | L5    | 2351 | OMC  | C2-N1  | 4.40  | 1.49        | 1.40     |
| 49  | S2    | 1391 | OMC  | C2-N1  | 4.39  | 1.49        | 1.40     |
| 49  | S2    | 1678 | A2M  | C6-N6  | 4.39  | 1.45        | 1.34     |
| 8   | L5    | 4228 | OMG  | C2-N2  | 4.39  | 1.44        | 1.34     |
| 49  | S2    | 159  | A2M  | C6-N6  | 4.36  | 1.45        | 1.34     |
| 49  | S2    | 1842 | 4AC  | O2-C2  | -4.35 | 1.15        | 1.23     |
| 49  | S2    | 1337 | 4AC  | O2-C2  | -4.35 | 1.15        | 1.23     |
| 8   | L5    | 3760 | A2M  | C6-N6  | 4.34  | 1.45        | 1.34     |
| 49  | S2    | 1383 | A2M  | C6-N6  | 4.30  | 1.44        | 1.34     |
| 8   | L5    | 2363 | A2M  | C6-N6  | 4.30  | 1.44        | 1.34     |
| 8   | L5    | 3701 | OMC  | C2-N1  | 4.29  | 1.49        | 1.40     |
| 49  | S2    | 1842 | 4AC  | C5-C4  | 4.29  | 1.50        | 1.40     |
| 49  | S2    | 174  | OMC  | C2-N1  | 4.28  | 1.49        | 1.40     |
| 8   | L5    | 3734 | PSU  | C1'-C5 | -4.26 | 1.40        | 1.50     |
| 8   | L5    | 2422 | OMC  | C2-N1  | 4.25  | 1.49        | 1.40     |
| 8   | L5    | 1881 | OMC  | C2-N1  | 4.22  | 1.49        | 1.40     |
| 8   | L5    | 1782 | PSU  | C1'-C5 | -4.19 | 1.40        | 1.50     |
| 8   | L5    | 2861 | OMC  | C2-N1  | 4.16  | 1.49        | 1.40     |
| 8   | L5    | 2365 | OMC  | C2-N1  | 4.12  | 1.48        | 1.40     |
| 49  | S2    | 1337 | 4AC  | C5-C4  | 4.11  | 1.49        | 1.40     |
| 49  | S2    | 1703 | OMC  | C2-N1  | 4.08  | 1.48        | 1.40     |
| 49  | S2    | 1288 | OMU  | C4-N3  | 4.08  | 1.45        | 1.38     |
| 8   | L5    | 4536 | OMC  | C2-N1  | 4.05  | 1.48        | 1.40     |
| 49  | S2    | 428  | OMU  | C4-N3  | 4.05  | 1.45        | 1.38     |
| 8   | L5    | 3841 | OMC  | C2-N1  | 4.04  | 1.48        | 1.40     |
| 8   | L5    | 1340 | OMC  | C2-N1  | 4.02  | 1.48        | 1.40     |
| 8   | L5    | 2804 | OMC  | C2-N1  | 4.02  | 1.48        | 1.40     |
| 49  | S2    | 1337 | 4AC  | C4-N4  | 4.00  | 1.45        | 1.39     |
| 10  | L8    | 14   | OMU  | C4-N3  | 4.00  | 1.45        | 1.38     |
| 49  | S2    | 1842 | 4AC  | C2-N1  | 3.97  | 1.48        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 3734 | PSU  | C4-N3   | 3.92  | 1.46        | 1.38     |
| 49  | S2    | 1442 | OMU  | C4-N3   | 3.90  | 1.45        | 1.38     |
| 8   | L5    | 3729 | PSU  | C4-N3   | 3.84  | 1.46        | 1.38     |
| 8   | L5    | 1782 | PSU  | C4-N3   | 3.83  | 1.46        | 1.38     |
| 49  | S2    | 1842 | 4AC  | C4-N4   | 3.80  | 1.45        | 1.39     |
| 8   | L5    | 4620 | OMU  | C4-N3   | 3.78  | 1.45        | 1.38     |
| 49  | S2    | 1337 | 4AC  | C2-N1   | 3.78  | 1.48        | 1.40     |
| 49  | S2    | 1639 | G7M  | C5-C6   | 3.78  | 1.53        | 1.43     |
| 8   | L5    | 3925 | OMU  | C4-N3   | 3.76  | 1.45        | 1.38     |
| 8   | L5    | 4353 | PSU  | C4-N3   | 3.64  | 1.45        | 1.38     |
| 8   | L5    | 3758 | PSU  | C4-N3   | 3.63  | 1.45        | 1.38     |
| 49  | S2    | 1850 | MA6  | C6-N6   | 3.63  | 1.47        | 1.36     |
| 10  | L8    | 55   | PSU  | C4-N3   | 3.62  | 1.45        | 1.38     |
| 49  | S2    | 1851 | MA6  | C6-N6   | 3.59  | 1.47        | 1.36     |
| 8   | L5    | 1683 | PSU  | C4-N3   | 3.57  | 1.45        | 1.38     |
| 49  | S2    | 1326 | UY1  | C4-N3   | 3.45  | 1.45        | 1.38     |
| 49  | S2    | 159  | A2M  | O3'-C3' | -3.32 | 1.35        | 1.43     |
| 49  | S2    | 1842 | 4AC  | C6-N1   | 3.26  | 1.45        | 1.38     |
| 49  | S2    | 1678 | A2M  | O3'-C3' | -3.21 | 1.35        | 1.43     |
| 49  | S2    | 159  | A2M  | C5-C4   | -3.20 | 1.33        | 1.39     |
| 8   | L5    | 1326 | A2M  | C5-C4   | -3.19 | 1.33        | 1.39     |
| 8   | L5    | 3760 | A2M  | C5-C4   | -3.17 | 1.33        | 1.39     |
| 8   | L5    | 1524 | A2M  | O3'-C3' | -3.16 | 1.35        | 1.43     |
| 8   | L5    | 1871 | A2M  | O3'-C3' | -3.16 | 1.35        | 1.43     |
| 8   | L5    | 2351 | OMC  | C6-N1   | 3.15  | 1.45        | 1.38     |
| 8   | L5    | 2363 | A2M  | O3'-C3' | -3.14 | 1.35        | 1.43     |
| 8   | L5    | 3760 | A2M  | O3'-C3' | -3.13 | 1.35        | 1.43     |
| 8   | L5    | 398  | A2M  | O3'-C3' | -3.13 | 1.35        | 1.43     |
| 8   | L5    | 3723 | A2M  | O3'-C3' | -3.13 | 1.35        | 1.43     |
| 49  | S2    | 1851 | MA6  | C5-C4   | -3.12 | 1.33        | 1.39     |
| 8   | L5    | 1326 | A2M  | O3'-C3' | -3.12 | 1.35        | 1.43     |
| 8   | L5    | 1316 | OMG  | C5-N7   | -3.12 | 1.33        | 1.39     |
| 8   | L5    | 1881 | OMC  | C6-N1   | 3.12  | 1.45        | 1.38     |
| 49  | S2    | 1031 | A2M  | C5-C4   | -3.11 | 1.33        | 1.39     |
| 8   | L5    | 3825 | A2M  | O3'-C3' | -3.10 | 1.35        | 1.43     |
| 8   | L5    | 3724 | A2M  | O3'-C3' | -3.10 | 1.35        | 1.43     |
| 8   | L5    | 4499 | OMG  | C5-N7   | -3.10 | 1.33        | 1.39     |
| 49  | S2    | 174  | OMC  | C6-N1   | 3.09  | 1.45        | 1.38     |
| 49  | S2    | 1703 | OMC  | C6-N1   | 3.09  | 1.45        | 1.38     |
| 8   | L5    | 4494 | OMG  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 8   | L5    | 1871 | A2M  | C5-C4   | -3.09 | 1.33        | 1.39     |
| 8   | L5    | 3627 | OMG  | C5-N7   | -3.09 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 4620 | OMU  | O4-C4   | -3.09 | 1.18        | 1.24     |
| 49  | S2    | 576  | A2M  | O3'-C3' | -3.09 | 1.35        | 1.43     |
| 8   | L5    | 3825 | A2M  | C5-C4   | -3.08 | 1.33        | 1.39     |
| 49  | S2    | 668  | A2M  | C5-C4   | -3.07 | 1.33        | 1.39     |
| 8   | L5    | 4590 | A2M  | O3'-C3' | -3.07 | 1.35        | 1.43     |
| 8   | L5    | 2365 | OMC  | C6-N1   | 3.06  | 1.45        | 1.38     |
| 8   | L5    | 4637 | OMG  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 8   | L5    | 3792 | OMG  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 8   | L5    | 1522 | OMG  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 49  | S2    | 27   | A2M  | O3'-C3' | -3.05 | 1.35        | 1.43     |
| 8   | L5    | 2424 | OMG  | C5-N7   | -3.05 | 1.33        | 1.39     |
| 49  | S2    | 1383 | A2M  | O3'-C3' | -3.04 | 1.35        | 1.43     |
| 49  | S2    | 644  | OMG  | C5-N7   | -3.03 | 1.33        | 1.39     |
| 8   | L5    | 2401 | A2M  | C5-C4   | -3.03 | 1.33        | 1.39     |
| 8   | L5    | 4590 | A2M  | C5-C4   | -3.02 | 1.33        | 1.39     |
| 8   | L5    | 3925 | OMU  | O4-C4   | -3.02 | 1.18        | 1.24     |
| 8   | L5    | 2422 | OMC  | C6-N1   | 3.01  | 1.45        | 1.38     |
| 8   | L5    | 2363 | A2M  | C5-C4   | -3.01 | 1.33        | 1.39     |
| 8   | L5    | 3760 | A2M  | C5-N7   | -3.01 | 1.33        | 1.39     |
| 49  | S2    | 1678 | A2M  | C5-C4   | -3.01 | 1.33        | 1.39     |
| 49  | S2    | 1031 | A2M  | O3'-C3' | -3.01 | 1.35        | 1.43     |
| 8   | L5    | 3718 | A2M  | C5-C4   | -3.01 | 1.33        | 1.39     |
| 8   | L5    | 2876 | OMG  | C5-N7   | -3.01 | 1.33        | 1.39     |
| 49  | S2    | 1442 | OMU  | O4-C4   | -3.01 | 1.18        | 1.24     |
| 8   | L5    | 3701 | OMC  | C6-N1   | 2.99  | 1.45        | 1.38     |
| 8   | L5    | 1625 | OMG  | C5-N7   | -2.99 | 1.33        | 1.39     |
| 8   | L5    | 3841 | OMC  | C6-N1   | 2.99  | 1.45        | 1.38     |
| 8   | L5    | 2815 | A2M  | O3'-C3' | -2.99 | 1.35        | 1.43     |
| 8   | L5    | 3718 | A2M  | O3'-C3' | -2.99 | 1.35        | 1.43     |
| 49  | S2    | 1703 | OMC  | O2-C2   | -2.99 | 1.18        | 1.23     |
| 49  | S2    | 1391 | OMC  | C6-N1   | 2.98  | 1.45        | 1.38     |
| 10  | L8    | 75   | OMG  | C5-N7   | -2.98 | 1.33        | 1.39     |
| 8   | L5    | 3724 | A2M  | C5-C4   | -2.98 | 1.33        | 1.39     |
| 8   | L5    | 2787 | A2M  | O3'-C3' | -2.98 | 1.36        | 1.43     |
| 8   | L5    | 398  | A2M  | C5-C4   | -2.97 | 1.33        | 1.39     |
| 49  | S2    | 27   | A2M  | C5-C4   | -2.97 | 1.33        | 1.39     |
| 49  | S2    | 1328 | OMG  | C5-N7   | -2.97 | 1.33        | 1.39     |
| 49  | S2    | 428  | OMU  | O4-C4   | -2.96 | 1.18        | 1.24     |
| 8   | L5    | 2401 | A2M  | O3'-C3' | -2.96 | 1.36        | 1.43     |
| 8   | L5    | 3744 | OMG  | C5-N7   | -2.96 | 1.33        | 1.39     |
| 8   | L5    | 2861 | OMC  | C6-N1   | 2.95  | 1.45        | 1.38     |
| 8   | L5    | 2787 | A2M  | C5-C4   | -2.94 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 49  | S2    | 601  | OMG  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 8   | L5    | 2364 | OMG  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 8   | L5    | 4623 | OMG  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 8   | L5    | 4618 | OMG  | C5-N7   | -2.94 | 1.33        | 1.39     |
| 8   | L5    | 1340 | OMC  | C6-N1   | 2.93  | 1.45        | 1.38     |
| 8   | L5    | 1524 | A2M  | C5-C4   | -2.93 | 1.33        | 1.39     |
| 8   | L5    | 3758 | PSU  | O4-C4   | -2.93 | 1.18        | 1.23     |
| 49  | S2    | 668  | A2M  | O3'-C3' | -2.93 | 1.36        | 1.43     |
| 8   | L5    | 4228 | OMG  | C5-N7   | -2.92 | 1.33        | 1.39     |
| 49  | S2    | 1383 | A2M  | C5-C4   | -2.91 | 1.33        | 1.39     |
| 49  | S2    | 1288 | OMU  | O4-C4   | -2.91 | 1.18        | 1.24     |
| 8   | L5    | 1871 | A2M  | C5-N7   | -2.91 | 1.33        | 1.39     |
| 8   | L5    | 4370 | OMG  | C5-N7   | -2.91 | 1.33        | 1.39     |
| 10  | L8    | 14   | OMU  | O4-C4   | -2.90 | 1.18        | 1.24     |
| 8   | L5    | 2815 | A2M  | C5-C4   | -2.89 | 1.33        | 1.39     |
| 49  | S2    | 683  | OMG  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 8   | L5    | 2401 | A2M  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 10  | L8    | 14   | OMU  | C6-N1   | 2.88  | 1.44        | 1.38     |
| 49  | S2    | 1850 | MA6  | C5-N7   | -2.86 | 1.33        | 1.39     |
| 49  | S2    | 159  | A2M  | C5-N7   | -2.86 | 1.33        | 1.39     |
| 49  | S2    | 428  | OMU  | C6-N1   | 2.86  | 1.44        | 1.38     |
| 8   | L5    | 3724 | A2M  | O2'-C2' | 2.86  | 1.49        | 1.42     |
| 8   | L5    | 3723 | A2M  | C5-C4   | -2.86 | 1.33        | 1.39     |
| 8   | L5    | 2861 | OMC  | O2-C2   | -2.85 | 1.18        | 1.23     |
| 8   | L5    | 3718 | A2M  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 49  | S2    | 576  | A2M  | C5-C4   | -2.85 | 1.33        | 1.39     |
| 8   | L5    | 2804 | OMC  | C6-N1   | 2.84  | 1.44        | 1.38     |
| 8   | L5    | 2365 | OMC  | O2-C2   | -2.83 | 1.18        | 1.23     |
| 8   | L5    | 4536 | OMC  | C6-N1   | 2.83  | 1.44        | 1.38     |
| 8   | L5    | 1524 | A2M  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 8   | L5    | 2351 | OMC  | O2-C2   | -2.81 | 1.18        | 1.23     |
| 8   | L5    | 2422 | OMC  | O2-C2   | -2.81 | 1.18        | 1.23     |
| 8   | L5    | 2804 | OMC  | O2-C2   | -2.81 | 1.18        | 1.23     |
| 49  | S2    | 1383 | A2M  | O2'-C2' | 2.81  | 1.49        | 1.42     |
| 49  | S2    | 1678 | A2M  | O2'-C2' | 2.80  | 1.49        | 1.42     |
| 8   | L5    | 4228 | OMG  | C2-N1   | 2.80  | 1.44        | 1.37     |
| 8   | L5    | 4536 | OMC  | O2-C2   | -2.80 | 1.18        | 1.23     |
| 49  | S2    | 159  | A2M  | O2'-C2' | 2.80  | 1.49        | 1.42     |
| 8   | L5    | 3841 | OMC  | O2-C2   | -2.79 | 1.18        | 1.23     |
| 49  | S2    | 1031 | A2M  | O2'-C2' | 2.79  | 1.49        | 1.42     |
| 8   | L5    | 2364 | OMG  | C2-N1   | 2.79  | 1.44        | 1.37     |
| 49  | S2    | 1337 | 4AC  | C6-N1   | 2.78  | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 49  | S2    | 668  | A2M  | O2'-C2' | 2.78  | 1.49        | 1.42     |
| 8   | L5    | 4353 | PSU  | O4-C4   | -2.78 | 1.18        | 1.23     |
| 8   | L5    | 4590 | A2M  | O2'-C2' | 2.78  | 1.49        | 1.42     |
| 8   | L5    | 2363 | A2M  | O2'-C2' | 2.78  | 1.49        | 1.42     |
| 8   | L5    | 3723 | A2M  | O2'-C2' | 2.78  | 1.49        | 1.42     |
| 8   | L5    | 1340 | OMC  | O2-C2   | -2.78 | 1.18        | 1.23     |
| 8   | L5    | 1326 | A2M  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 49  | S2    | 1391 | OMC  | O2-C2   | -2.78 | 1.18        | 1.23     |
| 49  | S2    | 1850 | MA6  | C8-N9   | -2.77 | 1.32        | 1.37     |
| 10  | L8    | 14   | OMU  | O2-C2   | -2.77 | 1.18        | 1.23     |
| 8   | L5    | 2787 | A2M  | C5-N7   | -2.77 | 1.33        | 1.39     |
| 49  | S2    | 601  | OMG  | C2-N1   | 2.77  | 1.44        | 1.37     |
| 8   | L5    | 1881 | OMC  | O2-C2   | -2.76 | 1.18        | 1.23     |
| 49  | S2    | 576  | A2M  | O2'-C2' | 2.76  | 1.49        | 1.42     |
| 49  | S2    | 683  | OMG  | C2-N1   | 2.76  | 1.44        | 1.37     |
| 8   | L5    | 3627 | OMG  | C2-N1   | 2.76  | 1.44        | 1.37     |
| 8   | L5    | 3825 | A2M  | O2'-C2' | 2.76  | 1.49        | 1.42     |
| 49  | S2    | 1288 | OMU  | C6-N1   | 2.75  | 1.44        | 1.38     |
| 8   | L5    | 2363 | A2M  | C5-N7   | -2.75 | 1.33        | 1.39     |
| 49  | S2    | 27   | A2M  | C5-N7   | -2.75 | 1.33        | 1.39     |
| 8   | L5    | 2815 | A2M  | C5-N7   | -2.75 | 1.33        | 1.39     |
| 8   | L5    | 1683 | PSU  | O4-C4   | -2.74 | 1.18        | 1.23     |
| 49  | S2    | 576  | A2M  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 49  | S2    | 1326 | UY1  | O4-C4   | -2.74 | 1.18        | 1.23     |
| 8   | L5    | 3744 | OMG  | C2-N1   | 2.73  | 1.44        | 1.37     |
| 8   | L5    | 4590 | A2M  | C5-N7   | -2.73 | 1.33        | 1.39     |
| 49  | S2    | 1678 | A2M  | C5-N7   | -2.73 | 1.33        | 1.39     |
| 10  | L8    | 75   | OMG  | C2-N1   | 2.73  | 1.44        | 1.37     |
| 8   | L5    | 3723 | A2M  | C5-N7   | -2.72 | 1.33        | 1.39     |
| 8   | L5    | 1871 | A2M  | O2'-C2' | 2.72  | 1.49        | 1.42     |
| 8   | L5    | 2401 | A2M  | O2'-C2' | 2.72  | 1.49        | 1.42     |
| 8   | L5    | 1326 | A2M  | O2'-C2' | 2.72  | 1.49        | 1.42     |
| 8   | L5    | 1625 | OMG  | C2-N1   | 2.71  | 1.44        | 1.37     |
| 8   | L5    | 3627 | OMG  | O6-C6   | -2.71 | 1.18        | 1.23     |
| 49  | S2    | 27   | A2M  | O2'-C2' | 2.70  | 1.49        | 1.42     |
| 8   | L5    | 398  | A2M  | O2'-C2' | 2.70  | 1.49        | 1.42     |
| 49  | S2    | 174  | OMC  | O2-C2   | -2.70 | 1.18        | 1.23     |
| 8   | L5    | 2815 | A2M  | O2'-C2' | 2.69  | 1.49        | 1.42     |
| 49  | S2    | 601  | OMG  | O6-C6   | -2.69 | 1.18        | 1.23     |
| 49  | S2    | 1442 | OMU  | C6-N1   | 2.69  | 1.44        | 1.38     |
| 49  | S2    | 1832 | 6MZ  | C5-C4   | -2.69 | 1.34        | 1.39     |
| 8   | L5    | 1782 | PSU  | O4-C4   | -2.69 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 398  | A2M  | C5-N7   | -2.69 | 1.33        | 1.39     |
| 8   | L5    | 3825 | A2M  | C5-N7   | -2.68 | 1.33        | 1.39     |
| 8   | L5    | 4618 | OMG  | C2-N1   | 2.68  | 1.44        | 1.37     |
| 49  | S2    | 1639 | G7M  | C2-N1   | 2.68  | 1.44        | 1.37     |
| 49  | S2    | 1850 | MA6  | C5-C4   | -2.68 | 1.34        | 1.39     |
| 8   | L5    | 1524 | A2M  | O2'-C2' | 2.67  | 1.49        | 1.42     |
| 8   | L5    | 3724 | A2M  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 8   | L5    | 2787 | A2M  | O2'-C2' | 2.67  | 1.49        | 1.42     |
| 8   | L5    | 1625 | OMG  | O6-C6   | -2.67 | 1.18        | 1.23     |
| 8   | L5    | 2424 | OMG  | C2-N1   | 2.67  | 1.44        | 1.37     |
| 8   | L5    | 4637 | OMG  | O6-C6   | -2.66 | 1.18        | 1.23     |
| 49  | S2    | 668  | A2M  | C5-N7   | -2.65 | 1.34        | 1.39     |
| 8   | L5    | 1522 | OMG  | O6-C6   | -2.65 | 1.18        | 1.23     |
| 49  | S2    | 644  | OMG  | O6-C6   | -2.65 | 1.18        | 1.23     |
| 49  | S2    | 1328 | OMG  | O6-C6   | -2.65 | 1.18        | 1.23     |
| 8   | L5    | 4494 | OMG  | O6-C6   | -2.64 | 1.18        | 1.23     |
| 8   | L5    | 3718 | A2M  | O2'-C2' | 2.64  | 1.49        | 1.42     |
| 8   | L5    | 2876 | OMG  | O6-C6   | -2.64 | 1.18        | 1.23     |
| 49  | S2    | 1031 | A2M  | C5-N7   | -2.63 | 1.34        | 1.39     |
| 8   | L5    | 4623 | OMG  | C2-N1   | 2.63  | 1.44        | 1.37     |
| 8   | L5    | 4494 | OMG  | C2-N1   | 2.63  | 1.44        | 1.37     |
| 8   | L5    | 4623 | OMG  | O6-C6   | -2.63 | 1.18        | 1.23     |
| 8   | L5    | 1522 | OMG  | C2-N1   | 2.63  | 1.44        | 1.37     |
| 49  | S2    | 1328 | OMG  | C2-N1   | 2.62  | 1.44        | 1.37     |
| 49  | S2    | 644  | OMG  | C2-N1   | 2.61  | 1.44        | 1.37     |
| 8   | L5    | 3760 | A2M  | O2'-C2' | 2.61  | 1.49        | 1.42     |
| 8   | L5    | 1316 | OMG  | C2-N1   | 2.61  | 1.44        | 1.37     |
| 10  | L8    | 55   | PSU  | O4-C4   | -2.60 | 1.18        | 1.23     |
| 8   | L5    | 2424 | OMG  | O6-C6   | -2.60 | 1.18        | 1.23     |
| 49  | S2    | 1639 | G7M  | O6-C6   | -2.60 | 1.18        | 1.23     |
| 8   | L5    | 4228 | OMG  | C6-N1   | 2.59  | 1.43        | 1.38     |
| 8   | L5    | 4228 | OMG  | O6-C6   | -2.57 | 1.18        | 1.23     |
| 8   | L5    | 2364 | OMG  | O6-C6   | -2.57 | 1.18        | 1.23     |
| 8   | L5    | 4370 | OMG  | C2-N1   | 2.57  | 1.44        | 1.37     |
| 8   | L5    | 4637 | OMG  | C2-N1   | 2.56  | 1.44        | 1.37     |
| 8   | L5    | 3734 | PSU  | O4-C4   | -2.56 | 1.18        | 1.23     |
| 49  | S2    | 1383 | A2M  | C5-N7   | -2.56 | 1.34        | 1.39     |
| 8   | L5    | 3744 | OMG  | O6-C6   | -2.56 | 1.18        | 1.23     |
| 8   | L5    | 4620 | OMU  | O2-C2   | -2.56 | 1.18        | 1.23     |
| 49  | S2    | 1678 | A2M  | C8-N9   | -2.55 | 1.32        | 1.37     |
| 49  | S2    | 683  | OMG  | O6-C6   | -2.55 | 1.18        | 1.23     |
| 8   | L5    | 3925 | OMU  | O2-C2   | -2.55 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 8   | L5    | 4499 | OMG  | C2-N1 | 2.55  | 1.44        | 1.37     |
| 8   | L5    | 4618 | OMG  | O6-C6 | -2.54 | 1.18        | 1.23     |
| 10  | L8    | 75   | OMG  | O6-C6 | -2.54 | 1.18        | 1.23     |
| 8   | L5    | 3701 | OMC  | O2-C2 | -2.54 | 1.19        | 1.23     |
| 8   | L5    | 4228 | OMG  | C4-N9 | -2.54 | 1.31        | 1.38     |
| 8   | L5    | 3744 | OMG  | C6-N1 | 2.54  | 1.43        | 1.38     |
| 8   | L5    | 3729 | PSU  | O4-C4 | -2.54 | 1.18        | 1.23     |
| 8   | L5    | 3792 | OMG  | C2-N1 | 2.53  | 1.43        | 1.37     |
| 8   | L5    | 4620 | OMU  | C6-N1 | 2.53  | 1.44        | 1.38     |
| 8   | L5    | 4370 | OMG  | O6-C6 | -2.53 | 1.18        | 1.23     |
| 8   | L5    | 2876 | OMG  | C2-N1 | 2.52  | 1.43        | 1.37     |
| 49  | S2    | 1832 | 6MZ  | C8-N9 | -2.52 | 1.33        | 1.37     |
| 49  | S2    | 1832 | 6MZ  | C5-N7 | -2.52 | 1.34        | 1.39     |
| 8   | L5    | 4499 | OMG  | O6-C6 | -2.51 | 1.18        | 1.23     |
| 8   | L5    | 3925 | OMU  | C6-N1 | 2.51  | 1.44        | 1.38     |
| 8   | L5    | 3627 | OMG  | C4-N9 | -2.51 | 1.31        | 1.38     |
| 8   | L5    | 3792 | OMG  | O6-C6 | -2.50 | 1.18        | 1.23     |
| 49  | S2    | 601  | OMG  | C5-C6 | 2.48  | 1.53        | 1.44     |
| 8   | L5    | 4370 | OMG  | C5-C6 | 2.48  | 1.53        | 1.44     |
| 8   | L5    | 1316 | OMG  | O6-C6 | -2.47 | 1.18        | 1.23     |
| 49  | S2    | 1442 | OMU  | O2-C2 | -2.47 | 1.18        | 1.23     |
| 8   | L5    | 4228 | OMG  | C5-C6 | 2.46  | 1.53        | 1.44     |
| 8   | L5    | 4618 | OMG  | C5-C6 | 2.46  | 1.53        | 1.44     |
| 8   | L5    | 4618 | OMG  | C6-N1 | 2.46  | 1.43        | 1.38     |
| 10  | L8    | 75   | OMG  | C6-N1 | 2.46  | 1.43        | 1.38     |
| 8   | L5    | 3744 | OMG  | C5-C6 | 2.44  | 1.53        | 1.44     |
| 49  | S2    | 428  | OMU  | O2-C2 | -2.44 | 1.18        | 1.23     |
| 49  | S2    | 683  | OMG  | C6-N1 | 2.43  | 1.43        | 1.38     |
| 8   | L5    | 4494 | OMG  | C6-N1 | 2.43  | 1.43        | 1.38     |
| 8   | L5    | 3718 | A2M  | C8-N9 | -2.43 | 1.33        | 1.37     |
| 49  | S2    | 683  | OMG  | C5-C6 | 2.43  | 1.53        | 1.44     |
| 8   | L5    | 2364 | OMG  | C5-C6 | 2.42  | 1.53        | 1.44     |
| 49  | S2    | 1851 | MA6  | C5-N7 | -2.42 | 1.34        | 1.39     |
| 8   | L5    | 3825 | A2M  | C8-N9 | -2.42 | 1.33        | 1.37     |
| 8   | L5    | 1625 | OMG  | C5-C6 | 2.41  | 1.53        | 1.44     |
| 49  | S2    | 1328 | OMG  | C5-C6 | 2.41  | 1.53        | 1.44     |
| 8   | L5    | 2424 | OMG  | C6-N1 | 2.41  | 1.43        | 1.38     |
| 8   | L5    | 1316 | OMG  | C5-C6 | 2.41  | 1.53        | 1.44     |
| 10  | L8    | 75   | OMG  | C5-C6 | 2.41  | 1.53        | 1.44     |
| 8   | L5    | 2424 | OMG  | C5-C6 | 2.41  | 1.53        | 1.44     |
| 8   | L5    | 3627 | OMG  | C6-N1 | 2.41  | 1.43        | 1.38     |
| 8   | L5    | 4637 | OMG  | C5-C6 | 2.40  | 1.53        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 8   | L5    | 2364 | OMG  | C6-N1 | 2.40  | 1.43        | 1.38     |
| 49  | S2    | 1248 | B8N  | O2-C2 | -2.40 | 1.18        | 1.22     |
| 49  | S2    | 644  | OMG  | C5-C6 | 2.39  | 1.53        | 1.44     |
| 8   | L5    | 4590 | A2M  | C8-N9 | -2.39 | 1.33        | 1.37     |
| 49  | S2    | 1703 | OMC  | C5-C4 | 2.39  | 1.48        | 1.42     |
| 8   | L5    | 1326 | A2M  | C8-N9 | -2.39 | 1.33        | 1.37     |
| 8   | L5    | 3792 | OMG  | C5-C6 | 2.39  | 1.53        | 1.44     |
| 8   | L5    | 2365 | OMC  | C5-C4 | 2.39  | 1.48        | 1.42     |
| 8   | L5    | 3760 | A2M  | C8-N9 | -2.39 | 1.33        | 1.37     |
| 8   | L5    | 4494 | OMG  | C5-C6 | 2.39  | 1.53        | 1.44     |
| 49  | S2    | 1031 | A2M  | C8-N9 | -2.38 | 1.33        | 1.37     |
| 8   | L5    | 2363 | A2M  | C8-N9 | -2.38 | 1.33        | 1.37     |
| 8   | L5    | 4623 | OMG  | C5-C6 | 2.38  | 1.53        | 1.44     |
| 8   | L5    | 1871 | A2M  | C8-N9 | -2.37 | 1.33        | 1.37     |
| 49  | S2    | 159  | A2M  | C8-N9 | -2.37 | 1.33        | 1.37     |
| 8   | L5    | 1522 | OMG  | C5-C6 | 2.37  | 1.53        | 1.44     |
| 49  | S2    | 683  | OMG  | C4-N9 | -2.37 | 1.31        | 1.38     |
| 8   | L5    | 2422 | OMC  | C5-C4 | 2.36  | 1.48        | 1.42     |
| 49  | S2    | 174  | OMC  | C5-C4 | 2.36  | 1.48        | 1.42     |
| 8   | L5    | 4623 | OMG  | C6-N1 | 2.34  | 1.43        | 1.38     |
| 49  | S2    | 27   | A2M  | C8-N9 | -2.34 | 1.33        | 1.37     |
| 8   | L5    | 4499 | OMG  | C5-C6 | 2.34  | 1.53        | 1.44     |
| 8   | L5    | 4623 | OMG  | C4-N9 | -2.34 | 1.32        | 1.38     |
| 8   | L5    | 2364 | OMG  | C4-N9 | -2.34 | 1.32        | 1.38     |
| 8   | L5    | 3627 | OMG  | C5-C6 | 2.34  | 1.53        | 1.44     |
| 49  | S2    | 1288 | OMU  | O2-C2 | -2.34 | 1.18        | 1.23     |
| 49  | S2    | 1328 | OMG  | C6-N1 | 2.34  | 1.43        | 1.38     |
| 8   | L5    | 1316 | OMG  | C6-N1 | 2.33  | 1.43        | 1.38     |
| 8   | L5    | 2401 | A2M  | C8-N9 | -2.33 | 1.33        | 1.37     |
| 49  | S2    | 1639 | G7M  | C6-N1 | 2.32  | 1.43        | 1.38     |
| 8   | L5    | 4618 | OMG  | C4-N9 | -2.32 | 1.32        | 1.38     |
| 8   | L5    | 4370 | OMG  | C6-N1 | 2.32  | 1.43        | 1.38     |
| 49  | S2    | 576  | A2M  | C8-N9 | -2.32 | 1.33        | 1.37     |
| 8   | L5    | 2876 | OMG  | C5-C6 | 2.32  | 1.53        | 1.44     |
| 8   | L5    | 1522 | OMG  | C4-N9 | -2.32 | 1.32        | 1.38     |
| 8   | L5    | 1881 | OMC  | C5-C4 | 2.32  | 1.48        | 1.42     |
| 8   | L5    | 3724 | A2M  | C8-N9 | -2.31 | 1.33        | 1.37     |
| 49  | S2    | 668  | A2M  | C8-N9 | -2.30 | 1.33        | 1.37     |
| 49  | S2    | 1288 | OMU  | C5-C4 | 2.30  | 1.48        | 1.43     |
| 49  | S2    | 1248 | B8N  | O4-C4 | -2.28 | 1.18        | 1.23     |
| 8   | L5    | 3744 | OMG  | C4-N9 | -2.28 | 1.32        | 1.38     |
| 49  | S2    | 1383 | A2M  | C8-N9 | -2.28 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 2876 | OMG  | C6-N1   | 2.27  | 1.43        | 1.38     |
| 8   | L5    | 1522 | OMG  | C6-N1   | 2.27  | 1.43        | 1.38     |
| 8   | L5    | 1625 | OMG  | C6-N1   | 2.26  | 1.43        | 1.38     |
| 8   | L5    | 2861 | OMC  | C5-C4   | 2.26  | 1.48        | 1.42     |
| 49  | S2    | 1391 | OMC  | C5-C4   | 2.26  | 1.48        | 1.42     |
| 8   | L5    | 3723 | A2M  | C8-N9   | -2.25 | 1.33        | 1.37     |
| 49  | S2    | 428  | OMU  | C5-C4   | 2.25  | 1.48        | 1.43     |
| 8   | L5    | 4499 | OMG  | C4-N9   | -2.25 | 1.32        | 1.38     |
| 49  | S2    | 644  | OMG  | C6-N1   | 2.25  | 1.43        | 1.38     |
| 8   | L5    | 2876 | OMG  | C4-N9   | -2.25 | 1.32        | 1.38     |
| 49  | S2    | 1248 | B8N  | C2-N3   | 2.24  | 1.42        | 1.38     |
| 8   | L5    | 1340 | OMC  | C5-C4   | 2.24  | 1.48        | 1.42     |
| 49  | S2    | 1328 | OMG  | C4-N9   | -2.23 | 1.32        | 1.38     |
| 8   | L5    | 4637 | OMG  | C6-N1   | 2.23  | 1.43        | 1.38     |
| 49  | S2    | 1031 | A2M  | O5'-C5' | -2.23 | 1.39        | 1.44     |
| 49  | S2    | 601  | OMG  | C4-N9   | -2.21 | 1.32        | 1.38     |
| 8   | L5    | 1316 | OMG  | C4-N9   | -2.21 | 1.32        | 1.38     |
| 8   | L5    | 1625 | OMG  | C4-N9   | -2.20 | 1.32        | 1.38     |
| 8   | L5    | 4370 | OMG  | C4-N9   | -2.20 | 1.32        | 1.38     |
| 8   | L5    | 398  | A2M  | C8-N9   | -2.19 | 1.33        | 1.37     |
| 8   | L5    | 4499 | OMG  | C6-N1   | 2.19  | 1.42        | 1.38     |
| 8   | L5    | 4536 | OMC  | C5-C4   | 2.19  | 1.47        | 1.42     |
| 49  | S2    | 1326 | UY1  | O2-C2   | -2.17 | 1.18        | 1.23     |
| 49  | S2    | 668  | A2M  | O5'-C5' | -2.17 | 1.39        | 1.44     |
| 10  | L8    | 75   | OMG  | C4-N9   | -2.17 | 1.32        | 1.38     |
| 8   | L5    | 2815 | A2M  | C8-N9   | -2.17 | 1.33        | 1.37     |
| 8   | L5    | 1524 | A2M  | C4-N9   | -2.16 | 1.32        | 1.37     |
| 8   | L5    | 3792 | OMG  | C4-N9   | -2.16 | 1.32        | 1.38     |
| 49  | S2    | 644  | OMG  | C4-N9   | -2.16 | 1.32        | 1.38     |
| 8   | L5    | 2424 | OMG  | C4-N9   | -2.15 | 1.32        | 1.38     |
| 8   | L5    | 4494 | OMG  | C4-N9   | -2.15 | 1.32        | 1.38     |
| 8   | L5    | 3841 | OMC  | C5-C4   | 2.15  | 1.47        | 1.42     |
| 10  | L8    | 14   | OMU  | C5-C4   | 2.14  | 1.48        | 1.43     |
| 8   | L5    | 2787 | A2M  | C8-N9   | -2.13 | 1.33        | 1.37     |
| 49  | S2    | 1442 | OMU  | C5-C4   | 2.13  | 1.48        | 1.43     |
| 49  | S2    | 27   | A2M  | O5'-C5' | -2.13 | 1.39        | 1.44     |
| 49  | S2    | 601  | OMG  | C6-N1   | 2.13  | 1.42        | 1.38     |
| 8   | L5    | 3792 | OMG  | C6-N1   | 2.12  | 1.42        | 1.38     |
| 49  | S2    | 1639 | G7M  | C4-N9   | -2.12 | 1.32        | 1.38     |
| 49  | S2    | 1851 | MA6  | C8-N9   | -2.12 | 1.33        | 1.37     |
| 8   | L5    | 3825 | A2M  | O5'-C5' | -2.12 | 1.39        | 1.44     |
| 8   | L5    | 3701 | OMC  | C5-C4   | 2.10  | 1.47        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L5    | 2351 | OMC  | C5-C4   | 2.09  | 1.47        | 1.42     |
| 8   | L5    | 4620 | OMU  | C5-C4   | 2.07  | 1.48        | 1.43     |
| 8   | L5    | 4637 | OMG  | C4-N9   | -2.07 | 1.32        | 1.38     |
| 8   | L5    | 1871 | A2M  | O5'-C5' | -2.07 | 1.39        | 1.44     |
| 8   | L5    | 2363 | A2M  | O5'-C5' | -2.06 | 1.39        | 1.44     |
| 8   | L5    | 2804 | OMC  | C5-C4   | 2.06  | 1.47        | 1.42     |
| 49  | S2    | 1248 | B8N  | C1'-C5  | 2.05  | 1.54        | 1.50     |
| 8   | L5    | 3925 | OMU  | C5-C4   | 2.05  | 1.48        | 1.43     |
| 8   | L5    | 398  | A2M  | O5'-C5' | -2.04 | 1.39        | 1.44     |
| 8   | L5    | 1326 | A2M  | O5'-C5' | -2.04 | 1.39        | 1.44     |
| 8   | L5    | 3760 | A2M  | O5'-C5' | -2.02 | 1.39        | 1.44     |
| 8   | L5    | 3724 | A2M  | O5'-C5' | -2.01 | 1.39        | 1.44     |
| 8   | L5    | 1524 | A2M  | O5'-C5' | -2.00 | 1.39        | 1.44     |

