



## Full wwPDB EM Validation Report ⓘ

Sep 17, 2026 – 02:28 pm BST

PDB ID : 9SMD / pdb\_00009smd  
EMDB ID : EMD-55029  
Title : Ribosome-dome complex including the Sec-translocon (SecYEG-SecA-SecDF)  
from antibiotics treated Mycoplasma pneumoniae cells (Combined)  
Authors : Xue, L.; Jensen, R.K.; Mahamid, J.  
Deposited on : 2025-09-07  
Resolution : 9.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

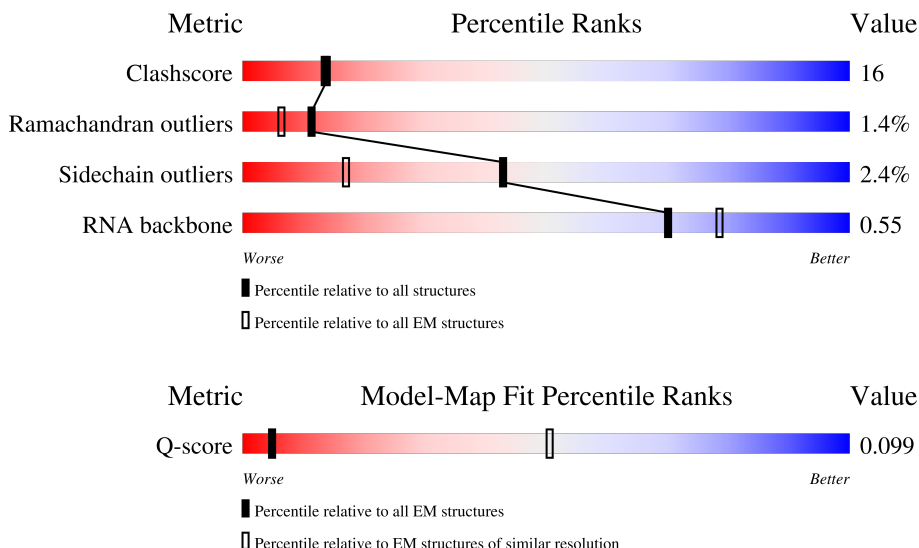
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.40 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                       | 224 ( 8.90 - 9.90 )                                      |

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   | 0     | 48     |                  |
| 2   | 1     | 59     |                  |
| 3   | 10    | 477    |                  |

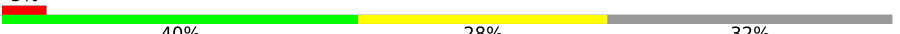
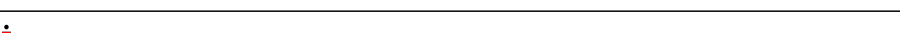
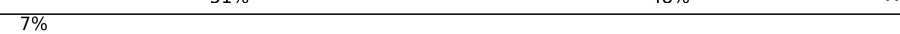
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 11    | 76     |                  |
| 5   | 12    | 125    |                  |
| 6   | 17    | 971    |                  |
| 7   | 2     | 37     |                  |
| 8   | 3     | 2907   |                  |
| 9   | 4     | 108    |                  |
| 10  | 5     | 1523   |                  |
| 11  | 6     | 1523   |                  |
| 12  | 7     | 76     |                  |
| 13  | 8     | 76     |                  |
| 14  | 9     | 808    |                  |
| 15  | A     | 294    |                  |
| 16  | AA    | 219    |                  |
| 17  | AB    | 21     |                  |
| 18  | AC    | 97     |                  |
| 18  | x     | 97     |                  |
| 19  | C     | 205    |                  |
| 20  | E     | 215    |                  |
| 21  | F     | 155    |                  |
| 22  | G     | 142    |                  |
| 23  | H     | 132    |                  |
| 24  | I     | 108    |                  |
| 25  | J     | 121    |                  |
| 26  | K     | 139    |                  |
| 27  | L     | 124    |                  |