All (566) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 49  | S2    | 1851 | MA6  | N1-C6-N6  | -13.85 | 101.94      | 117.08   |
| 49  | S2    | 1850 | MA6  | N1-C6-N6  | -11.56 | 104.44      | 117.08   |
| 49  | S2    | 601  | OMG  | C1'-N9-C8 | -8.84  | 101.52      | 126.70   |
| 8   | L5    | 2876 | OMG  | C1'-N9-C8 | -8.55  | 102.35      | 126.70   |
| 8   | L5    | 4637 | OMG  | C1'-N9-C8 | -8.45  | 102.64      | 126.70   |
| 8   | L5    | 3792 | OMG  | C1'-N9-C8 | -8.27  | 103.17      | 126.70   |
| 8   | L5    | 1625 | OMG  | C1'-N9-C8 | -8.07  | 103.72      | 126.70   |
| 8   | L5    | 1316 | OMG  | C1'-N9-C8 | -7.97  | 104.02      | 126.70   |
| 8   | L5    | 2424 | OMG  | C1'-N9-C8 | -7.90  | 104.21      | 126.70   |
| 8   | L5    | 4494 | OMG  | C1'-N9-C8 | -7.90  | 104.22      | 126.70   |
| 8   | L5    | 4499 | OMG  | C1'-N9-C8 | -7.88  | 104.27      | 126.70   |
| 49  | S2    | 644  | OMG  | C1'-N9-C8 | -7.86  | 104.33      | 126.70   |
| 8   | L5    | 2364 | OMG  | C1'-N9-C8 | -7.83  | 104.41      | 126.70   |
| 10  | L8    | 75   | OMG  | C1'-N9-C8 | -7.78  | 104.55      | 126.70   |
| 8   | L5    | 4370 | OMG  | C1'-N9-C8 | -7.78  | 104.56      | 126.70   |
| 49  | S2    | 601  | OMG  | C1'-N9-C4 | 7.77   | 149.59      | 126.50   |
| 49  | S2    | 1328 | OMG  | C1'-N9-C8 | -7.75  | 104.63      | 126.70   |
| 8   | L5    | 1522 | OMG  | C1'-N9-C8 | -7.68  | 104.84      | 126.70   |
| 8   | L5    | 4623 | OMG  | C1'-N9-C8 | -7.59  | 105.08      | 126.70   |
| 49  | S2    | 1639 | G7M  | C1'-N9-C4 | 7.58   | 149.02      | 126.50   |
| 8   | L5    | 4618 | OMG  | C1'-N9-C8 | -7.55  | 105.20      | 126.70   |
| 8   | L5    | 3744 | OMG  | C1'-N9-C8 | -7.51  | 105.32      | 126.70   |
| 49  | S2    | 1639 | G7M  | C1'-N9-C8 | -7.43  | 101.65      | 126.74   |
| 49  | S2    | 683  | OMG  | C1'-N9-C8 | -7.39  | 105.66      | 126.70   |
| 49  | S2    | 1851 | MA6  | C5-C6-N6  | 7.39   | 138.17      | 125.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8   | L5    | 3627 | OMG  | C1'-N9-C8 | -7.29 | 105.95      | 126.70   |
| 8   | L5    | 4637 | OMG  | C1'-N9-C4 | 7.28  | 148.13      | 126.50   |
| 8   | L5    | 2876 | OMG  | C1'-N9-C4 | 7.27  | 148.09      | 126.50   |
| 8   | L5    | 4228 | OMG  | C1'-N9-C8 | -7.18 | 106.25      | 126.70   |
| 8   | L5    | 3792 | OMG  | C1'-N9-C4 | 7.13  | 147.67      | 126.50   |
| 8   | L5    | 1625 | OMG  | C1'-N9-C4 | 6.93  | 147.09      | 126.50   |
| 8   | L5    | 2424 | OMG  | C1'-N9-C4 | 6.90  | 146.98      | 126.50   |
| 8   | L5    | 4494 | OMG  | C1'-N9-C4 | 6.83  | 146.80      | 126.50   |
| 8   | L5    | 4499 | OMG  | C1'-N9-C4 | 6.77  | 146.62      | 126.50   |
| 8   | L5    | 1316 | OMG  | C1'-N9-C4 | 6.75  | 146.56      | 126.50   |
| 10  | L8    | 75   | OMG  | C1'-N9-C4 | 6.73  | 146.49      | 126.50   |
| 49  | S2    | 644  | OMG  | C1'-N9-C4 | 6.69  | 146.37      | 126.50   |
| 8   | L5    | 4370 | OMG  | C1'-N9-C4 | 6.67  | 146.30      | 126.50   |
| 8   | L5    | 2364 | OMG  | C1'-N9-C4 | 6.63  | 146.18      | 126.50   |
| 49  | S2    | 1328 | OMG  | C1'-N9-C4 | 6.62  | 146.18      | 126.50   |
| 8   | L5    | 1522 | OMG  | C1'-N9-C4 | 6.58  | 146.04      | 126.50   |
| 8   | L5    | 4618 | OMG  | C1'-N9-C4 | 6.53  | 145.90      | 126.50   |
| 8   | L5    | 4623 | OMG  | C1'-N9-C4 | 6.45  | 145.65      | 126.50   |
| 8   | L5    | 3744 | OMG  | C1'-N9-C4 | 6.40  | 145.50      | 126.50   |
| 49  | S2    | 1850 | MA6  | C5-C6-N6  | 6.39  | 136.43      | 125.30   |
| 8   | L5    | 3627 | OMG  | C1'-N9-C4 | 6.10  | 144.63      | 126.50   |
| 49  | S2    | 683  | OMG  | C1'-N9-C4 | 6.07  | 144.53      | 126.50   |
| 8   | L5    | 3760 | A2M  | N3-C2-N1  | -5.97 | 119.27      | 128.60   |
| 8   | L5    | 4228 | OMG  | C1'-N9-C4 | 5.96  | 144.20      | 126.50   |
| 49  | S2    | 27   | A2M  | N3-C2-N1  | -5.84 | 119.46      | 128.60   |
| 49  | S2    | 1832 | 6MZ  | N1-C2-N3  | -5.80 | 119.52      | 128.60   |
| 49  | S2    | 1248 | B8N  | C31-N3-C2 | 5.79  | 126.34      | 117.67   |
| 8   | L5    | 1871 | A2M  | N3-C2-N1  | -5.78 | 119.57      | 128.60   |
| 49  | S2    | 1678 | A2M  | C5-C4-N3  | -5.75 | 119.25      | 126.75   |
| 49  | S2    | 1031 | A2M  | C5-C4-N3  | -5.74 | 119.26      | 126.75   |
| 8   | L5    | 1326 | A2M  | N3-C2-N1  | -5.73 | 119.64      | 128.60   |
| 8   | L5    | 2815 | A2M  | C5-C4-N3  | -5.73 | 119.28      | 126.75   |
| 8   | L5    | 4590 | A2M  | N3-C2-N1  | -5.70 | 119.69      | 128.60   |
| 8   | L5    | 2815 | A2M  | N3-C2-N1  | -5.63 | 119.80      | 128.60   |
| 49  | S2    | 1850 | MA6  | C5-C4-N3  | -5.62 | 119.42      | 126.75   |
| 49  | S2    | 576  | A2M  | C5-C4-N3  | -5.60 | 119.44      | 126.75   |
| 49  | S2    | 1851 | MA6  | N1-C2-N3  | -5.59 | 119.86      | 128.60   |
| 8   | L5    | 3825 | A2M  | C5-C4-N3  | -5.58 | 119.47      | 126.75   |
| 49  | S2    | 668  | A2M  | N3-C2-N1  | -5.58 | 119.88      | 128.60   |
| 8   | L5    | 3724 | A2M  | N3-C2-N1  | -5.57 | 119.88      | 128.60   |
| 49  | S2    | 1031 | A2M  | N3-C2-N1  | -5.57 | 119.89      | 128.60   |
| 8   | L5    | 3723 | A2M  | N3-C2-N1  | -5.56 | 119.90      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8   | L5    | 2363 | A2M  | N3-C2-N1 | -5.56 | 119.90      | 128.60   |
| 8   | L5    | 398  | A2M  | N3-C2-N1 | -5.55 | 119.92      | 128.60   |
| 8   | L5    | 2401 | A2M  | N3-C2-N1 | -5.55 | 119.92      | 128.60   |
| 49  | S2    | 159  | A2M  | C5-C4-N3 | -5.52 | 119.54      | 126.75   |
| 49  | S2    | 1383 | A2M  | N3-C2-N1 | -5.52 | 119.97      | 128.60   |
| 8   | L5    | 2363 | A2M  | C5-C4-N3 | -5.51 | 119.56      | 126.75   |
| 8   | L5    | 4590 | A2M  | C5-C4-N3 | -5.49 | 119.59      | 126.75   |
| 8   | L5    | 2787 | A2M  | N3-C2-N1 | -5.48 | 120.02      | 128.60   |
| 8   | L5    | 2787 | A2M  | C5-C4-N3 | -5.45 | 119.64      | 126.75   |
| 8   | L5    | 3718 | A2M  | C5-C4-N3 | -5.45 | 119.64      | 126.75   |
| 8   | L5    | 398  | A2M  | C5-C4-N3 | -5.41 | 119.69      | 126.75   |
| 49  | S2    | 576  | A2M  | N3-C2-N1 | -5.41 | 120.14      | 128.60   |
| 49  | S2    | 159  | A2M  | N3-C2-N1 | -5.38 | 120.19      | 128.60   |
| 8   | L5    | 1326 | A2M  | C5-C4-N3 | -5.38 | 119.74      | 126.75   |
| 49  | S2    | 1678 | A2M  | N3-C2-N1 | -5.37 | 120.20      | 128.60   |
| 8   | L5    | 2401 | A2M  | C5-C4-N3 | -5.37 | 119.74      | 126.75   |
| 8   | L5    | 4620 | OMU  | C4-N3-C2 | -5.36 | 119.52      | 126.58   |
| 8   | L5    | 3724 | A2M  | C5-C4-N3 | -5.35 | 119.76      | 126.75   |
| 8   | L5    | 3825 | A2M  | N3-C2-N1 | -5.32 | 120.28      | 128.60   |
| 49  | S2    | 1383 | A2M  | C5-C4-N3 | -5.31 | 119.83      | 126.75   |
| 49  | S2    | 1442 | OMU  | C4-N3-C2 | -5.29 | 119.60      | 126.58   |
| 8   | L5    | 3718 | A2M  | N3-C2-N1 | -5.28 | 120.34      | 128.60   |
| 8   | L5    | 1524 | A2M  | N3-C2-N1 | -5.27 | 120.36      | 128.60   |
| 49  | S2    | 428  | OMU  | C4-N3-C2 | -5.21 | 119.70      | 126.58   |
| 49  | S2    | 1288 | OMU  | C4-N3-C2 | -5.20 | 119.72      | 126.58   |
| 8   | L5    | 1871 | A2M  | C5-C4-N3 | -5.20 | 119.97      | 126.75   |
| 49  | S2    | 1383 | A2M  | N6-C6-N1 | -5.19 | 107.00      | 118.35   |
| 8   | L5    | 3723 | A2M  | C5-C4-N3 | -5.16 | 120.02      | 126.75   |
| 49  | S2    | 1851 | MA6  | C5-C4-N3 | -5.14 | 120.05      | 126.75   |
| 8   | L5    | 3925 | OMU  | C4-N3-C2 | -5.12 | 119.82      | 126.58   |
| 49  | S2    | 27   | A2M  | C5-C4-N3 | -5.12 | 120.07      | 126.75   |
| 8   | L5    | 2363 | A2M  | N6-C6-N1 | -5.09 | 107.20      | 118.35   |
| 49  | S2    | 159  | A2M  | N6-C6-N1 | -5.09 | 107.21      | 118.35   |
| 49  | S2    | 27   | A2M  | N6-C6-N1 | -5.08 | 107.23      | 118.35   |
| 49  | S2    | 1832 | 6MZ  | C5-C4-N3 | -5.06 | 120.14      | 126.75   |
| 49  | S2    | 1850 | MA6  | N1-C2-N3 | -5.06 | 120.68      | 128.60   |
| 8   | L5    | 2815 | A2M  | N6-C6-N1 | -5.03 | 107.32      | 118.35   |
| 8   | L5    | 4637 | OMG  | C5-C4-N3 | -5.03 | 120.29      | 128.46   |
| 49  | S2    | 601  | OMG  | C5-C4-N3 | -5.01 | 120.33      | 128.46   |
| 8   | L5    | 4590 | A2M  | N6-C6-N1 | -5.01 | 107.38      | 118.35   |
| 49  | S2    | 668  | A2M  | N6-C6-N1 | -5.00 | 107.39      | 118.35   |
| 49  | S2    | 668  | A2M  | C5-C4-N3 | -4.99 | 120.24      | 126.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 49  | S2    | 1678 | A2M  | N6-C6-N1 | -4.98 | 107.45      | 118.35   |
| 49  | S2    | 1850 | MA6  | C4-C5-C6 | 4.97  | 121.44      | 115.88   |
| 8   | L5    | 3718 | A2M  | N6-C6-N1 | -4.96 | 107.49      | 118.35   |
| 10  | L8    | 14   | OMU  | C4-N3-C2 | -4.96 | 120.04      | 126.58   |
| 8   | L5    | 1524 | A2M  | N6-C6-N1 | -4.92 | 107.58      | 118.35   |
| 8   | L5    | 3825 | A2M  | N6-C6-N1 | -4.90 | 107.62      | 118.35   |
| 8   | L5    | 398  | A2M  | N6-C6-N1 | -4.90 | 107.62      | 118.35   |
| 8   | L5    | 2787 | A2M  | N6-C6-N1 | -4.90 | 107.63      | 118.35   |
| 8   | L5    | 3724 | A2M  | N6-C6-N1 | -4.88 | 107.66      | 118.35   |
| 49  | S2    | 1326 | UY1  | C4-N3-C2 | -4.88 | 119.31      | 126.34   |
| 8   | L5    | 4494 | OMG  | C5-C4-N3 | -4.84 | 120.61      | 128.46   |
| 8   | L5    | 3723 | A2M  | N6-C6-N1 | -4.84 | 107.76      | 118.35   |
| 49  | S2    | 1031 | A2M  | N6-C6-N1 | -4.79 | 107.86      | 118.35   |
| 49  | S2    | 1248 | B8N  | C5-C4-N3 | 4.79  | 125.03      | 116.17   |
| 8   | L5    | 3760 | A2M  | N6-C6-N1 | -4.78 | 107.88      | 118.35   |
| 8   | L5    | 2401 | A2M  | N6-C6-N1 | -4.78 | 107.89      | 118.35   |
| 49  | S2    | 644  | OMG  | C5-C4-N3 | -4.77 | 120.72      | 128.46   |
| 49  | S2    | 1248 | B8N  | C4-N3-C2 | -4.74 | 119.46      | 125.46   |
| 8   | L5    | 1326 | A2M  | N6-C6-N1 | -4.74 | 107.96      | 118.35   |
| 8   | L5    | 1316 | OMG  | C5-C4-N3 | -4.73 | 120.79      | 128.46   |
| 8   | L5    | 2424 | OMG  | C5-C4-N3 | -4.73 | 120.79      | 128.46   |
| 8   | L5    | 1871 | A2M  | N6-C6-N1 | -4.72 | 108.01      | 118.35   |
| 49  | S2    | 576  | A2M  | N6-C6-N1 | -4.71 | 108.05      | 118.35   |
| 8   | L5    | 3792 | OMG  | C5-C4-N3 | -4.69 | 120.85      | 128.46   |
| 8   | L5    | 3760 | A2M  | C5-C4-N3 | -4.69 | 120.63      | 126.75   |
| 8   | L5    | 1625 | OMG  | C5-C4-N3 | -4.65 | 120.91      | 128.46   |
| 8   | L5    | 4499 | OMG  | C5-C4-N3 | -4.65 | 120.92      | 128.46   |
| 10  | L8    | 75   | OMG  | C5-C4-N3 | -4.63 | 120.94      | 128.46   |
| 8   | L5    | 4370 | OMG  | C5-C4-N3 | -4.62 | 120.97      | 128.46   |
| 8   | L5    | 2876 | OMG  | C5-C4-N3 | -4.61 | 120.97      | 128.46   |
| 8   | L5    | 4353 | PSU  | C4-N3-C2 | -4.59 | 119.72      | 126.34   |
| 8   | L5    | 3758 | PSU  | C4-N3-C2 | -4.56 | 119.76      | 126.34   |
| 49  | S2    | 1851 | MA6  | N9-C8-N7 | -4.56 | 107.68      | 113.91   |
| 49  | S2    | 1328 | OMG  | C5-C4-N3 | -4.53 | 121.11      | 128.46   |
| 49  | S2    | 668  | A2M  | N9-C8-N7 | -4.51 | 107.75      | 113.91   |
| 8   | L5    | 4618 | OMG  | C5-C4-N3 | -4.47 | 121.20      | 128.46   |
| 8   | L5    | 3744 | OMG  | C5-C4-N3 | -4.47 | 121.21      | 128.46   |
| 8   | L5    | 1522 | OMG  | C5-C4-N3 | -4.46 | 121.22      | 128.46   |
| 8   | L5    | 1524 | A2M  | C5-C6-N6 | 4.46  | 133.13      | 123.43   |
| 8   | L5    | 4494 | OMG  | C2-N3-C4 | 4.42  | 120.17      | 112.30   |
| 49  | S2    | 601  | OMG  | C2-N3-C4 | 4.41  | 120.16      | 112.30   |
| 8   | L5    | 1683 | PSU  | C4-N3-C2 | -4.40 | 120.00      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 49  | S2    | 1639 | G7M  | C2-N3-C4 | 4.39  | 120.12      | 112.30   |
| 49  | S2    | 27   | A2M  | C5-C6-N6 | 4.38  | 132.97      | 123.43   |
| 8   | L5    | 2364 | OMG  | C5-C4-N3 | -4.37 | 121.38      | 128.46   |
| 8   | L5    | 2424 | OMG  | C2-N3-C4 | 4.36  | 120.06      | 112.30   |
| 49  | S2    | 668  | A2M  | C5-C6-N6 | 4.35  | 132.89      | 123.43   |
| 8   | L5    | 1782 | PSU  | C4-N3-C2 | -4.34 | 120.08      | 126.34   |
| 8   | L5    | 1316 | OMG  | C2-N3-C4 | 4.34  | 120.03      | 112.30   |
| 49  | S2    | 644  | OMG  | C2-N3-C4 | 4.34  | 120.03      | 112.30   |
| 8   | L5    | 4623 | OMG  | C5-C4-N3 | -4.32 | 121.46      | 128.46   |
| 8   | L5    | 1326 | A2M  | N9-C8-N7 | -4.32 | 108.01      | 113.91   |
| 49  | S2    | 1832 | 6MZ  | N9-C8-N7 | -4.31 | 108.01      | 113.91   |
| 8   | L5    | 1524 | A2M  | C5-C4-N3 | -4.31 | 121.13      | 126.75   |
| 8   | L5    | 3724 | A2M  | N9-C8-N7 | -4.30 | 108.03      | 113.91   |
| 49  | S2    | 1383 | A2M  | C5-C6-N6 | 4.30  | 132.79      | 123.43   |
| 8   | L5    | 3744 | OMG  | C2-N3-C4 | 4.30  | 119.96      | 112.30   |
| 8   | L5    | 4590 | A2M  | N9-C8-N7 | -4.29 | 108.05      | 113.91   |
| 49  | S2    | 159  | A2M  | N9-C8-N7 | -4.28 | 108.06      | 113.91   |
| 8   | L5    | 3729 | PSU  | C4-N3-C2 | -4.28 | 120.17      | 126.34   |
| 49  | S2    | 683  | OMG  | C5-C4-N3 | -4.28 | 121.53      | 128.46   |
| 10  | L8    | 75   | OMG  | C2-N3-C4 | 4.25  | 119.87      | 112.30   |
| 8   | L5    | 3718 | A2M  | C5-C6-N6 | 4.25  | 132.67      | 123.43   |
| 49  | S2    | 1328 | OMG  | C2-N3-C4 | 4.23  | 119.84      | 112.30   |
| 8   | L5    | 4370 | OMG  | C2-N3-C4 | 4.23  | 119.84      | 112.30   |
| 8   | L5    | 1522 | OMG  | C2-N3-C4 | 4.23  | 119.84      | 112.30   |
| 8   | L5    | 4637 | OMG  | C2-N3-C4 | 4.22  | 119.82      | 112.30   |
| 8   | L5    | 2876 | OMG  | C2-N3-C4 | 4.21  | 119.80      | 112.30   |
| 8   | L5    | 3734 | PSU  | N1-C2-N3 | 4.21  | 119.90      | 115.13   |
| 8   | L5    | 3792 | OMG  | C2-N3-C4 | 4.21  | 119.80      | 112.30   |
| 49  | S2    | 159  | A2M  | C5-C6-N6 | 4.20  | 132.58      | 123.43   |
| 49  | S2    | 1678 | A2M  | N9-C8-N7 | -4.20 | 108.17      | 113.91   |
| 8   | L5    | 3734 | PSU  | C4-N3-C2 | -4.18 | 120.31      | 126.34   |
| 8   | L5    | 4618 | OMG  | C2-N3-C4 | 4.18  | 119.75      | 112.30   |
| 8   | L5    | 4499 | OMG  | C2-N3-C4 | 4.18  | 119.74      | 112.30   |
| 8   | L5    | 3627 | OMG  | C5-C4-N3 | -4.17 | 121.69      | 128.46   |
| 8   | L5    | 2815 | A2M  | C5-C6-N6 | 4.16  | 132.48      | 123.43   |
| 8   | L5    | 4590 | A2M  | C5-C6-N6 | 4.16  | 132.48      | 123.43   |
| 8   | L5    | 4623 | OMG  | C2-N3-C4 | 4.16  | 119.71      | 112.30   |
| 8   | L5    | 2363 | A2M  | C5-C6-N6 | 4.16  | 132.47      | 123.43   |
| 8   | L5    | 1625 | OMG  | C2-N3-C4 | 4.15  | 119.70      | 112.30   |