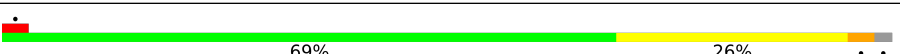
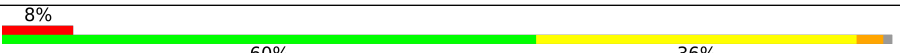
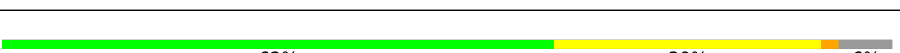
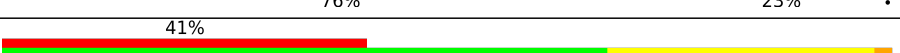
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28  | M     | 61     |    |
| 29  | N     | 86     |    |
| 30  | O     | 94     |    |
| 31  | P     | 85     |    |
| 32  | Q     | 104    |    |
| 33  | R     | 87     |    |
| 34  | S     | 87     |    |
| 35  | T     | 60     |    |
| 36  | W     | 273    |    |
| 37  | Y     | 21     |    |
| 38  | Z     | 36     |    |
| 39  | a     | 287    |    |
| 40  | b     | 287    |  |
| 41  | c     | 212    |  |
| 42  | d     | 180    |  |
| 43  | e     | 184    |  |
| 44  | f     | 149    |  |
| 45  | g     | 161    |  |
| 46  | h     | 137    |  |
| 47  | i     | 146    |  |
| 48  | j     | 122    |  |
| 49  | k     | 151    |  |
| 50  | l     | 139    |  |
| 51  | m     | 124    |  |
| 52  | n     | 116    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 53  | o     | 119    |    |
| 54  | p     | 127    |    |
| 55  | q     | 100    |    |
| 56  | r     | 159    |    |
| 57  | s     | 194    |    |
| 58  | t     | 111    |    |
| 59  | u     | 104    |    |
| 60  | v     | 65     |    |
| 61  | w     | 111    |    |
| 62  | y     | 57     |    |
| 63  | z     | 53     |    |
| 64  | 13    | 1217   |    |
| 65  | 14    | 1298   |  |
| 66  | 15    | 1274   |  |
| 67  | 16    | 276    |  |
| 67  | 18    | 276    |  |

## 2 Entry composition [i](#)

There are 72 unique types of molecules in this entry. The entry contains 202419 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 0     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 380   | 236 | 81 | 61 | 2 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 477   | 300 | 99 | 77 | 1 |         |       |

- Molecule 3 is a protein called Protein translocase subunit SecY.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 10    | 454      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3487  | 2284 | 568 | 628 | 7 |         |       |

- Molecule 4 is a protein called Probable protein-export membrane protein SecG.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | 11    | 76       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 585   | 391 | 93 | 96 | 5 |         |       |

- Molecule 5 is a protein called SecE.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | 12    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 848   | 563 | 142 | 142 | 1 |         |       |

- Molecule 6 is a protein called SecDF.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 6   | 17    | 964      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7613  | 4947 | 1255 | 1401 | 10 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | 2     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 304   | 189 | 65 | 46 | 4 |         |       |

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 8   | 3     | 2893     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 61992 | 27701 | 11293 | 20105 | 2893 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 9   | 4     | 108      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2305  | 1030 | 415 | 752 | 108 |         |       |

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 10  | 5     | 1507     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32256 | 14418 | 5847 | 10484 | 1507 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| 5     | 525     | G7M      | -      | insertion | GB 26117688 |
| 5     | 1003    | A        | G      | conflict  | GB 26117688 |
| 5     | 1493    | MA6      | -      | insertion | GB 26117688 |
| 5     | 1494    | MA6      | -      | insertion | GB 26117688 |

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|-------|
| 11  | 6     | 2        | Total | C  | N | O  | P | 0       | 0     |
|     |       |          | 42    | 19 | 8 | 13 | 2 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| 6     | 574     | 7MG      | -      | insertion | GB 26117688 |
| 6     | 1053    | A        | G      | conflict  | GB 26117688 |
| 6     | 1543    | MA6      | -      | insertion | GB 26117688 |

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| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| 6     | 1544    | MA6      | -      | insertion | GB 26117688 |

- Molecule 12 is a RNA chain called tRNA-Asp (P-site).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 12  | 7     | 76       | Total | C   | N   | O   | P  | S       | 0     | 0 |
|     |       |          | 1638  | 734 | 291 | 535 | 76 | 2       |       |   |

- Molecule 13 is a RNA chain called tRNA-Lys (A-site).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 13  | 8     | 76       | Total | C   | N   | O   | P  | S       | 0     | 0 |
|     |       |          | 1635  | 733 | 284 | 541 | 76 | 1       |       |   |

- Molecule 14 is a protein called Protein translocase subunit SecA.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 14  | 9     | 808      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6467  | 4097 | 1141 | 1207 | 22 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | A     | 266      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2138  | 1359 | 376 | 394 | 9 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | AA    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1191  | 753 | 228 | 207 | 3 |         |       |

- Molecule 17 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 17  | AB    | 21       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 440   | 198 | 75 | 146 | 21 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 18  | AC    | 43       | Total | C   | N  | O  |   | 0       | 0     |
|     |       |          | 342   | 214 | 65 | 63 |   |         |       |
| 18  | x     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 366   | 235 | 59 | 68 | 4 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | C     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1669  | 1057 | 316 | 292 | 4 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | E     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1509  | 950 | 270 | 287 | 2 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | F     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1254  | 790 | 240 | 217 | 7 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | G     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1110  | 723 | 193 | 192 | 2 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1041  | 661 | 196 | 183 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| H     | 27      | HIS      | LYS    | conflict | UNP P75179 |

- Molecule 24 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | I     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 536 | 147 | 148 | 1 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | J     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 829   | 514 | 153 | 156 | 6 |         |       |

- Molecule 26 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | K     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1071  | 677 | 212 | 180 | 2 |         |       |

- Molecule 27 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 27  | L     | 121      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 975   | 609 | 197 | 169 |  |         |       |

- Molecule 28 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | M     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 474   | 302 | 96 | 72 | 4 |         |       |

- Molecule 29 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 29  | N     | 85       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 689   | 436 | 130 | 123 |  |         |       |

- Molecule 30 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | O     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 453 | 130 | 118 | 4 |         |       |

- Molecule 31 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | P     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 436 | 138 | 118 | 1 |         |       |

- Molecule 32 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 32  | Q     | 71       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 590   | 378 | 115 | 93 | 4 |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | R     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 700   | 444 | 132 | 122 | 2 |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 34  | S     | 79       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 643   | 391 | 138 | 114 |  |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 35  | T     | 59       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 519   | 326 | 111 | 80 | 2 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | W     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 1116 | 326 | 317 | 5 |         |       |

- Molecule 37 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 37  | Y     | 6        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 126   | 57 | 22 | 41 | 6 |         |       |

- Molecule 38 is a protein called Nascent peptide.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 38  | Z     | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 187   | 112 | 37 | 38 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | a     | 285      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2225  | 1385 | 437 | 397 | 6 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | b     | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1778  | 1129 | 320 | 322 | 7 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | c     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1654  | 1053 | 299 | 299 | 3 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | d     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1416  | 910 | 251 | 251 | 4 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 43  | e     | 176      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1396  | 899 | 247 | 250 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | f     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 779 | 212 | 214 | 3 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | g     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 951   | 606 | 165 | 177 | 3 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | h     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 959   | 616 | 160 | 177 | 6 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | i     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1164  | 737 | 213 | 209 | 5 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | j     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 944   | 595 | 178 | 167 | 4 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | k     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1170  | 741 | 228 | 200 | 1 |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | l     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1079  | 694 | 196 | 182 | 7 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | m     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 609 | 175 | 171 | 3 |         |       |

- Molecule 52 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | n     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 918   | 573 | 181 | 162 | 2 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | o     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 966   | 609 | 186 | 170 | 1 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | p     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 624 | 194 | 161 | 2 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | q     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 525 | 148 | 134 | 4 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | r     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1091  | 677 | 212 | 195 | 7 |         |       |

- Molecule 57 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | s     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 740   | 486 | 125 | 128 | 1 |         |       |

- Molecule 58 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | t     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 871   | 550 | 166 | 152 | 3 |         |       |

- Molecule 59 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | u     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 416 | 132 | 121 | 1 |         |       |

- Molecule 60 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 60  | v     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 520   | 320 | 109 | 90 | 1 |         |       |

- Molecule 61 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | w     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 576 | 168 | 162 |   |         |       |

- Molecule 62 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 62  | y     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 274 | 98 | 75 | 5 |         |       |

- Molecule 63 is a protein called 50S ribosomal protein L33 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 63  | z     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 408   | 255 | 81 | 68 | 4 |         |       |

- Molecule 64 is a protein called Uncharacterized lipoprotein MG307 homolog.