| 8   | L5    | 3760 | A2M  | C5-C6-N6 | 4.15  | 132.46      | 123.43   |
| 8   | L5    | 1683 | PSU  | N1-C2-N3 | 4.14  | 119.83      | 115.13   |
| 8   | L5    | 398  | A2M  | N9-C8-N7 | -4.14 | 108.26      | 113.91   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8   | L5    | 2364 | OMG  | C2-N3-C4 | 4.13  | 119.65      | 112.30   |
| 8   | L5    | 3627 | OMG  | C2-N3-C4 | 4.12  | 119.65      | 112.30   |
| 8   | L5    | 3760 | A2M  | N9-C8-N7 | -4.12 | 108.28      | 113.91   |
| 8   | L5    | 4353 | PSU  | N1-C2-N3 | 4.12  | 119.79      | 115.13   |
| 8   | L5    | 3723 | A2M  | C5-C6-N6 | 4.11  | 132.38      | 123.43   |
| 49  | S2    | 1326 | UY1  | N1-C2-N3 | 4.11  | 119.79      | 115.13   |
| 49  | S2    | 1678 | A2M  | C5-C6-N6 | 4.11  | 132.37      | 123.43   |
| 49  | S2    | 683  | OMG  | C2-N3-C4 | 4.11  | 119.62      | 112.30   |
| 49  | S2    | 1031 | A2M  | N9-C8-N7 | -4.10 | 108.31      | 113.91   |
| 8   | L5    | 3723 | A2M  | N9-C8-N7 | -4.10 | 108.31      | 113.91   |
| 10  | L8    | 14   | OMU  | N3-C2-N1 | 4.10  | 120.33      | 114.89   |
| 49  | S2    | 1383 | A2M  | N9-C8-N7 | -4.09 | 108.32      | 113.91   |
| 8   | L5    | 2787 | A2M  | C5-C6-N6 | 4.09  | 132.32      | 123.43   |
| 8   | L5    | 3825 | A2M  | N9-C8-N7 | -4.09 | 108.33      | 113.91   |
| 8   | L5    | 4620 | OMU  | N3-C2-N1 | 4.08  | 120.31      | 114.89   |
| 49  | S2    | 27   | A2M  | N9-C8-N7 | -4.08 | 108.33      | 113.91   |
| 8   | L5    | 1871 | A2M  | N9-C8-N7 | -4.08 | 108.34      | 113.91   |
| 8   | L5    | 4228 | OMG  | C2-N3-C4 | 4.07  | 119.55      | 112.30   |
| 8   | L5    | 3724 | A2M  | C5-C6-N6 | 4.07  | 132.28      | 123.43   |
| 8   | L5    | 398  | A2M  | C5-C6-N6 | 4.06  | 132.27      | 123.43   |
| 8   | L5    | 2815 | A2M  | N9-C8-N7 | -4.06 | 108.36      | 113.91   |
| 49  | S2    | 576  | A2M  | N9-C8-N7 | -4.05 | 108.37      | 113.91   |
| 8   | L5    | 2401 | A2M  | C5-C6-N6 | 4.05  | 132.24      | 123.43   |
| 8   | L5    | 2401 | A2M  | N9-C8-N7 | -4.05 | 108.38      | 113.91   |
| 8   | L5    | 4228 | OMG  | C5-C4-N3 | -4.04 | 121.91      | 128.46   |
| 49  | S2    | 1639 | G7M  | C5-C4-N3 | -4.03 | 120.42      | 128.15   |
| 8   | L5    | 1782 | PSU  | N1-C2-N3 | 4.02  | 119.69      | 115.13   |
| 8   | L5    | 3825 | A2M  | C5-C6-N6 | 4.02  | 132.17      | 123.43   |
| 8   | L5    | 3718 | A2M  | N9-C8-N7 | -4.02 | 108.42      | 113.91   |
| 8   | L5    | 2787 | A2M  | N9-C8-N7 | -4.01 | 108.42      | 113.91   |
| 8   | L5    | 3729 | PSU  | N1-C2-N3 | 4.01  | 119.67      | 115.13   |
| 8   | L5    | 2363 | A2M  | N9-C8-N7 | -3.99 | 108.46      | 113.91   |
| 8   | L5    | 1326 | A2M  | C5-C6-N6 | 3.96  | 132.04      | 123.43   |
| 8   | L5    | 1871 | A2M  | C5-C6-N6 | 3.95  | 132.03      | 123.43   |
| 49  | S2    | 1832 | 6MZ  | C4-C5-C6 | 3.95  | 119.87      | 116.81   |
| 49  | S2    | 576  | A2M  | C5-C6-N6 | 3.94  | 132.00      | 123.43   |
| 8   | L5    | 3758 | PSU  | N1-C2-N3 | 3.93  | 119.59      | 115.13   |
| 8   | L5    | 1524 | A2M  | N9-C8-N7 | -3.93 | 108.54      | 113.91   |
| 49  | S2    | 1442 | OMU  | N3-C2-N1 | 3.88  | 120.04      | 114.89   |
| 49  | S2    | 1639 | G7M  | C5-C6-N1 | 3.84  | 119.82      | 111.79   |
| 49  | S2    | 683  | OMG  | N9-C8-N7 | -3.80 | 106.24      | 113.39   |
| 49  | S2    | 1850 | MA6  | N3-C4-N9 | 3.80  | 133.34      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8   | L5    | 2815 | A2M  | C2-N3-C4  | 3.80  | 120.72      | 111.75   |
| 49  | S2    | 1031 | A2M  | C2-N3-C4  | 3.78  | 120.68      | 111.75   |
| 49  | S2    | 1851 | MA6  | C4-C5-C6  | 3.77  | 120.10      | 115.88   |
| 49  | S2    | 1031 | A2M  | C5-C6-N6  | 3.77  | 131.63      | 123.43   |
| 10  | L8    | 55   | PSU  | N1-C2-N3  | 3.76  | 119.39      | 115.13   |
| 8   | L5    | 3925 | OMU  | N3-C2-N1  | 3.76  | 119.88      | 114.89   |
| 49  | S2    | 1288 | OMU  | N3-C2-N1  | 3.75  | 119.87      | 114.89   |
| 10  | L8    | 55   | PSU  | C6-N1-C2  | -3.72 | 118.88      | 122.68   |
| 8   | L5    | 4228 | OMG  | N9-C8-N7  | -3.72 | 106.39      | 113.39   |
| 49  | S2    | 428  | OMU  | N3-C2-N1  | 3.71  | 119.82      | 114.89   |
| 8   | L5    | 4590 | A2M  | C2-N3-C4  | 3.70  | 120.48      | 111.75   |
| 8   | L5    | 1326 | A2M  | C2-N3-C4  | 3.69  | 120.47      | 111.75   |
| 8   | L5    | 2363 | A2M  | C2-N3-C4  | 3.68  | 120.45      | 111.75   |
| 49  | S2    | 1678 | A2M  | C2-N3-C4  | 3.68  | 120.44      | 111.75   |
| 8   | L5    | 398  | A2M  | C2-N3-C4  | 3.62  | 120.30      | 111.75   |
| 8   | L5    | 3825 | A2M  | C2-N3-C4  | 3.62  | 120.30      | 111.75   |
| 8   | L5    | 1871 | A2M  | C2-N3-C4  | 3.61  | 120.28      | 111.75   |
| 8   | L5    | 2787 | A2M  | C2-N3-C4  | 3.61  | 120.27      | 111.75   |
| 49  | S2    | 27   | A2M  | C2-N3-C4  | 3.61  | 120.27      | 111.75   |
| 8   | L5    | 3724 | A2M  | C2-N3-C4  | 3.60  | 120.26      | 111.75   |
| 8   | L5    | 1316 | OMG  | N9-C8-N7  | -3.59 | 106.63      | 113.39   |
| 49  | S2    | 576  | A2M  | C2-N3-C4  | 3.59  | 120.23      | 111.75   |
| 49  | S2    | 159  | A2M  | C2-N3-C4  | 3.58  | 120.21      | 111.75   |
| 49  | S2    | 1851 | MA6  | C2-N3-C4  | 3.57  | 120.20      | 111.75   |
| 49  | S2    | 1383 | A2M  | C2-N3-C4  | 3.57  | 120.19      | 111.75   |
| 49  | S2    | 644  | OMG  | N9-C8-N7  | -3.56 | 106.68      | 113.39   |
| 8   | L5    | 3627 | OMG  | N9-C8-N7  | -3.56 | 106.69      | 113.39   |
| 8   | L5    | 2876 | OMG  | N9-C8-N7  | -3.55 | 106.70      | 113.39   |
| 10  | L8    | 55   | PSU  | C4-N3-C2  | -3.55 | 121.23      | 126.34   |
| 49  | S2    | 1832 | 6MZ  | C2-N3-C4  | 3.54  | 120.11      | 111.75   |
| 8   | L5    | 2401 | A2M  | C2-N3-C4  | 3.53  | 120.09      | 111.75   |
| 8   | L5    | 2364 | OMG  | N9-C8-N7  | -3.53 | 106.75      | 113.39   |
| 8   | L5    | 4623 | OMG  | N9-C8-N7  | -3.51 | 106.77      | 113.39   |
| 8   | L5    | 3718 | A2M  | C2-N3-C4  | 3.51  | 120.04      | 111.75   |
| 8   | L5    | 3723 | A2M  | C2-N3-C4  | 3.51  | 120.03      | 111.75   |
| 8   | L5    | 3744 | OMG  | N9-C8-N7  | -3.50 | 106.80      | 113.39   |
| 49  | S2    | 576  | A2M  | N3-C4-N9  | 3.48  | 132.82      | 127.08   |
| 49  | S2    | 668  | A2M  | C2-N3-C4  | 3.48  | 119.97      | 111.75   |
| 10  | L8    | 14   | OMU  | C1'-N1-C2 | 3.47  | 123.85      | 117.57   |
| 49  | S2    | 1832 | 6MZ  | C5-N7-C8  | 3.46  | 108.43      | 103.51   |
| 49  | S2    | 1851 | MA6  | C2-N1-C6  | 3.45  | 119.91      | 111.75   |
| 49  | S2    | 1031 | A2M  | N3-C4-N9  | 3.45  | 132.77      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 49  | S2    | 1328 | OMG  | N9-C8-N7   | -3.44 | 106.92      | 113.39   |
| 49  | S2    | 1850 | MA6  | C2-N1-C6   | 3.44  | 119.87      | 111.75   |
| 8   | L5    | 3760 | A2M  | C2-N3-C4   | 3.41  | 119.81      | 111.75   |
| 8   | L5    | 1522 | OMG  | N9-C8-N7   | -3.40 | 106.99      | 113.39   |
| 49  | S2    | 1678 | A2M  | N3-C4-N9   | 3.39  | 132.67      | 127.08   |
| 8   | L5    | 3734 | PSU  | C6-N1-C2   | -3.39 | 119.22      | 122.68   |
| 49  | S2    | 428  | OMU  | C5-C4-N3   | 3.38  | 119.89      | 114.84   |
| 8   | L5    | 4370 | OMG  | N9-C8-N7   | -3.37 | 107.05      | 113.39   |
| 49  | S2    | 1442 | OMU  | C5-C4-N3   | 3.37  | 119.88      | 114.84   |
| 8   | L5    | 2815 | A2M  | N3-C4-N9   | 3.36  | 132.63      | 127.08   |
| 8   | L5    | 3792 | OMG  | N9-C8-N7   | -3.35 | 107.08      | 113.39   |
| 8   | L5    | 1625 | OMG  | N9-C8-N7   | -3.35 | 107.08      | 113.39   |
| 8   | L5    | 4637 | OMG  | N9-C8-N7   | -3.31 | 107.15      | 113.39   |
| 10  | L8    | 75   | OMG  | N9-C8-N7   | -3.31 | 107.16      | 113.39   |
| 8   | L5    | 4590 | A2M  | C5-N7-C8   | 3.30  | 108.19      | 103.51   |
| 49  | S2    | 1850 | MA6  | C2-N3-C4   | 3.27  | 119.47      | 111.75   |
| 8   | L5    | 4494 | OMG  | N9-C8-N7   | -3.27 | 107.24      | 113.39   |
| 8   | L5    | 4499 | OMG  | N9-C8-N7   | -3.27 | 107.24      | 113.39   |
| 49  | S2    | 1288 | OMU  | C5-C4-N3   | 3.26  | 119.72      | 114.84   |
| 49  | S2    | 668  | A2M  | C5-N7-C8   | 3.26  | 108.14      | 103.51   |
| 8   | L5    | 4637 | OMG  | N9-C4-N3   | 3.26  | 132.49      | 125.94   |
| 8   | L5    | 3925 | OMU  | C5-C4-N3   | 3.26  | 119.71      | 114.84   |
| 49  | S2    | 1678 | A2M  | C5-N7-C8   | 3.26  | 108.14      | 103.51   |
| 8   | L5    | 3724 | A2M  | C5-N7-C8   | 3.24  | 108.11      | 103.51   |
| 8   | L5    | 4618 | OMG  | N9-C8-N7   | -3.24 | 107.28      | 113.39   |
| 49  | S2    | 159  | A2M  | C5-N7-C8   | 3.24  | 108.11      | 103.51   |
| 8   | L5    | 3825 | A2M  | N3-C4-N9   | 3.22  | 132.40      | 127.08   |
| 8   | L5    | 1683 | PSU  | C6-N1-C2   | -3.22 | 119.39      | 122.68   |
| 8   | L5    | 4620 | OMU  | C5-C4-N3   | 3.22  | 119.65      | 114.84   |
| 8   | L5    | 1326 | A2M  | N3-C4-N9   | 3.21  | 132.38      | 127.08   |
| 8   | L5    | 2363 | A2M  | N3-C4-N9   | 3.21  | 132.37      | 127.08   |
| 49  | S2    | 159  | A2M  | N3-C4-N9   | 3.20  | 132.36      | 127.08   |
| 8   | L5    | 4590 | A2M  | N3-C4-N9   | 3.19  | 132.34      | 127.08   |
| 8   | L5    | 1326 | A2M  | C5-N7-C8   | 3.19  | 108.04      | 103.51   |
| 8   | L5    | 2815 | A2M  | C5-N7-C8   | 3.19  | 108.04      | 103.51   |
| 8   | L5    | 398  | A2M  | N3-C4-N9   | 3.17  | 132.30      | 127.08   |
| 8   | L5    | 4637 | OMG  | C2-N1-C6   | -3.15 | 119.36      | 125.10   |
| 8   | L5    | 1524 | A2M  | C2'-C1'-N9 | -3.14 | 108.24      | 113.53   |
| 49  | S2    | 1851 | MA6  | N3-C4-N9   | 3.14  | 132.26      | 127.08   |
| 10  | L8    | 14   | OMU  | C5-C4-N3   | 3.13  | 119.52      | 114.84   |
| 8   | L5    | 2401 | A2M  | N3-C4-N9   | 3.12  | 132.23      | 127.08   |
| 8   | L5    | 3718 | A2M  | C5-N7-C8   | 3.12  | 107.94      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8   | L5    | 2424 | OMG  | N9-C8-N7 | -3.12 | 107.52      | 113.39   |
| 8   | L5    | 2787 | A2M  | N3-C4-N9 | 3.11  | 132.21      | 127.08   |
| 49  | S2    | 1639 | G7M  | O6-C6-C5 | -3.10 | 121.07      | 128.06   |
| 49  | S2    | 1639 | G7M  | N9-C4-N3 | 3.10  | 132.16      | 125.94   |
| 49  | S2    | 601  | OMG  | N9-C4-N3 | 3.09  | 132.14      | 125.94   |
| 8   | L5    | 1871 | A2M  | N3-C4-N9 | 3.08  | 132.16      | 127.08   |
| 8   | L5    | 2787 | A2M  | C5-N7-C8 | 3.08  | 107.89      | 103.51   |
| 8   | L5    | 3718 | A2M  | N3-C4-N9 | 3.08  | 132.15      | 127.08   |
| 8   | L5    | 2363 | A2M  | C5-N7-C8 | 3.08  | 107.88      | 103.51   |
| 8   | L5    | 3729 | PSU  | C6-N1-C2 | -3.07 | 119.54      | 122.68   |
| 8   | L5    | 3758 | PSU  | C6-N1-C2 | -3.07 | 119.54      | 122.68   |
| 8   | L5    | 3825 | A2M  | C5-N7-C8 | 3.07  | 107.87      | 103.51   |
| 49  | S2    | 1850 | MA6  | N9-C8-N7 | -3.07 | 109.72      | 113.91   |
| 8   | L5    | 1782 | PSU  | C6-N1-C2 | -3.07 | 119.55      | 122.68   |
| 8   | L5    | 3724 | A2M  | N3-C4-N9 | 3.07  | 132.13      | 127.08   |
| 8   | L5    | 1524 | A2M  | C2-N3-C4 | 3.06  | 118.97      | 111.75   |
| 8   | L5    | 2401 | A2M  | C5-N7-C8 | 3.05  | 107.85      | 103.51   |
| 49  | S2    | 1031 | A2M  | C5-N7-C8 | 3.05  | 107.84      | 103.51   |
| 8   | L5    | 398  | A2M  | C5-N7-C8 | 3.04  | 107.83      | 103.51   |
| 8   | L5    | 3723 | A2M  | C5-N7-C8 | 3.04  | 107.82      | 103.51   |
| 49  | S2    | 1337 | 4AC  | N4-C4-N3 | 3.04  | 118.95      | 113.85   |
| 49  | S2    | 576  | A2M  | C5-N7-C8 | 3.03  | 107.81      | 103.51   |
| 49  | S2    | 1383 | A2M  | C5-N7-C8 | 3.02  | 107.80      | 103.51   |
| 49  | S2    | 601  | OMG  | C2-N1-C6 | -3.02 | 119.60      | 125.10   |
| 49  | S2    | 601  | OMG  | N9-C8-N7 | -3.01 | 107.71      | 113.39   |
| 8   | L5    | 4228 | OMG  | C2-N1-C6 | -2.99 | 119.64      | 125.10   |
| 49  | S2    | 1851 | MA6  | C5-N7-C8 | 2.99  | 107.75      | 103.51   |
| 49  | S2    | 27   | A2M  | C5-N7-C8 | 2.98  | 107.74      | 103.51   |
| 8   | L5    | 3723 | A2M  | N3-C4-N9 | 2.97  | 131.98      | 127.08   |
| 8   | L5    | 2424 | OMG  | C2-N1-C6 | -2.97 | 119.68      | 125.10   |
| 49  | S2    | 1639 | G7M  | C2-N1-C6 | -2.97 | 119.68      | 125.10   |
| 8   | L5    | 1625 | OMG  | C2-N1-C6 | -2.96 | 119.71      | 125.10   |
| 8   | L5    | 4494 | OMG  | N9-C4-N3 | 2.94  | 131.84      | 125.94   |
| 49  | S2    | 1383 | A2M  | N3-C4-N9 | 2.93  | 131.91      | 127.08   |
| 49  | S2    | 1248 | B8N  | N3-C2-N1 | 2.93  | 120.90      | 116.76   |
| 49  | S2    | 644  | OMG  | C2-N1-C6 | -2.92 | 119.78      | 125.10   |
| 8   | L5    | 1871 | A2M  | C5-N7-C8 | 2.91  | 107.65      | 103.51   |
| 8   | L5    | 1316 | OMG  | C2-N1-C6 | -2.91 | 119.80      | 125.10   |
| 8   | L5    | 4618 | OMG  | C2-N1-C6 | -2.91 | 119.80      | 125.10   |
| 8   | L5    | 4620 | OMU  | O4-C4-C5 | -2.91 | 120.05      | 125.16   |
| 49  | S2    | 1442 | OMU  | O4-C4-C5 | -2.90 | 120.05      | 125.16   |
| 8   | L5    | 4353 | PSU  | C6-N1-C2 | -2.90 | 119.72      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 10  | L8    | 75   | OMG  | C2-N1-C6   | -2.89 | 119.82      | 125.10   |
| 8   | L5    | 2876 | OMG  | C2-N1-C6   | -2.89 | 119.83      | 125.10   |
| 49  | S2    | 428  | OMU  | O4-C4-C5   | -2.89 | 120.08      | 125.16   |
| 8   | L5    | 1522 | OMG  | C2-N1-C6   | -2.89 | 119.83      | 125.10   |
| 8   | L5    | 2424 | OMG  | N9-C4-N3   | 2.87  | 131.70      | 125.94   |
| 8   | L5    | 2876 | OMG  | N9-C4-N3   | 2.87  | 131.70      | 125.94   |
| 49  | S2    | 27   | A2M  | N3-C4-N9   | 2.86  | 131.80      | 127.08   |
| 8   | L5    | 4494 | OMG  | C2-N1-C6   | -2.86 | 119.88      | 125.10   |
| 49  | S2    | 1288 | OMU  | O4-C4-C5   | -2.86 | 120.13      | 125.16   |
| 49  | S2    | 644  | OMG  | N9-C4-N3   | 2.86  | 131.69      | 125.94   |
| 49  | S2    | 683  | OMG  | C2-N1-C6   | -2.86 | 119.89      | 125.10   |
| 8   | L5    | 4499 | OMG  | C2-N1-C6   | -2.86 | 119.89      | 125.10   |
| 8   | L5    | 3792 | OMG  | N9-C4-N3   | 2.86  | 131.67      | 125.94   |
| 8   | L5    | 3744 | OMG  | C2-N1-C6   | -2.85 | 119.91      | 125.10   |
| 49  | S2    | 668  | A2M  | N3-C4-N9   | 2.85  | 131.77      | 127.08   |
| 8   | L5    | 1316 | OMG  | N9-C4-N3   | 2.84  | 131.65      | 125.94   |
| 8   | L5    | 4499 | OMG  | N9-C4-N3   | 2.84  | 131.65      | 125.94   |
| 49  | S2    | 1832 | 6MZ  | N3-C4-N9   | 2.84  | 131.76      | 127.08   |
| 8   | L5    | 2424 | OMG  | C5-C6-N1   | 2.83  | 120.36      | 113.19   |
| 8   | L5    | 4370 | OMG  | C2-N1-C6   | -2.82 | 119.95      | 125.10   |
| 8   | L5    | 3792 | OMG  | C2-N1-C6   | -2.82 | 119.96      | 125.10   |
| 8   | L5    | 1625 | OMG  | N9-C4-N3   | 2.82  | 131.59      | 125.94   |
| 8   | L5    | 2364 | OMG  | C2-N1-C6   | -2.82 | 119.97      | 125.10   |
| 8   | L5    | 4623 | OMG  | C2-N1-C6   | -2.81 | 119.98      | 125.10   |
| 8   | L5    | 3760 | A2M  | C5-N7-C8   | 2.80  | 107.49      | 103.51   |
| 8   | L5    | 4637 | OMG  | C5-C6-N1   | 2.77  | 120.24      | 113.19   |
| 8   | L5    | 1871 | A2M  | C2'-C1'-N9 | -2.77 | 108.87      | 113.53   |
| 8   | L5    | 3925 | OMU  | O4-C4-C5   | -2.76 | 120.30      | 125.16   |
| 49  | S2    | 1832 | 6MZ  | C4-C5-N7   | -2.75 | 107.27      | 110.62   |
| 49  | S2    | 644  | OMG  | C5-C6-N1   | 2.74  | 120.16      | 113.19   |
| 8   | L5    | 4370 | OMG  | N9-C4-N3   | 2.73  | 131.43      | 125.94   |
| 49  | S2    | 1328 | OMG  | C2-N1-C6   | -2.73 | 120.12      | 125.10   |
| 8   | L5    | 4494 | OMG  | C5-C6-N1   | 2.72  | 120.10      | 113.19   |
| 10  | L8    | 14   | OMU  | O4-C4-C5   | -2.72 | 120.38      | 125.16   |
| 10  | L8    | 75   | OMG  | N9-C4-N3   | 2.70  | 131.37      | 125.94   |
| 8   | L5    | 1625 | OMG  | C5-C6-N1   | 2.70  | 120.04      | 113.19   |
| 8   | L5    | 3627 | OMG  | C2-N1-C6   | -2.70 | 120.18      | 125.10   |
| 8   | L5    | 2876 | OMG  | C5-C6-N1   | 2.69  | 120.02      | 113.19   |
| 49  | S2    | 601  | OMG  | C5-C6-N1   | 2.68  | 120.00      | 113.19   |
| 49  | S2    | 1639 | G7M  | CN7-N7-C5  | 2.68  | 130.10      | 126.77   |
| 8   | L5    | 1522 | OMG  | C5-C6-N1   | 2.67  | 119.98      | 113.19   |
| 8   | L5    | 3729 | PSU  | C6-C5-C4   | 2.67  | 120.06      | 118.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8   | L5    | 4499 | OMG  | C5-C6-N1   | 2.67  | 119.96      | 113.19   |
| 8   | L5    | 3792 | OMG  | C5-C6-N1   | 2.67  | 119.96      | 113.19   |
| 8   | L5    | 4370 | OMG  | C5-C6-N1   | 2.66  | 119.95      | 113.19   |
| 8   | L5    | 3760 | A2M  | N3-C4-N9   | 2.66  | 131.46      | 127.08   |
| 49  | S2    | 1337 | 4AC  | C5-C4-N3   | -2.65 | 118.33      | 122.59   |
| 49  | S2    | 683  | OMG  | C5-C6-N1   | 2.64  | 119.90      | 113.19   |
| 8   | L5    | 4228 | OMG  | C5-C6-N1   | 2.64  | 119.90      | 113.19   |
| 8   | L5    | 4353 | PSU  | C6-C5-C4   | 2.64  | 120.04      | 118.20   |
| 8   | L5    | 1316 | OMG  | C5-C6-N1   | 2.63  | 119.88      | 113.19   |
| 8   | L5    | 4618 | OMG  | C5-C6-N1   | 2.63  | 119.87      | 113.19   |
| 10  | L8    | 75   | OMG  | C5-C6-N1   | 2.63  | 119.87      | 113.19   |
| 8   | L5    | 3744 | OMG  | C5-C6-N1   | 2.62  | 119.86      | 113.19   |
| 8   | L5    | 4623 | OMG  | C5-C6-N1   | 2.62  | 119.84      | 113.19   |
| 49  | S2    | 1326 | UY1  | C6-C5-C4   | 2.61  | 120.03      | 118.20   |
| 49  | S2    | 1851 | MA6  | C4-N9-C8   | 2.61  | 108.56      | 105.73   |
| 49  | S2    | 1328 | OMG  | N9-C4-N3   | 2.61  | 131.17      | 125.94   |
| 49  | S2    | 1328 | OMG  | C5-C6-N1   | 2.60  | 119.79      | 113.19   |
| 8   | L5    | 4637 | OMG  | O6-C6-C5   | -2.58 | 119.77      | 126.60   |
| 8   | L5    | 3627 | OMG  | C5-C6-N1   | 2.57  | 119.71      | 113.19   |
| 8   | L5    | 2424 | OMG  | O6-C6-C5   | -2.56 | 119.81      | 126.60   |
| 8   | L5    | 2364 | OMG  | C5-C6-N1   | 2.56  | 119.68      | 113.19   |
| 8   | L5    | 1522 | OMG  | N9-C4-N3   | 2.53  | 131.02      | 125.94   |
| 8   | L5    | 4494 | OMG  | O6-C6-C5   | -2.53 | 119.89      | 126.60   |
| 8   | L5    | 2364 | OMG  | N9-C4-N3   | 2.53  | 131.02      | 125.94   |
| 8   | L5    | 1524 | A2M  | C5-N7-C8   | 2.52  | 107.09      | 103.51   |
| 8   | L5    | 3718 | A2M  | C2'-C1'-N9 | -2.51 | 109.30      | 113.53   |
| 49  | S2    | 683  | OMG  | C8-N7-C5   | 2.51  | 108.78      | 104.24   |
| 10  | L8    | 75   | OMG  | O6-C6-C5   | -2.50 | 119.96      | 126.60   |
| 8   | L5    | 3729 | PSU  | O2-C2-N1   | -2.50 | 120.04      | 122.79   |
| 8   | L5    | 1316 | OMG  | C8-N7-C5   | 2.50  | 108.76      | 104.24   |
| 8   | L5    | 2876 | OMG  | O6-C6-C5   | -2.49 | 119.99      | 126.60   |
| 8   | L5    | 4228 | OMG  | N2-C2-N1   | 2.49  | 122.01      | 116.71   |
| 49  | S2    | 1326 | UY1  | C6-N1-C2   | -2.48 | 120.15      | 122.68   |
| 8   | L5    | 1625 | OMG  | O6-C6-C5   | -2.48 | 120.02      | 126.60   |
| 8   | L5    | 4618 | OMG  | O6-C6-C5   | -2.47 | 120.04      | 126.60   |
| 8   | L5    | 4228 | OMG  | O6-C6-C5   | -2.47 | 120.04      | 126.60   |
| 8   | L5    | 4618 | OMG  | N9-C4-N3   | 2.47  | 130.89      | 125.94   |
| 8   | L5    | 2364 | OMG  | O6-C6-C5   | -2.46 | 120.07      | 126.60   |
| 8   | L5    | 3744 | OMG  | N9-C4-N3   | 2.46  | 130.88      | 125.94   |
| 8   | L5    | 4499 | OMG  | O6-C6-C5   | -2.46 | 120.09      | 126.60   |
| 49  | S2    | 644  | OMG  | C8-N7-C5   | 2.45  | 108.68      | 104.24   |
| 49  | S2    | 1842 | 4AC  | N4-C4-N3   | 2.45  | 117.96      | 113.85   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8   | L5    | 3744 | OMG  | O6-C6-C5   | -2.45 | 120.11      | 126.60   |
| 49  | S2    | 683  | OMG  | O6-C6-C5   | -2.44 | 120.12      | 126.60   |
| 8   | L5    | 1683 | PSU  | O2-C2-N1   | -2.43 | 120.12      | 122.79   |
| 8   | L5    | 1522 | OMG  | O6-C6-C5   | -2.42 | 120.19      | 126.60   |
| 49  | S2    | 1248 | B8N  | O2-C2-N1   | -2.42 | 116.21      | 121.23   |
| 49  | S2    | 683  | OMG  | N9-C4-N3   | 2.41  | 130.78      | 125.94   |
| 8   | L5    | 4228 | OMG  | C8-N7-C5   | 2.41  | 108.59      | 104.24   |
| 8   | L5    | 3627 | OMG  | O6-C6-C5   | -2.40 | 120.23      | 126.60   |
| 8   | L5    | 1782 | PSU  | O2-C2-N1   | -2.40 | 120.15      | 122.79   |
| 49  | S2    | 1248 | B8N  | C32-C31-N3 | 2.40  | 116.49      | 112.00   |
| 8   | L5    | 3758 | PSU  | O2-C2-N1   | -2.40 | 120.15      | 122.79   |
| 8   | L5    | 1316 | OMG  | O6-C6-C5   | -2.39 | 120.25      | 126.60   |
| 49  | S2    | 644  | OMG  | O6-C6-C5   | -2.39 | 120.26      | 126.60   |
| 8   | L5    | 3792 | OMG  | O6-C6-C5   | -2.39 | 120.27      | 126.60   |
| 49  | S2    | 1678 | A2M  | C4-C5-N7   | -2.38 | 107.72      | 110.62   |
| 8   | L5    | 4623 | OMG  | N9-C4-N3   | 2.37  | 130.70      | 125.94   |
| 49  | S2    | 576  | A2M  | C6-C5-C4   | 2.37  | 120.36      | 117.18   |
| 8   | L5    | 3744 | OMG  | C8-N7-C5   | 2.36  | 108.52      | 104.24   |
| 49  | S2    | 1678 | A2M  | C2'-C1'-N9 | 2.35  | 117.48      | 113.53   |
| 8   | L5    | 4370 | OMG  | O6-C6-C5   | -2.35 | 120.38      | 126.60   |
| 8   | L5    | 3718 | A2M  | C6-C5-C4   | 2.34  | 120.33      | 117.18   |
| 8   | L5    | 2364 | OMG  | C8-N7-C5   | 2.34  | 108.47      | 104.24   |
| 10  | L8    | 55   | PSU  | O2-C2-N1   | -2.33 | 120.22      | 122.79   |
| 8   | L5    | 4590 | A2M  | C4-C5-N7   | -2.32 | 107.79      | 110.62   |
| 8   | L5    | 2876 | OMG  | C8-N7-C5   | 2.32  | 108.44      | 104.24   |
| 49  | S2    | 1328 | OMG  | O6-C6-C5   | -2.32 | 120.46      | 126.60   |
| 49  | S2    | 668  | A2M  | C4-N9-C8   | 2.31  | 108.23      | 105.73   |
| 8   | L5    | 4623 | OMG  | C8-N7-C5   | 2.31  | 108.42      | 104.24   |
| 49  | S2    | 1328 | OMG  | C8-N7-C5   | 2.31  | 108.42      | 104.24   |
| 49  | S2    | 1678 | A2M  | C6-C5-C4   | 2.31  | 120.29      | 117.18   |
| 8   | L5    | 3627 | OMG  | C8-N7-C5   | 2.30  | 108.41      | 104.24   |
| 8   | L5    | 4623 | OMG  | O6-C6-C5   | -2.30 | 120.49      | 126.60   |
| 8   | L5    | 3792 | OMG  | C8-N7-C5   | 2.30  | 108.41      | 104.24   |
| 8   | L5    | 3724 | A2M  | C4-C5-N7   | -2.30 | 107.81      | 110.62   |
| 8   | L5    | 3627 | OMG  | N2-C2-N1   | 2.30  | 121.61      | 116.71   |
| 8   | L5    | 4353 | PSU  | O2-C2-N1   | -2.30 | 120.26      | 122.79   |
| 8   | L5    | 3734 | PSU  | O2-C2-N1   | -2.28 | 120.28      | 122.79   |
| 49  | S2    | 1832 | 6MZ  | C4-N9-C8   | 2.28  | 108.20      | 105.73   |
| 8   | L5    | 4620 | OMU  | O2-C2-N1   | -2.28 | 119.76      | 122.79   |
| 8   | L5    | 3718 | A2M  | C4-C5-N7   | -2.28 | 107.84      | 110.62   |
| 8   | L5    | 1522 | OMG  | C8-N7-C5   | 2.28  | 108.36      | 104.24   |
| 49  | S2    | 601  | OMG  | O6-C6-C5   | -2.27 | 120.58      | 126.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 49  | S2    | 1383 | A2M  | C4-C5-N7    | -2.27 | 107.85      | 110.62   |
| 49  | S2    | 159  | A2M  | C6-C5-C4    | 2.27  | 120.23      | 117.18   |
| 8   | L5    | 4370 | OMG  | C8-N7-C5    | 2.27  | 108.34      | 104.24   |
| 8   | L5    | 3627 | OMG  | N9-C4-N3    | 2.26  | 130.49      | 125.94   |
| 8   | L5    | 3734 | PSU  | C6-C5-C4    | 2.26  | 119.78      | 118.20   |
| 8   | L5    | 4637 | OMG  | C8-N7-C5    | 2.26  | 108.33      | 104.24   |
| 49  | S2    | 1326 | UY1  | O2-C2-N1    | -2.26 | 120.30      | 122.79   |
| 49  | S2    | 576  | A2M  | C2'-C1'-N9  | -2.26 | 109.73      | 113.53   |
| 8   | L5    | 3744 | OMG  | N2-C2-N1    | 2.25  | 121.51      | 116.71   |
| 8   | L5    | 4494 | OMG  | C8-N7-C5    | 2.25  | 108.32      | 104.24   |
| 8   | L5    | 2401 | A2M  | C6-C5-C4    | 2.25  | 120.21      | 117.18   |
| 49  | S2    | 668  | A2M  | C4-C5-N7    | -2.25 | 107.88      | 110.62   |
| 49  | S2    | 1850 | MA6  | C5-N7-C8    | 2.23  | 106.68      | 103.51   |
| 8   | L5    | 1625 | OMG  | C8-N7-C5    | 2.22  | 108.26      | 104.24   |
| 49  | S2    | 1842 | 4AC  | C6-C5-C4    | 2.22  | 119.67      | 116.96   |
| 49  | S2    | 159  | A2M  | C4-C5-N7    | -2.21 | 107.92      | 110.62   |
| 8   | L5    | 3825 | A2M  | C4-C5-N7    | -2.21 | 107.93      | 110.62   |
| 10  | L8    | 75   | OMG  | C8-N7-C5    | 2.21  | 108.23      | 104.24   |
| 8   | L5    | 1524 | A2M  | N3-C4-N9    | 2.19  | 130.69      | 127.08   |
| 49  | S2    | 1842 | 4AC  | C5-C4-N3    | -2.19 | 119.07      | 122.59   |
| 49  | S2    | 1850 | MA6  | C6-C5-N7    | -2.18 | 129.62      | 133.28   |
| 8   | L5    | 2815 | A2M  | C4-C5-N7    | -2.18 | 107.96      | 110.62   |
| 8   | L5    | 2363 | A2M  | C4-C5-N7    | -2.18 | 107.97      | 110.62   |
| 8   | L5    | 1683 | PSU  | C6-C5-C4    | 2.17  | 119.72      | 118.20   |
| 8   | L5    | 2815 | A2M  | C6-C5-C4    | 2.16  | 120.08      | 117.18   |
| 49  | S2    | 1248 | B8N  | O36-C34-C33 | 2.16  | 120.72      | 113.38   |
| 8   | L5    | 3825 | A2M  | C6-C5-C4    | 2.15  | 120.08      | 117.18   |
| 49  | S2    | 1639 | G7M  | CN7-N7-C8   | -2.15 | 121.52      | 124.84   |
| 8   | L5    | 2364 | OMG  | N2-C2-N1    | 2.15  | 121.28      | 116.71   |
| 49  | S2    | 27   | A2M  | C4-C5-N7    | -2.14 | 108.01      | 110.62   |
| 49  | S2    | 1337 | 4AC  | C6-C5-C4    | 2.14  | 119.58      | 116.96   |
| 8   | L5    | 2787 | A2M  | C4-C5-N7    | -2.13 | 108.02      | 110.62   |
| 49  | S2    | 1383 | A2M  | C5-C4-N9    | 2.13  | 108.26      | 105.78   |
| 49  | S2    | 1248 | B8N  | C31-N3-C4   | -2.13 | 114.17      | 117.31   |
| 49  | S2    | 668  | A2M  | C3'-C2'-C1' | 2.13  | 106.89      | 102.89   |
| 8   | L5    | 2787 | A2M  | C6-C5-C4    | 2.12  | 120.04      | 117.18   |
| 8   | L5    | 4499 | OMG  | C8-N7-C5    | 2.12  | 108.08      | 104.24   |
| 8   | L5    | 4618 | OMG  | C8-N7-C5    | 2.12  | 108.07      | 104.24   |
| 49  | S2    | 1031 | A2M  | C4-C5-N7    | -2.11 | 108.04      | 110.62   |
| 8   | L5    | 3723 | A2M  | C4-C5-N7    | -2.11 | 108.04      | 110.62   |
| 10  | L8    | 14   | OMU  | C6-N1-C2    | -2.11 | 118.29      | 120.99   |
| 49  | S2    | 1248 | B8N  | O36-C34-O35 | -2.11 | 119.30      | 124.09   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 49  | S2    | 1288 | OMU  | O2-C2-N1   | -2.10 | 119.99      | 122.79   |
| 49  | S2    | 1639 | G7M  | N9-C8-N7   | -2.10 | 107.01      | 112.21   |
| 8   | L5    | 3723 | A2M  | C6-C5-C4   | 2.10  | 120.01      | 117.18   |
| 10  | L8    | 14   | OMU  | O2-C2-N3   | -2.10 | 117.59      | 121.50   |
| 8   | L5    | 1326 | A2M  | C4-C5-N7   | -2.10 | 108.06      | 110.62   |
| 49  | S2    | 1031 | A2M  | C6-C5-C4   | 2.09  | 120.00      | 117.18   |
| 49  | S2    | 1442 | OMU  | O2-C2-N1   | -2.09 | 120.00      | 122.79   |
| 8   | L5    | 1326 | A2M  | C4-N9-C8   | 2.09  | 108.00      | 105.73   |
| 8   | L5    | 398  | A2M  | C6-C5-C4   | 2.09  | 120.00      | 117.18   |
| 49  | S2    | 1337 | 4AC  | CM7-C7-N4  | 2.09  | 118.91      | 115.29   |
| 8   | L5    | 3724 | A2M  | C6-C5-C4   | 2.09  | 119.99      | 117.18   |
| 8   | L5    | 3718 | A2M  | C5-C4-N9   | 2.08  | 108.21      | 105.78   |
| 8   | L5    | 4590 | A2M  | C6-C5-C4   | 2.08  | 119.97      | 117.18   |
| 8   | L5    | 2401 | A2M  | C4-C5-N7   | -2.07 | 108.10      | 110.62   |
| 8   | L5    | 4228 | OMG  | C4-C5-N7   | -2.06 | 107.45      | 110.72   |
| 8   | L5    | 4228 | OMG  | N9-C4-N3   | 2.06  | 130.08      | 125.94   |
| 8   | L5    | 4618 | OMG  | N2-C2-N1   | 2.06  | 121.10      | 116.71   |
| 8   | L5    | 1524 | A2M  | C5-C4-N9   | 2.06  | 108.17      | 105.78   |
| 8   | L5    | 398  | A2M  | C4-C5-N7   | -2.05 | 108.12      | 110.62   |
| 49  | S2    | 428  | OMU  | O2-C2-N1   | -2.05 | 120.07      | 122.79   |
| 8   | L5    | 2424 | OMG  | C8-N7-C5   | 2.04  | 107.94      | 104.24   |
| 8   | L5    | 1326 | A2M  | C6-C5-C4   | 2.04  | 119.93      | 117.18   |
| 8   | L5    | 3724 | A2M  | C4-N9-C8   | 2.04  | 107.94      | 105.73   |
| 8   | L5    | 4623 | OMG  | N2-C2-N1   | 2.04  | 121.05      | 116.71   |
| 49  | S2    | 683  | OMG  | C4-C5-N7   | -2.04 | 107.50      | 110.72   |
| 49  | S2    | 1842 | 4AC  | CM7-C7-N4  | 2.04  | 118.81      | 115.29   |
| 8   | L5    | 2787 | A2M  | C5-C4-N9   | 2.03  | 108.15      | 105.78   |
| 8   | L5    | 1871 | A2M  | C6-C5-C4   | 2.03  | 119.92      | 117.18   |
| 8   | L5    | 2363 | A2M  | C6-C5-C4   | 2.03  | 119.91      | 117.18   |
| 49  | S2    | 683  | OMG  | C2'-C1'-N9 | -2.03 | 110.29      | 114.22   |
| 8   | L5    | 3825 | A2M  | C5-C4-N9   | 2.02  | 108.13      | 105.78   |
| 49  | S2    | 27   | A2M  | C5-C4-N9   | 2.01  | 108.12      | 105.78   |
| 49  | S2    | 576  | A2M  | C4-C5-N7   | -2.00 | 108.18      | 110.62   |
| 8   | L5    | 3925 | OMU  | O2-C2-N1   | -2.00 | 120.12      | 122.79   |
| 8   | L5    | 1522 | OMG  | N2-C2-N1   | 2.00  | 120.98      | 116.71   |
| 8   | L5    | 4590 | A2M  | C4-N9-C8   | 2.00  | 107.90      | 105.73   |
| 49  | S2    | 576  | A2M  | C4-N9-C8   | 2.00  | 107.90      | 105.73   |