| Mol | Chain | Residues | Atoms |      |      |      |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---|---------|-------|
| 64  | 13    | 1216     | Total | C    | N    | O    | S | 0       | 0     |
|     |       |          | 9604  | 6055 | 1627 | 1915 | 7 |         |       |

- Molecule 65 is a protein called Uncharacterized lipoprotein MG309 homolog.

| Mol | Chain | Residues | Atoms |      |      |      |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---|---------|-------|
| 65  | 14    | 1297     | Total | C    | N    | O    | S | 0       | 0     |
|     |       |          | 10101 | 6304 | 1723 | 2068 | 6 |         |       |

- Molecule 66 is a protein called Uncharacterized lipoprotein MG338 homolog.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 66  | 15    | 1273     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9894  | 6200 | 1706 | 1977 | 11 |         |       |

- Molecule 67 is a protein called Uncharacterized lipoprotein MG348 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|--|---------|-------|
| 67  | 18    | 275      | Total | C    | N   | O   |  | 0       | 0     |
|     |       |          | 2141  | 1329 | 379 | 433 |  |         |       |
| 67  | 16    | 275      | Total | C    | N   | O   |  | 0       | 0     |
|     |       |          | 2141  | 1329 | 379 | 433 |  |         |       |

- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 68  | 2     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | M     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | Q     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | x     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 68  | y     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | z     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 69 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

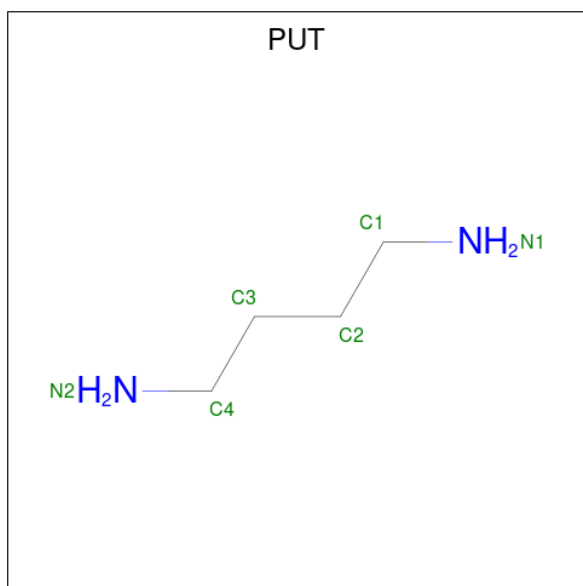
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 69  | 3     | 213      | Total | Mg  | 0       |
|     |       |          | 213   | 213 |         |
| 69  | 4     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 69  | 5     | 88       | Total | Mg  | 0       |
|     |       |          | 88    | 88  |         |
| 69  | 6     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 69  | 7     | 3        | Total | Mg  | 0       |
|     |       |          | 3     | 3   |         |
| 69  | 8     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 69  | AB    | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 69  | K     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 69  | P     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 69  | Y     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 69  | b     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 69  | i     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 69  | y     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 70 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 70  | 3     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 3     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 3     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 3     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

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| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 70  | 3     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 3     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 5     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 5     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 5     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | 5     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 70  | b     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

- Molecule 71 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 71  | 3     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 72 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 72  | 3     | 16       | Total | O  | 0       |
|     |       |          | 16    | 16 |         |
| 72  | 5     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 72  | A     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 72  | i     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

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

- Molecule 1: Large ribosomal subunit protein bL34

Chain 0: 