There are no chirality outliers.

All (104) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | L8    | 14   | OMU  | O4'-C1'-N1-C2   |
| 10  | L8    | 14   | OMU  | O4'-C1'-N1-C6   |
| 10  | L8    | 14   | OMU  | C1'-C2'-O2'-CM2 |
| 10  | L8    | 55   | PSU  | C3'-C4'-C5'-O5' |
| 10  | L8    | 55   | PSU  | O4'-C4'-C5'-O5' |
| 8   | L5    | 1316 | OMG  | C1'-C2'-O2'-CM2 |
| 8   | L5    | 1326 | A2M  | C1'-C2'-O2'-CM' |
| 8   | L5    | 1625 | OMG  | O4'-C4'-C5'-O5' |
| 8   | L5    | 2351 | OMC  | C1'-C2'-O2'-CM2 |
| 8   | L5    | 2401 | A2M  | C3'-C4'-C5'-O5' |
| 8   | L5    | 2424 | OMG  | O4'-C4'-C5'-O5' |
| 8   | L5    | 2424 | OMG  | C3'-C4'-C5'-O5' |
| 8   | L5    | 2861 | OMC  | C1'-C2'-O2'-CM2 |
| 8   | L5    | 2876 | OMG  | O4'-C4'-C5'-O5' |
| 8   | L5    | 3701 | OMC  | C2'-C1'-N1-C2   |
| 8   | L5    | 3701 | OMC  | C2'-C1'-N1-C6   |
| 8   | L5    | 3723 | A2M  | C1'-C2'-O2'-CM' |
| 8   | L5    | 3724 | A2M  | C1'-C2'-O2'-CM' |
| 8   | L5    | 3841 | OMC  | C1'-C2'-O2'-CM2 |
| 8   | L5    | 3925 | OMU  | C1'-C2'-O2'-CM2 |
| 8   | L5    | 4590 | A2M  | C4'-C5'-O5'-P   |
| 8   | L5    | 4620 | OMU  | O4'-C4'-C5'-O5' |
| 8   | L5    | 4623 | OMG  | C3'-C4'-C5'-O5' |
| 49  | S2    | 27   | A2M  | C1'-C2'-O2'-CM' |
| 49  | S2    | 159  | A2M  | C3'-C4'-C5'-O5' |
| 49  | S2    | 601  | OMG  | C1'-C2'-O2'-CM2 |
| 49  | S2    | 601  | OMG  | O4'-C1'-N9-C4   |
| 49  | S2    | 644  | OMG  | O4'-C4'-C5'-O5' |
| 49  | S2    | 644  | OMG  | C3'-C4'-C5'-O5' |
| 49  | S2    | 644  | OMG  | C1'-C2'-O2'-CM2 |
| 49  | S2    | 668  | A2M  | O4'-C4'-C5'-O5' |
| 49  | S2    | 683  | OMG  | O4'-C4'-C5'-O5' |
| 49  | S2    | 1248 | B8N  | C2'-C1'-C5-C4   |
| 49  | S2    | 1248 | B8N  | C32-C31-N3-C2   |
| 49  | S2    | 1248 | B8N  | C32-C31-N3-C4   |
| 49  | S2    | 1288 | OMU  | O4'-C4'-C5'-O5' |
| 49  | S2    | 1326 | UY1  | C2'-C1'-C5-C6   |
| 49  | S2    | 1383 | A2M  | C1'-C2'-O2'-CM' |
| 49  | S2    | 1442 | OMU  | C1'-C2'-O2'-CM2 |
| 49  | S2    | 1678 | A2M  | C1'-C2'-O2'-CM' |
| 49  | S2    | 1832 | 6MZ  | N1-C6-N6-C9     |
| 49  | S2    | 1832 | 6MZ  | O4'-C4'-C5'-O5' |
| 49  | S2    | 1851 | MA6  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 49  | S2    | 601  | OMG  | O4'-C1'-N9-C8   |
| 10  | L8    | 14   | OMU  | C3'-C4'-C5'-O5' |
| 8   | L5    | 398  | A2M  | C3'-C4'-C5'-O5' |
| 8   | L5    | 1625 | OMG  | C3'-C4'-C5'-O5' |
| 8   | L5    | 2351 | OMC  | O4'-C4'-C5'-O5' |
| 8   | L5    | 2876 | OMG  | C3'-C4'-C5'-O5' |
| 8   | L5    | 3627 | OMG  | O4'-C4'-C5'-O5' |
| 8   | L5    | 4620 | OMU  | C3'-C4'-C5'-O5' |
| 8   | L5    | 4623 | OMG  | O4'-C4'-C5'-O5' |
| 49  | S2    | 159  | A2M  | O4'-C4'-C5'-O5' |
| 49  | S2    | 601  | OMG  | O4'-C4'-C5'-O5' |
| 49  | S2    | 601  | OMG  | C3'-C4'-C5'-O5' |
| 49  | S2    | 668  | A2M  | C3'-C4'-C5'-O5' |
| 49  | S2    | 683  | OMG  | C3'-C4'-C5'-O5' |
| 49  | S2    | 1288 | OMU  | C3'-C4'-C5'-O5' |
| 49  | S2    | 1832 | 6MZ  | C3'-C4'-C5'-O5' |
| 49  | S2    | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 10  | L8    | 14   | OMU  | O4'-C4'-C5'-O5' |
| 8   | L5    | 2364 | OMG  | O4'-C4'-C5'-O5' |
| 8   | L5    | 2401 | A2M  | O4'-C4'-C5'-O5' |
| 8   | L5    | 2422 | OMC  | C3'-C4'-C5'-O5' |
| 8   | L5    | 3627 | OMG  | C3'-C4'-C5'-O5' |
| 8   | L5    | 3729 | PSU  | O4'-C4'-C5'-O5' |
| 49  | S2    | 428  | OMU  | C3'-C4'-C5'-O5' |
| 49  | S2    | 428  | OMU  | O4'-C4'-C5'-O5' |
| 8   | L5    | 398  | A2M  | O4'-C4'-C5'-O5' |
| 8   | L5    | 2422 | OMC  | O4'-C4'-C5'-O5' |
| 8   | L5    | 3734 | PSU  | O4'-C4'-C5'-O5' |
| 49  | S2    | 1703 | OMC  | O4'-C4'-C5'-O5' |
| 49  | S2    | 1850 | MA6  | C5-C6-N6-C10    |
| 49  | S2    | 1851 | MA6  | C5-C6-N6-C10    |
| 8   | L5    | 2787 | A2M  | C2'-C1'-N9-C8   |
| 49  | S2    | 428  | OMU  | C2'-C1'-N1-C6   |
| 8   | L5    | 3729 | PSU  | C3'-C4'-C5'-O5' |
| 8   | L5    | 2804 | OMC  | C1'-C2'-O2'-CM2 |
| 49  | S2    | 644  | OMG  | C4'-C5'-O5'-P   |
| 8   | L5    | 2351 | OMC  | C3'-C4'-C5'-O5' |
| 49  | S2    | 576  | A2M  | C3'-C4'-C5'-O5' |
| 8   | L5    | 1524 | A2M  | C3'-C2'-O2'-CM' |
| 49  | S2    | 428  | OMU  | O4'-C1'-N1-C6   |
| 8   | L5    | 2364 | OMG  | C3'-C4'-C5'-O5' |
| 49  | S2    | 1248 | B8N  | N3-C31-C32-C33  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 49  | S2    | 576  | A2M  | C4'-C5'-O5'-P   |
| 8   | L5    | 3701 | OMC  | O4'-C1'-N1-C6   |
| 8   | L5    | 2787 | A2M  | C2'-C1'-N9-C4   |
| 49  | S2    | 428  | OMU  | O4'-C1'-N1-C2   |
| 8   | L5    | 3734 | PSU  | C3'-C4'-C5'-O5' |
| 49  | S2    | 1248 | B8N  | O4'-C4'-C5'-O5' |
| 49  | S2    | 1248 | B8N  | O4'-C1'-C5-C4   |
| 8   | L5    | 3701 | OMC  | O4'-C1'-N1-C2   |
| 49  | S2    | 428  | OMU  | C2'-C1'-N1-C2   |
| 8   | L5    | 4590 | A2M  | C3'-C4'-C5'-O5' |
| 8   | L5    | 2787 | A2M  | O4'-C1'-N9-C8   |
| 8   | L5    | 2351 | OMC  | C2'-C1'-N1-C2   |
| 49  | S2    | 1703 | OMC  | C3'-C4'-C5'-O5' |
| 49  | S2    | 1639 | G7M  | C3'-C4'-C5'-O5' |
| 49  | S2    | 668  | A2M  | C2'-C1'-N9-C8   |
| 49  | S2    | 1326 | UY1  | O4'-C1'-C5-C6   |
| 8   | L5    | 3701 | OMC  | C4'-C5'-O5'-P   |
| 49  | S2    | 1248 | B8N  | C3'-C4'-C5'-O5' |
| 8   | L5    | 2351 | OMC  | C4'-C5'-O5'-P   |

There are no ring outliers.

42 monomers are involved in 75 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 49  | S2    | 27   | A2M  | 2       | 0            |
| 49  | S2    | 644  | OMG  | 2       | 0            |
| 10  | L8    | 14   | OMU  | 4       | 0            |
| 8   | L5    | 3724 | A2M  | 1       | 0            |
| 8   | L5    | 4228 | OMG  | 1       | 0            |
| 49  | S2    | 174  | OMC  | 1       | 0            |
| 10  | L8    | 55   | PSU  | 3       | 0            |
| 8   | L5    | 3744 | OMG  | 1       | 0            |
| 8   | L5    | 4623 | OMG  | 1       | 0            |
| 8   | L5    | 1340 | OMC  | 2       | 0            |
| 8   | L5    | 3723 | A2M  | 2       | 0            |
| 8   | L5    | 3760 | A2M  | 1       | 0            |
| 8   | L5    | 1871 | A2M  | 1       | 0            |
| 49  | S2    | 1678 | A2M  | 2       | 0            |
| 49  | S2    | 1832 | 6MZ  | 1       | 0            |
| 49  | S2    | 1288 | OMU  | 1       | 0            |
| 8   | L5    | 1326 | A2M  | 3       | 0            |
| 8   | L5    | 1625 | OMG  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 49  | S2    | 1383 | A2M  | 1       | 0            |
| 49  | S2    | 1442 | OMU  | 1       | 0            |
| 8   | L5    | 398  | A2M  | 1       | 0            |
| 8   | L5    | 3627 | OMG  | 1       | 0            |
| 8   | L5    | 2861 | OMC  | 1       | 0            |
| 8   | L5    | 3701 | OMC  | 1       | 0            |
| 8   | L5    | 4536 | OMC  | 3       | 0            |
| 8   | L5    | 2424 | OMG  | 1       | 0            |
| 49  | S2    | 1842 | 4AC  | 1       | 0            |
| 8   | L5    | 3718 | A2M  | 3       | 0            |
| 8   | L5    | 1524 | A2M  | 1       | 0            |
| 49  | S2    | 576  | A2M  | 3       | 0            |
| 49  | S2    | 428  | OMU  | 1       | 0            |
| 49  | S2    | 1337 | 4AC  | 5       | 0            |
| 8   | L5    | 1316 | OMG  | 1       | 0            |
| 49  | S2    | 1850 | MA6  | 6       | 0            |
| 8   | L5    | 3841 | OMC  | 1       | 0            |
| 8   | L5    | 2876 | OMG  | 2       | 0            |
| 8   | L5    | 2804 | OMC  | 3       | 0            |
| 49  | S2    | 601  | OMG  | 2       | 0            |
| 8   | L5    | 3925 | OMU  | 2       | 0            |
| 8   | L5    | 2815 | A2M  | 1       | 0            |
| 8   | L5    | 2363 | A2M  | 1       | 0            |
| 10  | L8    | 75   | OMG  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 340 ligands modelled in this entry, 337 are monoatomic - leaving 3 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 |
| 87  | PUT  | L5    | 5287 | -    | 5,5,5        | 0.23 | 0        | 4,4,4       | 0.24 | 0        |
| 86  | SPD  | L5    | 5286 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.39 | 0        |
| 89  | HYG  | S2    | 1901 | 84   | 35,39,39     | 2.58 | 10 (28%) | 43,60,60    | 1.18 | 4 (9%)   |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 87  | PUT  | L5    | 5287 | -    | -       | 0/3/3/3    | -       |
| 86  | SPD  | L5    | 5286 | -    | -       | 0/7/7/7    | -       |
| 89  | HYG  | S2    | 1901 | 84   | -       | 3/12/87/87 | 0/4/4/4 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 89  | S2    | 1901 | HYG  | O29-C12 | 8.46  | 1.57        | 1.43     |
| 89  | S2    | 1901 | HYG  | O22-C17 | 6.40  | 1.53        | 1.43     |
| 89  | S2    | 1901 | HYG  | O14-C13 | 5.92  | 1.56        | 1.41     |
| 89  | S2    | 1901 | HYG  | C17-C12 | -3.71 | 1.45        | 1.53     |
| 89  | S2    | 1901 | HYG  | C16-C15 | 3.40  | 1.60        | 1.53     |
| 89  | S2    | 1901 | HYG  | C25-C24 | -3.00 | 1.48        | 1.53     |
| 89  | S2    | 1901 | HYG  | O28-C23 | 2.86  | 1.43        | 1.40     |
| 89  | S2    | 1901 | HYG  | C16-C17 | -2.69 | 1.45        | 1.52     |
| 89  | S2    | 1901 | HYG  | O18-C13 | -2.34 | 1.35        | 1.41     |
| 89  | S2    | 1901 | HYG  | C13-C12 | -2.03 | 1.47        | 1.52     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 89  | S2    | 1901 | HYG  | O14-C13-C12 | -3.51 | 102.55      | 109.51   |
| 89  | S2    | 1901 | HYG  | O22-C17-C16 | 3.30  | 119.25      | 111.22   |
| 89  | S2    | 1901 | HYG  | O11-C5-C4   | -2.37 | 104.56      | 109.47   |
| 89  | S2    | 1901 | HYG  | C23-O28-C27 | -2.05 | 108.08      | 112.00   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 89  | S2    | 1901 | HYG  | C26-C27-C33-C34 |

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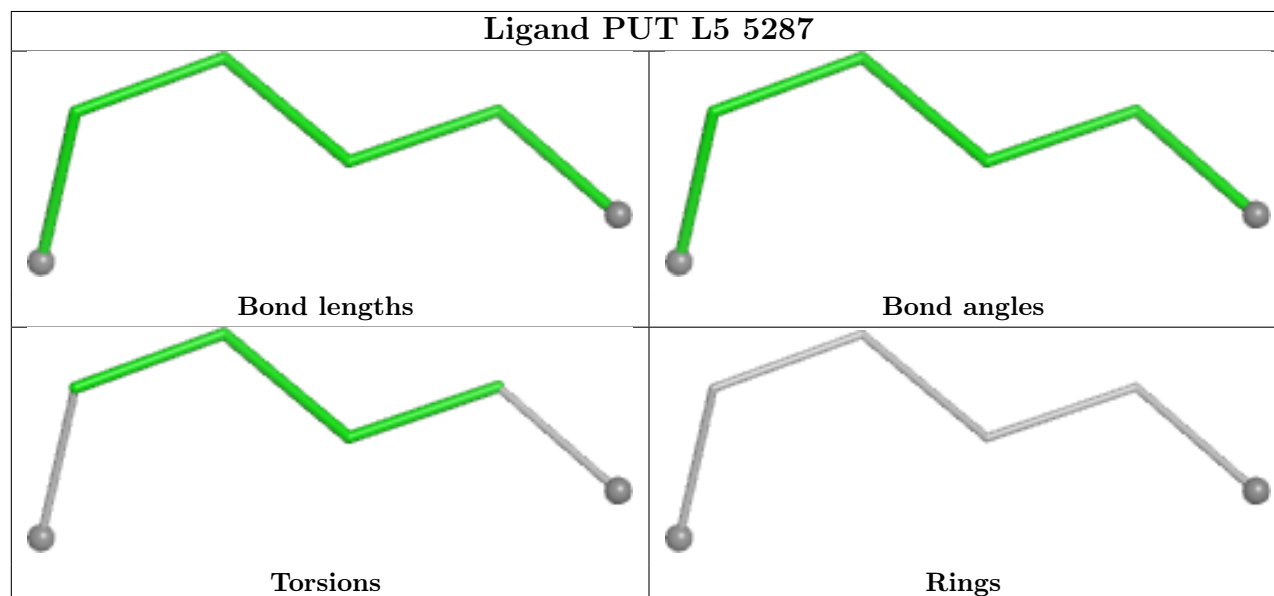
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 89  | S2    | 1901 | HYG  | O28-C27-C33-C34 |
| 89  | S2    | 1901 | HYG  | O14-C13-O18-C6  |

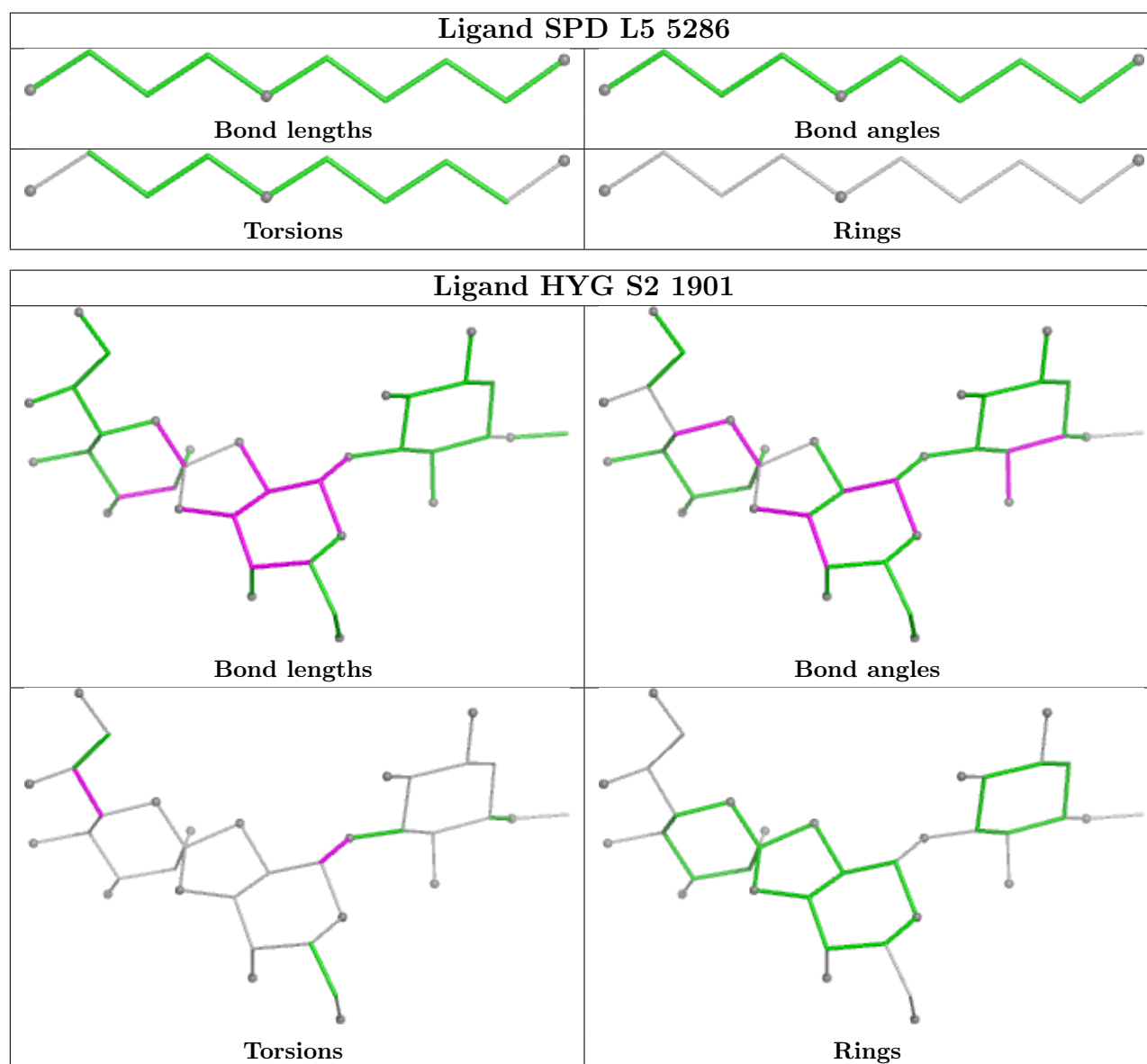
There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 87  | L5    | 5287 | PUT  | 1       | 0            |
| 86  | L5    | 5286 | SPD  | 2       | 0            |

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





## 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 |
|-----|-------|------------------|
| 49  | S2    | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | S2    | 1832:6MZ  | O3'    | 1833:C    | P      | 4.54         |
| 1     | S2    | 1248:B8N  | O3'    | 1249:C    | P      | 3.93         |

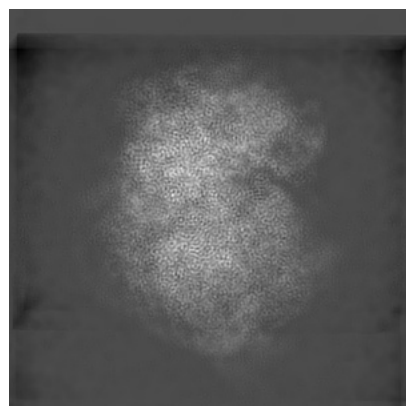
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52565. These allow visual inspection of the internal detail of the map and identification of artifacts.