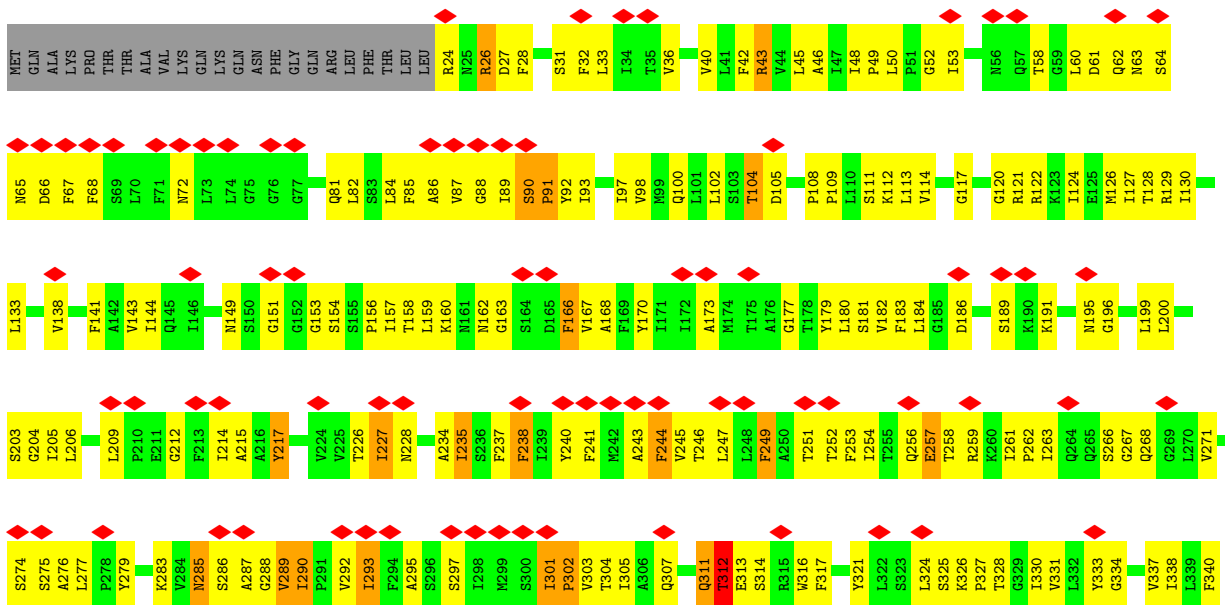
- Molecule 2: 50S ribosomal protein L35

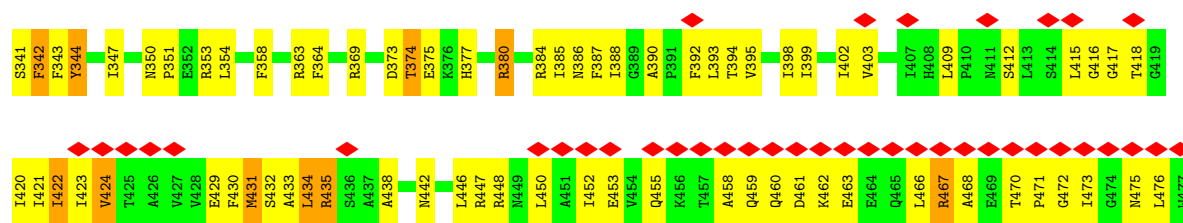
Chain 1: 



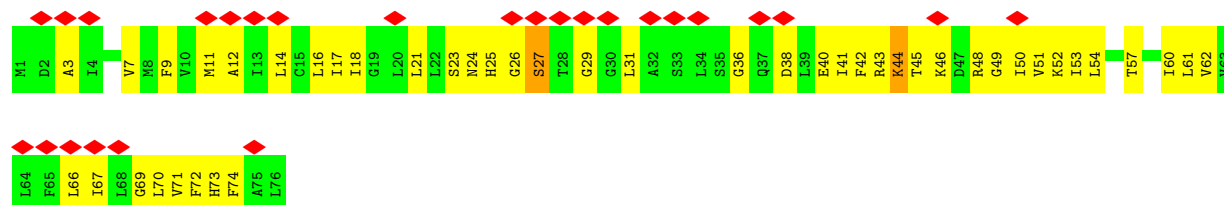
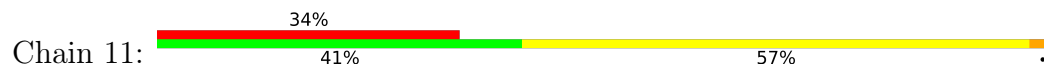
- Molecule 3: Protein translocase subunit SecY

Chain 10: 