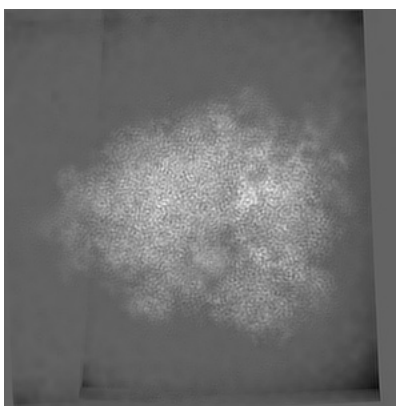
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

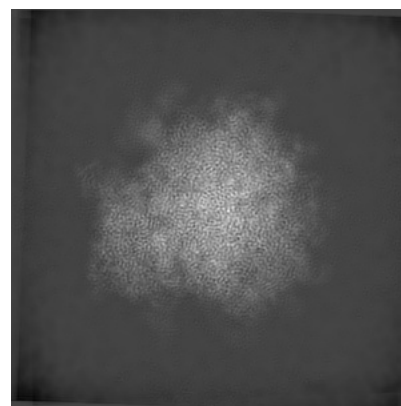
#### 6.1.1 Primary map



X

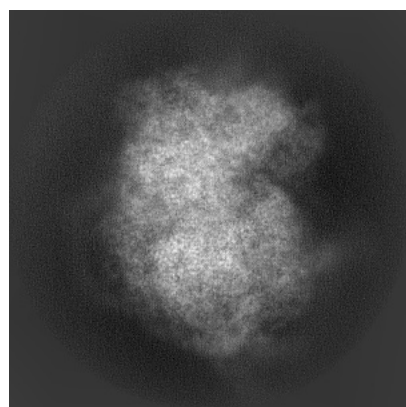


Y

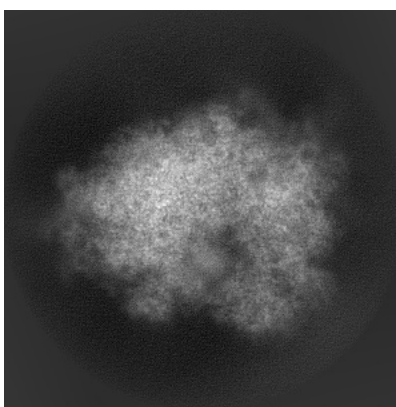


Z

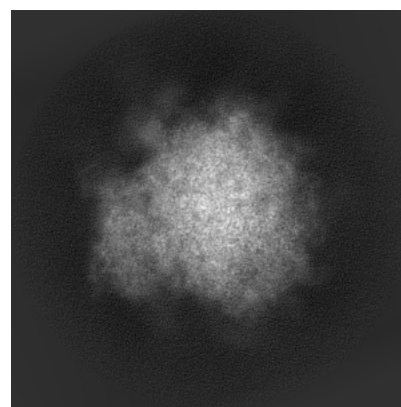
#### 6.1.2 Raw map



X



Y

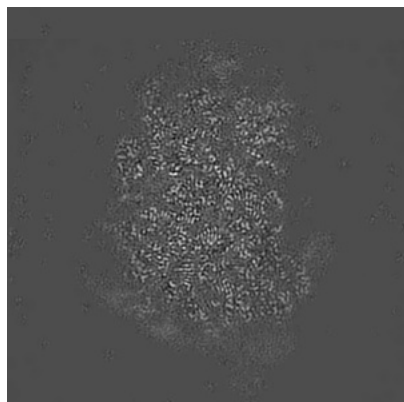


Z

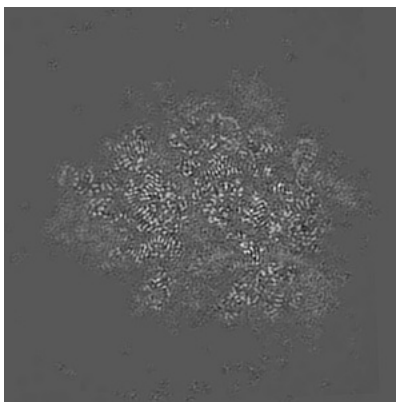
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

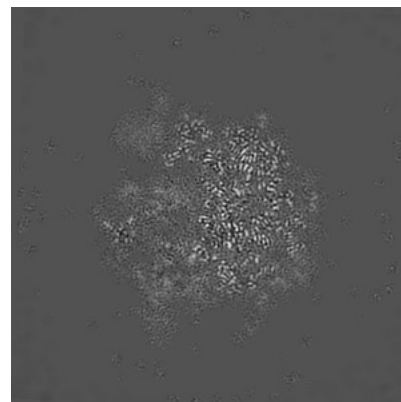
### 6.2.1 Primary map



X Index: 240

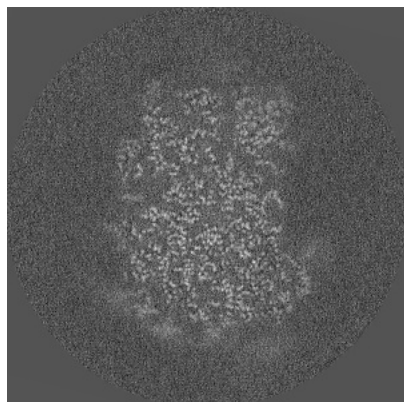


Y Index: 240

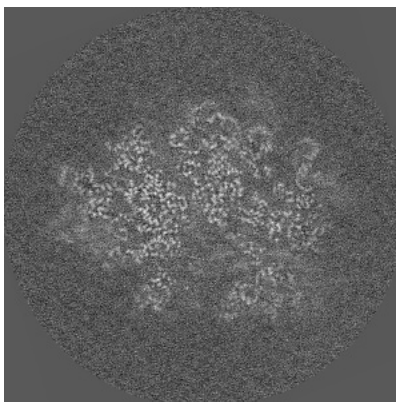


Z Index: 240

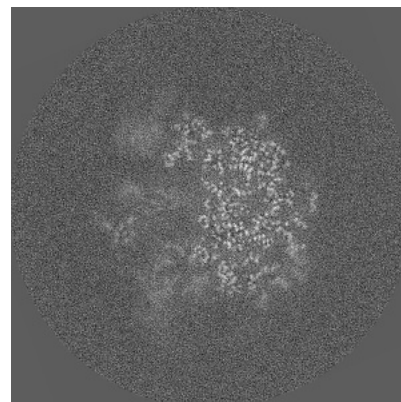
### 6.2.2 Raw map



X Index: 240



Y Index: 240

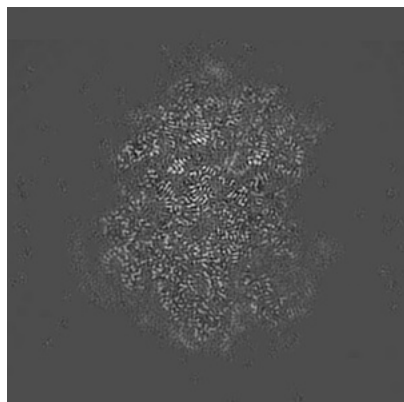


Z Index: 240

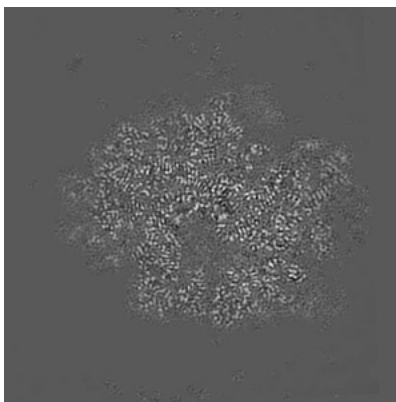
The images above show central slices of the map in three orthogonal directions.

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

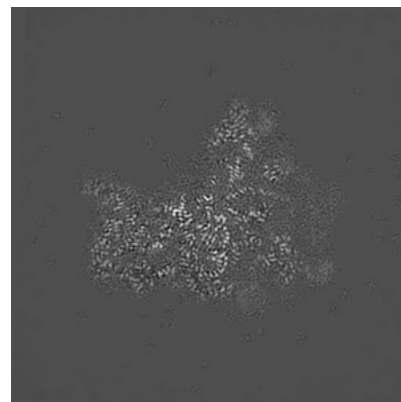
### 6.3.1 Primary map



X Index: 261

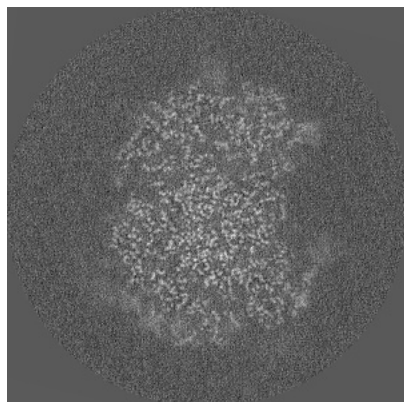


Y Index: 220

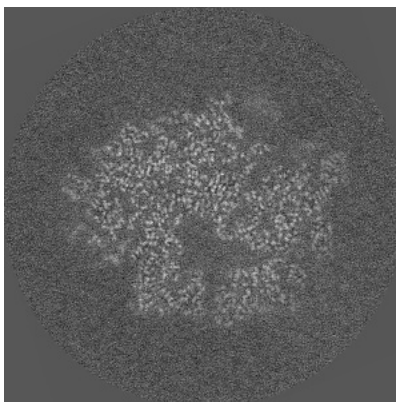


Z Index: 288

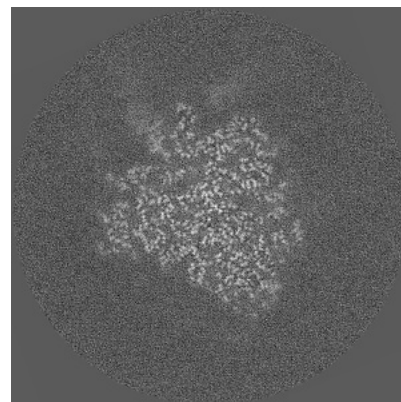
### 6.3.2 Raw map



X Index: 254



Y Index: 221

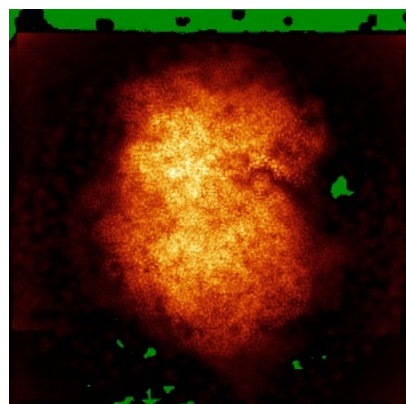


Z Index: 197

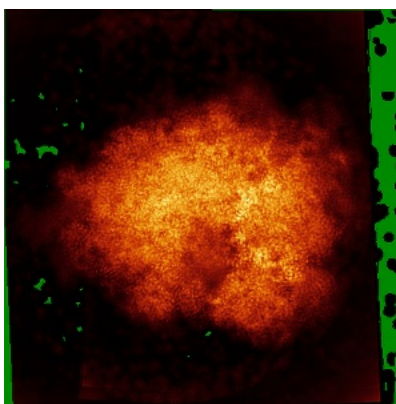
The images above show the largest variance slices of the map in three orthogonal directions.

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

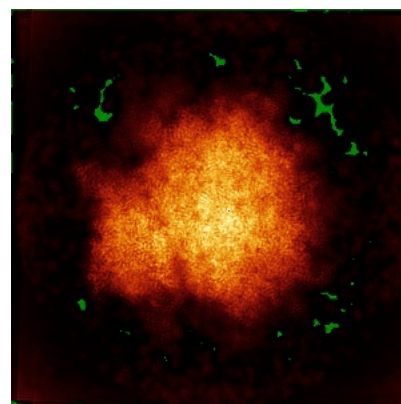
### 6.4.1 Primary map



X

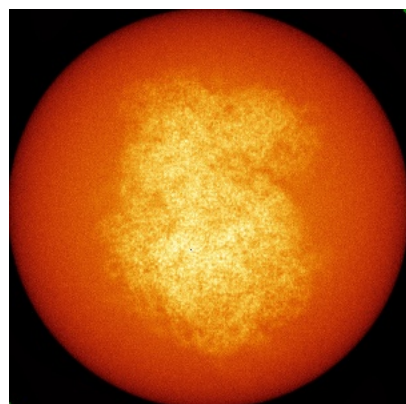


Y

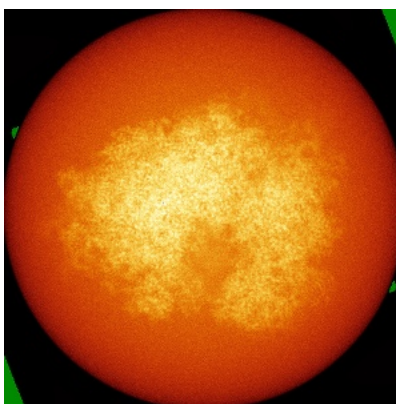


Z

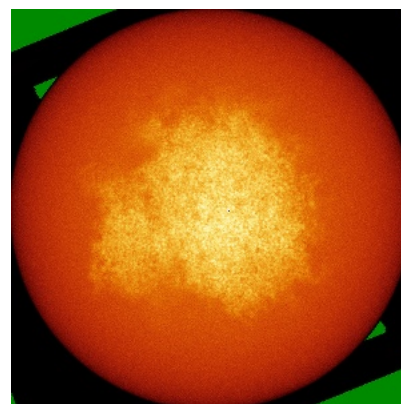
### 6.4.2 Raw map



X



Y

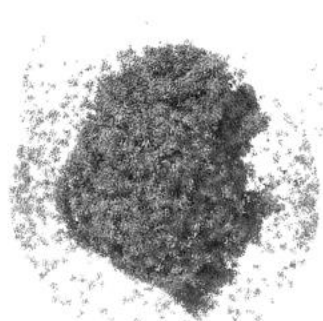


Z

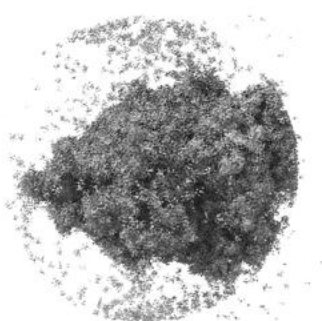
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

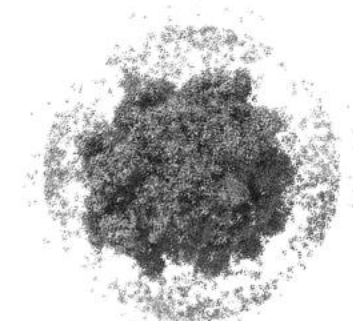
### 6.5.1 Primary map



X



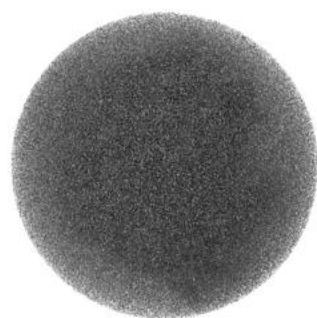
Y



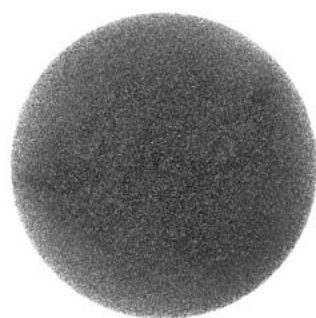
Z

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.

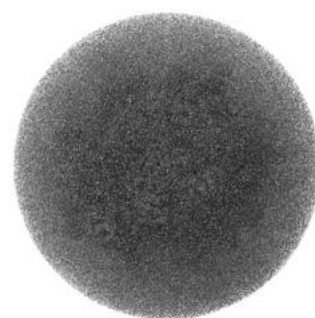
### 6.5.2 Raw map



X



Y



Z

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

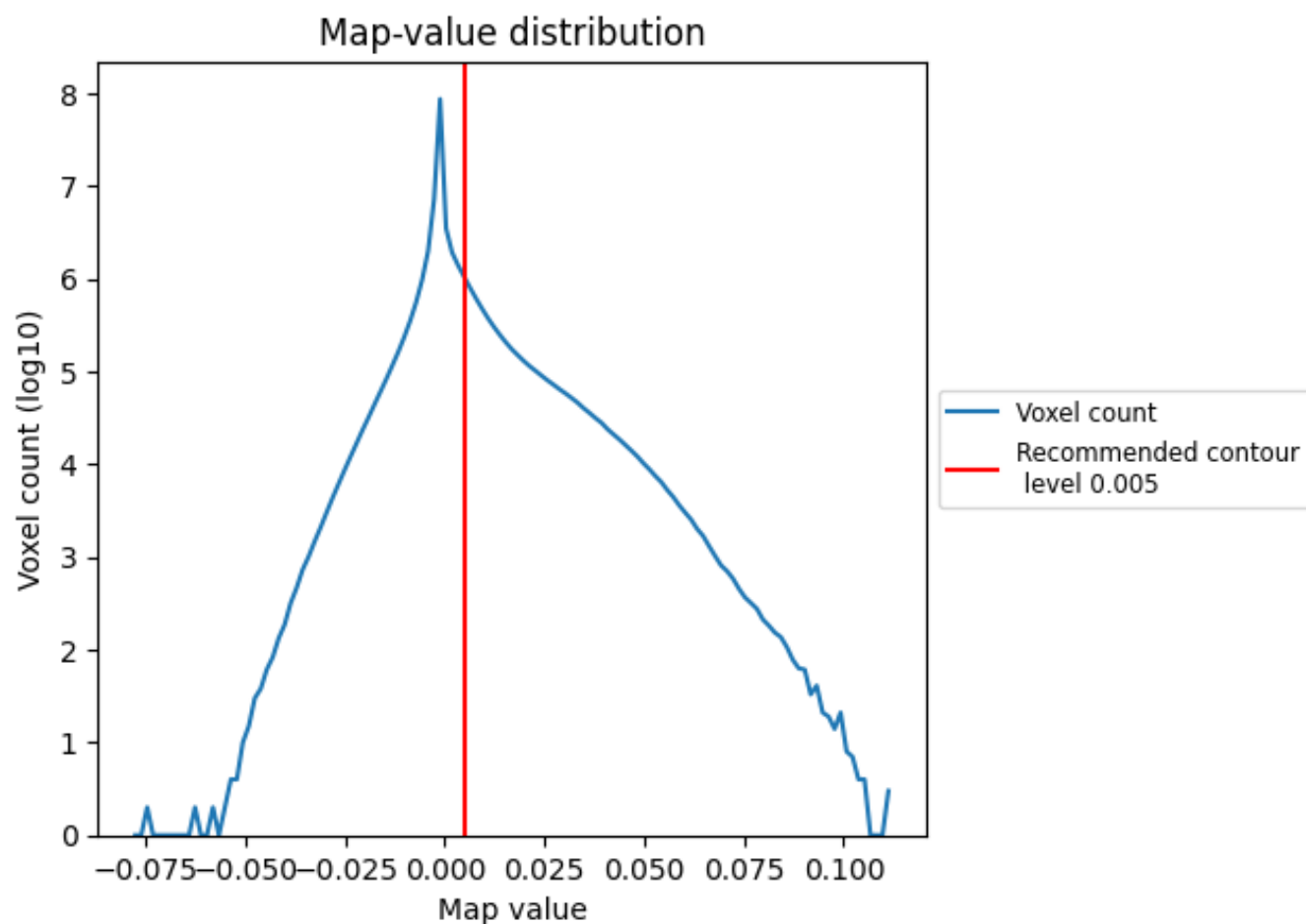
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

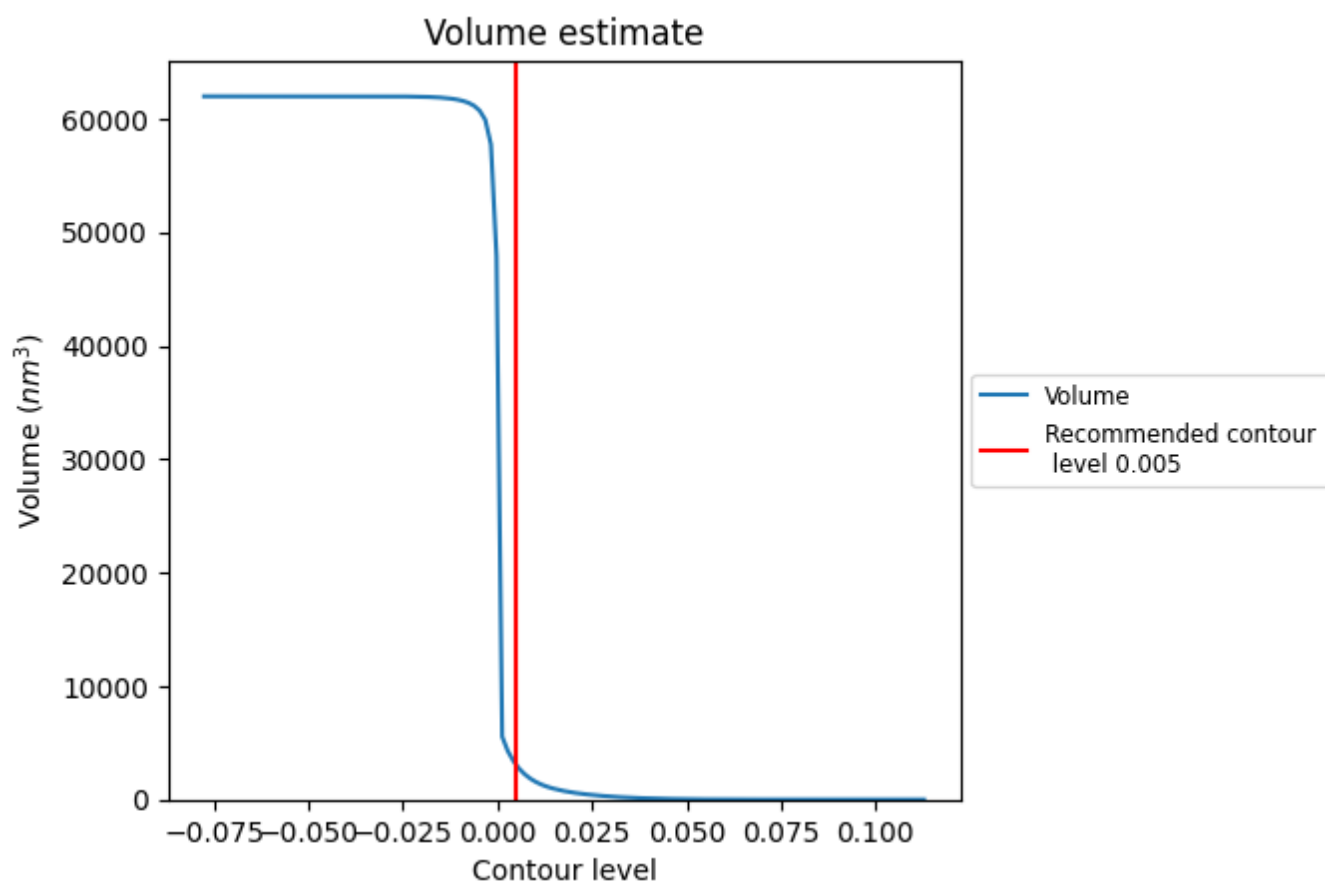
This section contains the results of statistical analysis of the map.

### 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.

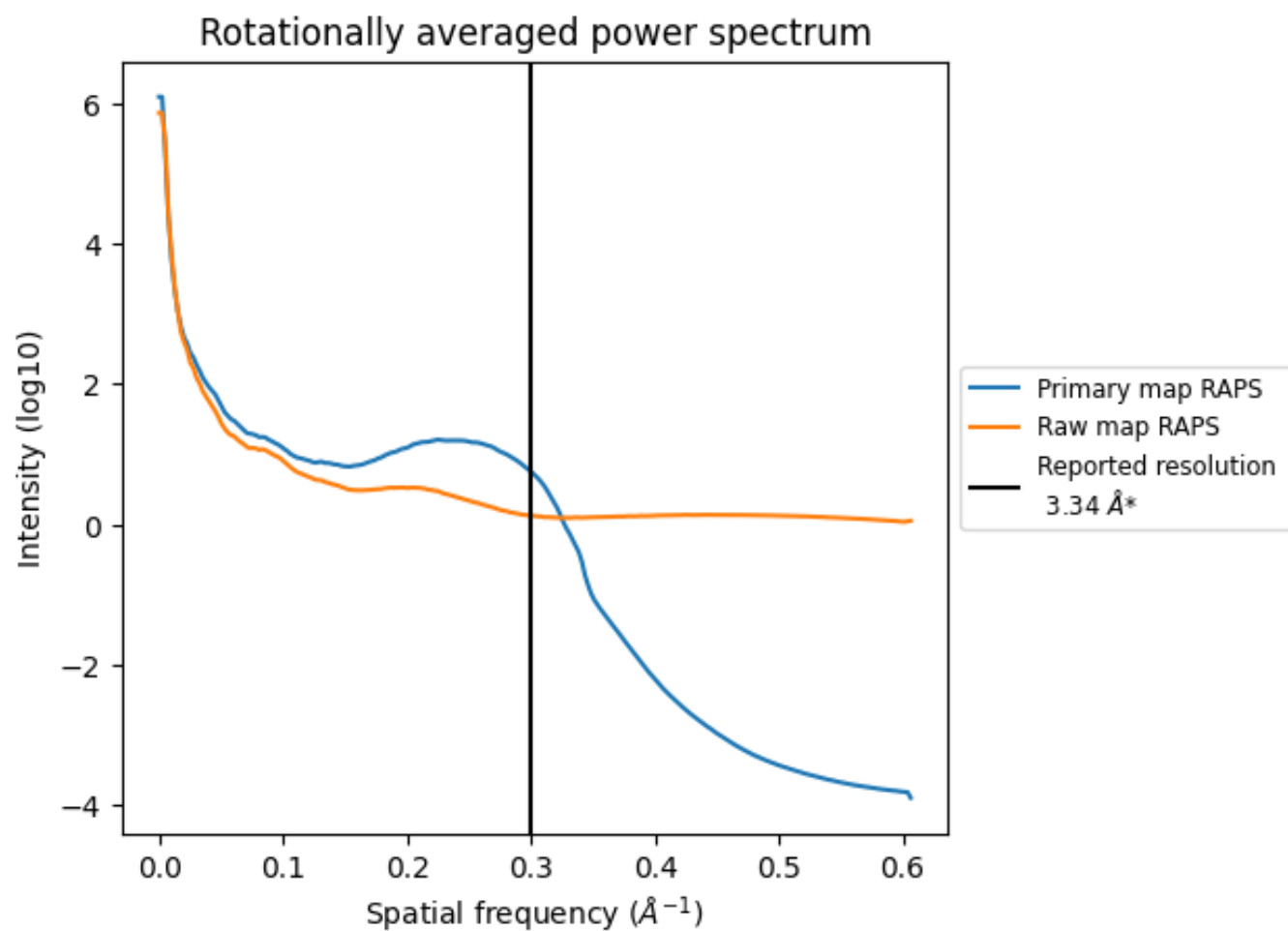
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3036  $\text{nm}^3$ ; this corresponds to an approximate mass of 2742 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 ⓘ

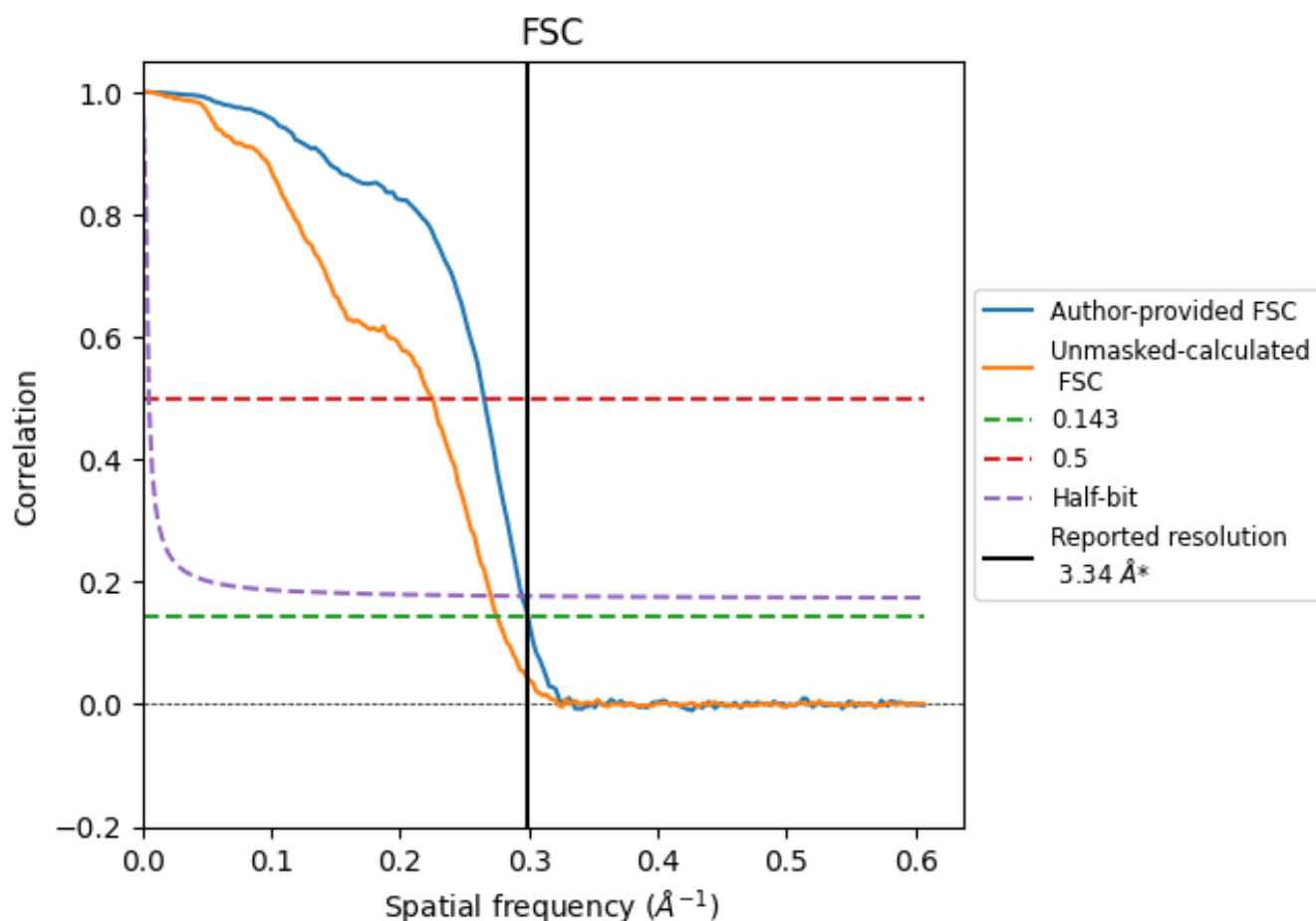


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.299  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

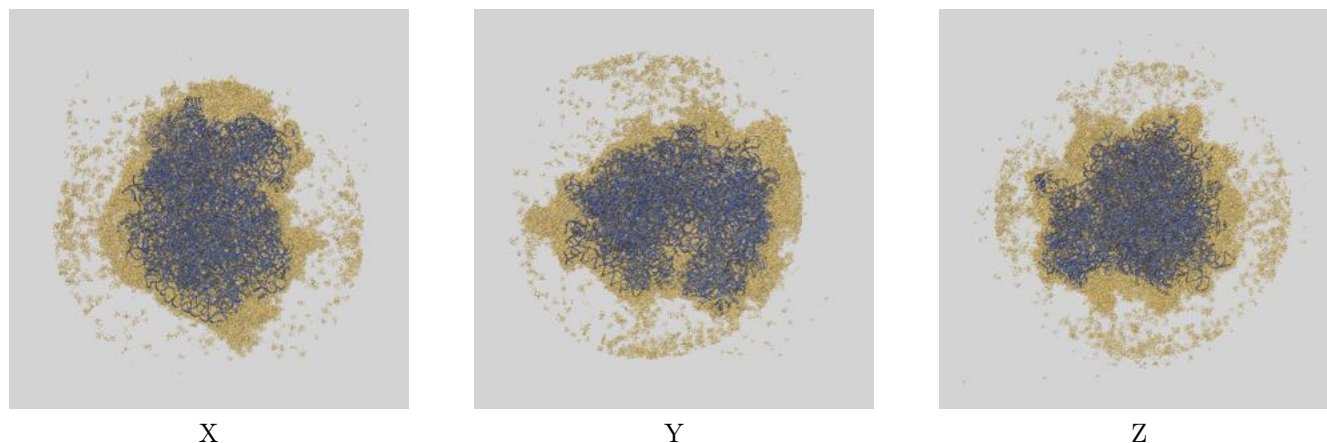
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.34                               | -    | -        |
| Author-provided FSC curve | 3.34                               | 3.77 | 3.39     |
| Unmasked-calculated*      | 3.63                               | 4.44 | 3.70     |

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

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

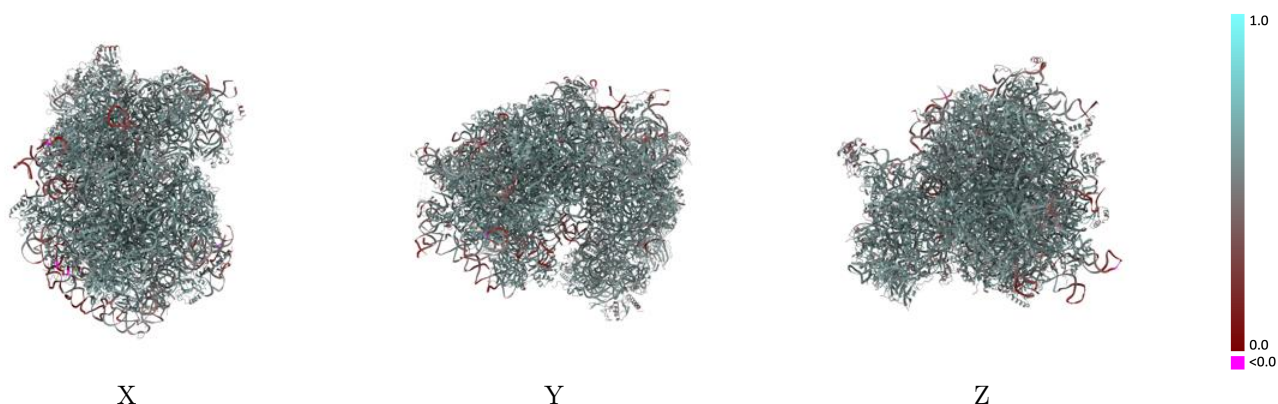
This section contains information regarding the fit between EMDB map EMD-52565 and PDB model 9I14. Per-residue inclusion information can be found in section [3](#) on page [24](#).

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



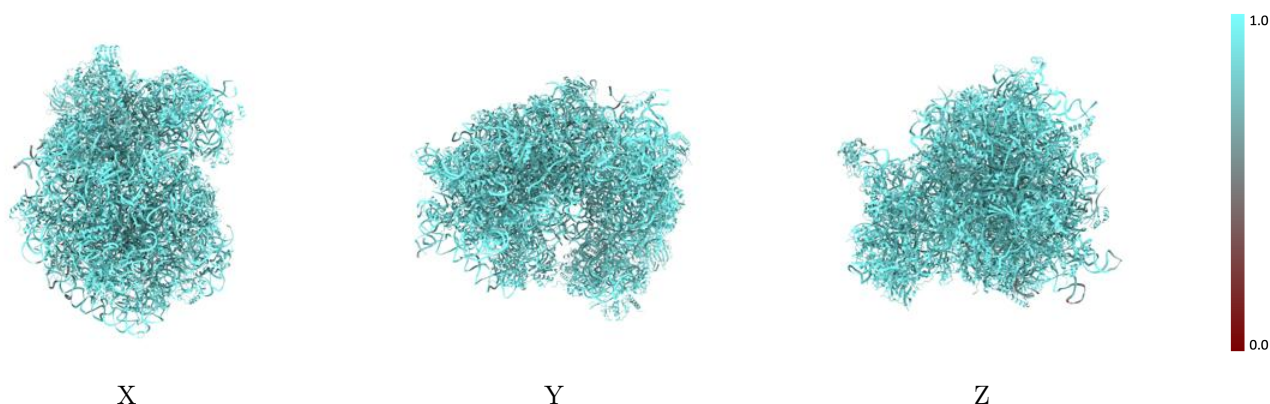
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



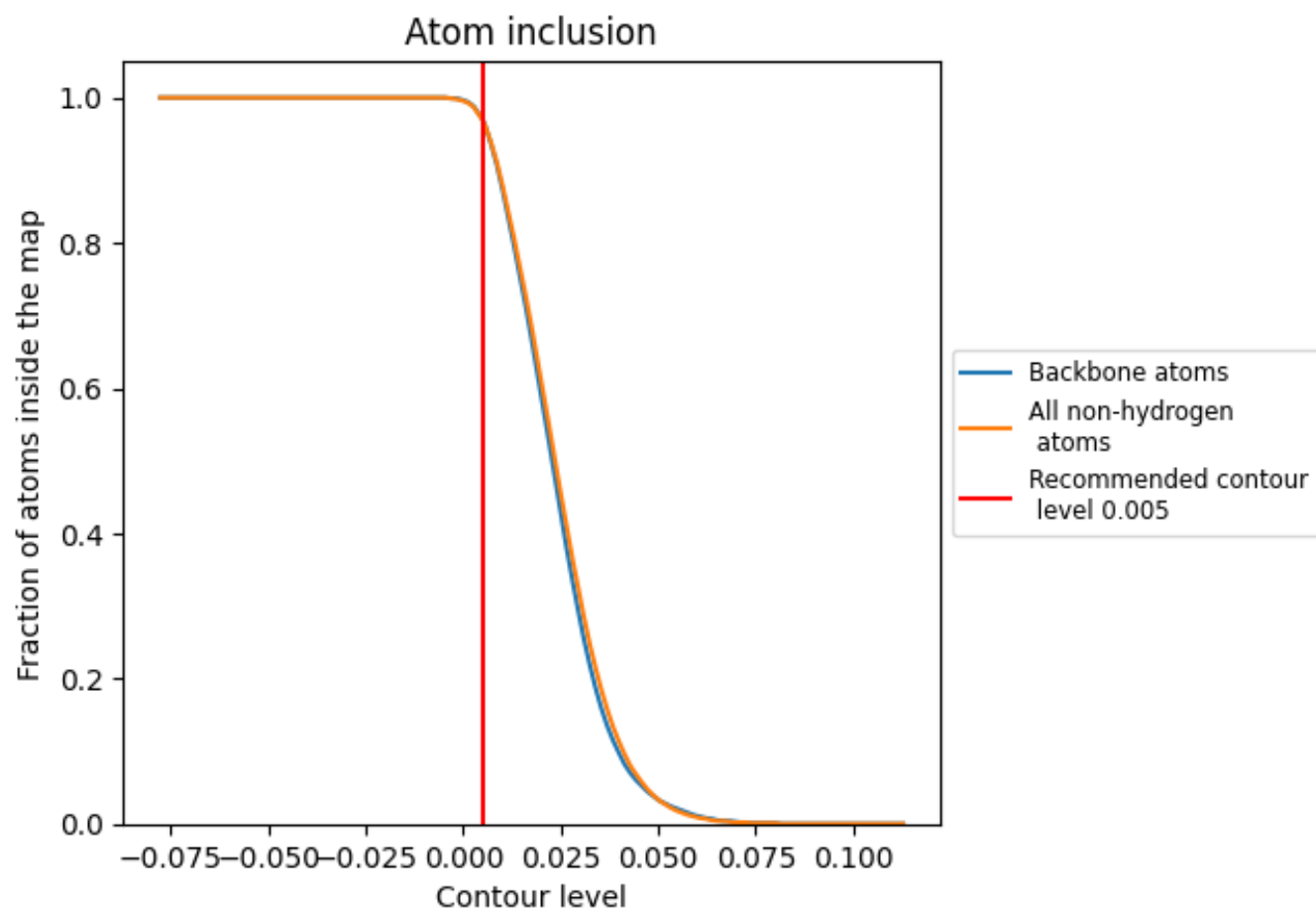
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 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   |  0.9690   |  0.5510   |
| A4    |  0.9790   |  0.5320   |
| B4    |  0.9500   |  0.4080   |
| D4    |  0.9110   |  0.3570   |
| L5    |  0.9660   |  0.5340   |
| L7    |  0.9930   |  0.5760   |
| L8    |  0.9860   |  0.5630   |
| LA    |  0.9840   |  0.5980   |
| LB    |  0.9760   |  0.5860   |
| LC    |  0.9720   |  0.5850   |
| LD    |  0.9590   |  0.5690   |
| LE    |  0.9680   |  0.5660   |
| LF    |  0.9690   |  0.5850   |
| LG    |  0.9560   |  0.5580   |
| LH    |  0.9590  |  0.5740  |
| LI    |  0.9660 |  0.5810 |
| LJ    |  0.9660 |  0.5630 |
| LL    |  0.9640 |  0.5700 |
| LM    |  0.9650 |  0.5730 |
| LN    |  0.9830 |  0.6020 |
| LO    |  0.9710 |  0.5850 |
| LP    |  0.9690 |  0.5900 |
| LQ    |  0.9810 |  0.5980 |
| LR    |  0.9760 |  0.5660 |
| LS    |  0.9800 |  0.5970 |
| LT    |  0.9750 |  0.5820 |
| LU    |  0.9290 |  0.5080 |
| LV    |  0.9840 |  0.5830 |
| LW    |  0.9800 |  0.5490 |
| LX    |  0.9710 |  0.5760 |
| LY    |  0.9630 |  0.5860 |
| LZ    |  0.9710 |  0.5710 |
| La    |  0.9770 |  0.5980 |
| Lb    |  0.9670 |  0.5600 |
| Lc    |  0.9630 |  0.5530 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Ld    |  0.9770   |  0.5780   |
| Le    |  0.9870   |  0.5970   |
| Lf    |  0.9860   |  0.6000   |
| Lg    |  0.9770   |  0.5790   |
| Lh    |  0.9560   |  0.5650   |
| Li    |  0.9550   |  0.5630   |
| Lj    |  0.9870   |  0.5950   |
| Lk    |  0.9460   |  0.5290   |
| Ll    |  0.9780   |  0.5860   |
| Lm    |  0.9750   |  0.5720   |
| Ln    |  0.9950   |  0.5820   |
| Lo    |  0.9820   |  0.5770   |
| Lp    |  0.9910   |  0.5870   |
| Lr    |  0.9740   |  0.5860   |
| S2    |  0.9830   |  0.5550   |
| SA    |  0.9500   |  0.5560   |
| SB    |  0.9680   |  0.5670   |
| SC    |  0.9750   |  0.5670   |
| SD    |  0.9560   |  0.5470   |
| SE    |  0.9650  |  0.5630  |
| SF    |  0.9680 |  0.5670 |
| SG    |  0.9720 |  0.5400 |
| SH    |  0.9390 |  0.5080 |
| SI    |  0.9810 |  0.5510 |
| SJ    |  0.9580 |  0.5460 |
| SK    |  0.9430 |  0.5620 |
| SL    |  0.9780 |  0.5670 |
| SM    |  0.8330 |  0.4440 |
| SN    |  0.9790 |  0.5650 |
| SO    |  0.9680 |  0.5710 |
| SP    |  0.9730 |  0.5650 |
| SQ    |  0.9610 |  0.5770 |
| SR    |  0.9340 |  0.5310 |
| SS    |  0.9650 |  0.5680 |
| ST    |  0.9640 |  0.5780 |
| SU    |  0.9280 |  0.5270 |
| SV    |  0.9410 |  0.5610 |
| SW    |  0.9770 |  0.5750 |
| SX    |  0.9630 |  0.5640 |
| SY    |  0.9660 |  0.5580 |
| SZ    |  0.9550 |  0.5570 |
| Sa    |  0.9750 |  0.5740 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Sb    |  0.9440 |  0.5090 |
| Sc    |  0.9830 |  0.5520 |
| Sd    |  0.9810 |  0.5830 |
| Se    |  0.9820 |  0.5640 |
| Sf    |  0.8910 |  0.4750 |
| Sg    |  0.9330 |  0.5460 |