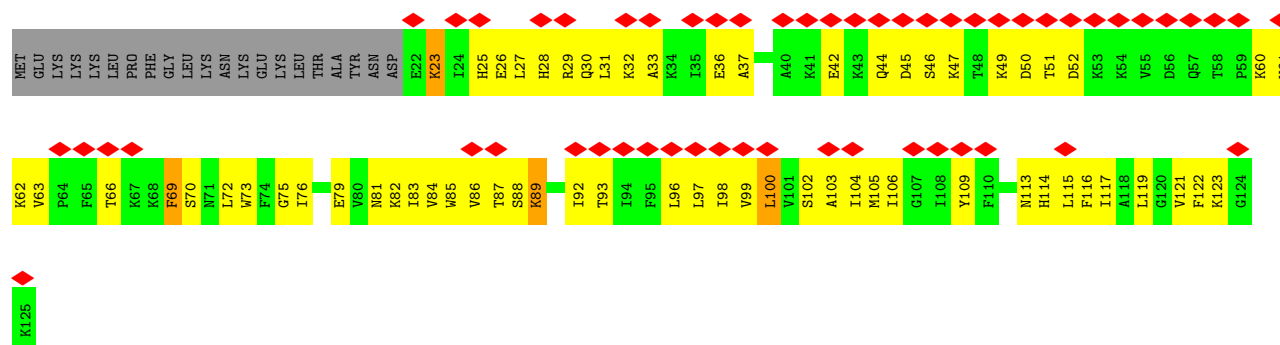




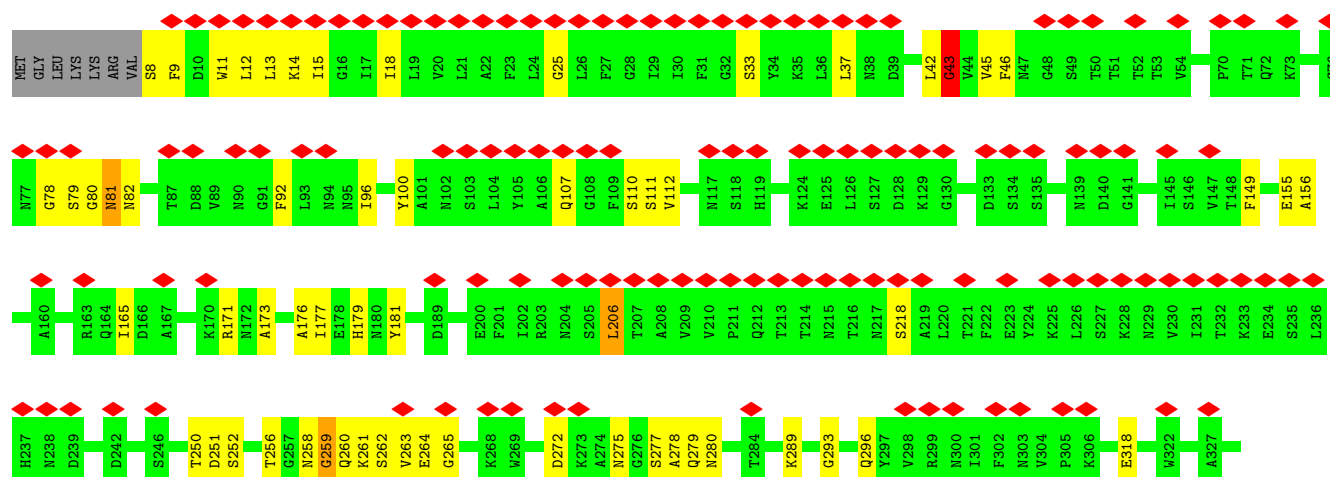
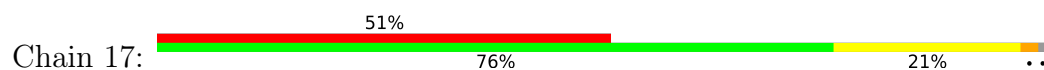
• Molecule 4: Probable protein-export membrane protein SecG

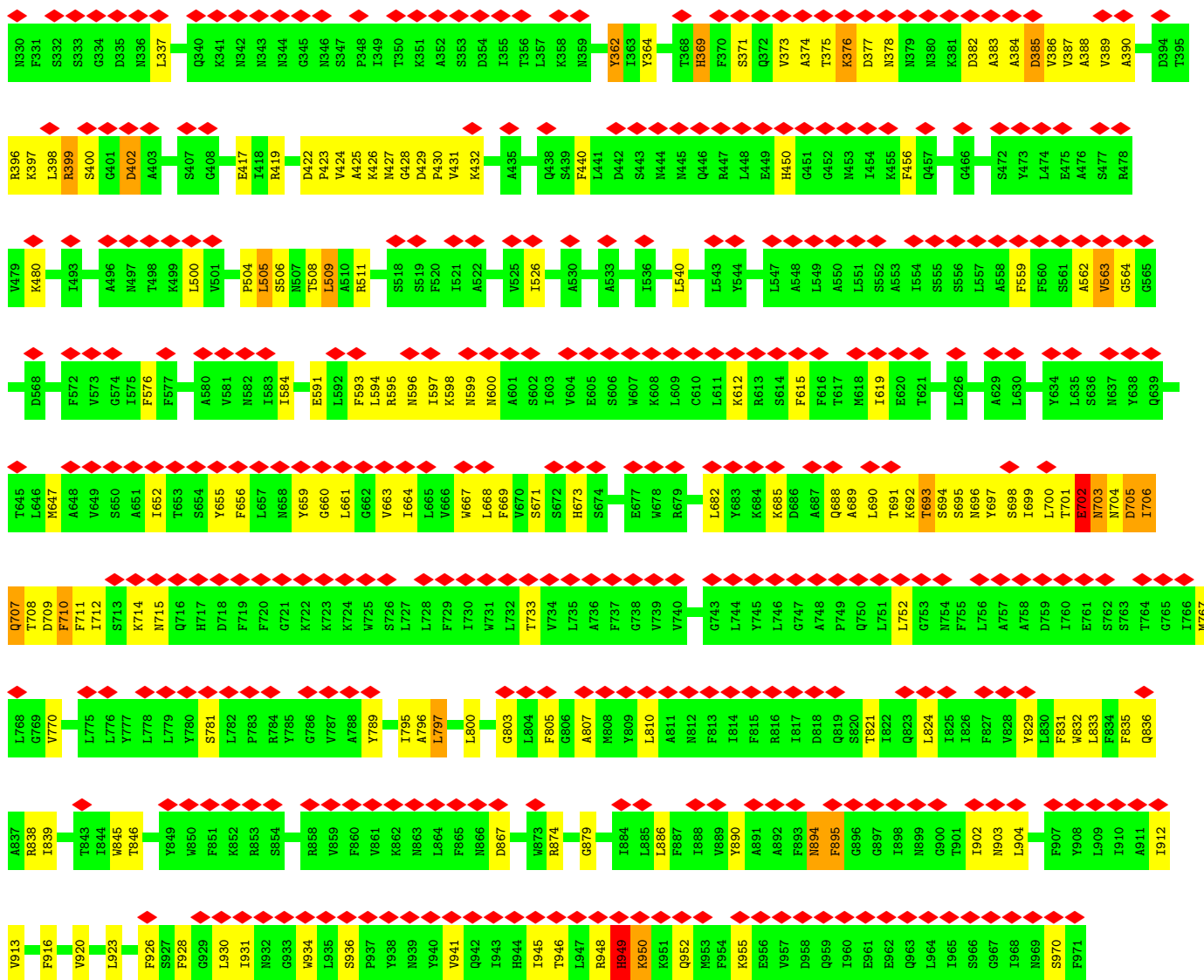


• Molecule 5: SecE



• Molecule 6: SecDF





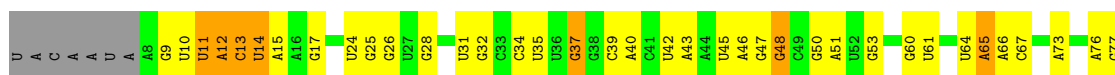
• Molecule 7: 50S ribosomal protein L36

Chain 2: 89% 11%



• Molecule 8: 23S ribosomal RNA

Chain 3: 55% 38% 7%

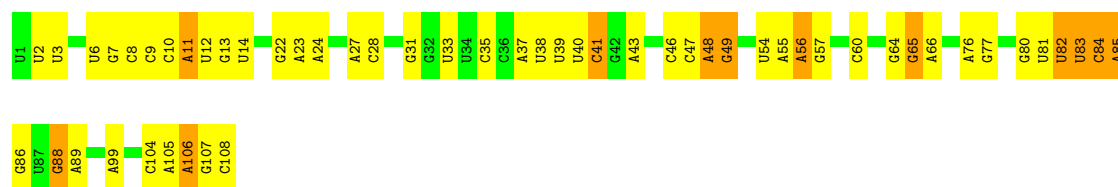


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U192  | G193  | U193  | G194  | U195  | G196  | A200  | C201  | A202  | C202  | U204  | C207  | G219  | A220  | A223  | G224  | A225  | A226  | A227  | G230  | A231  | A232  | U233  | G234  | U235  | G236  | A237  | U238  | U245  | G246  | G252  | C253  | G254  | G258  | A259  | A269  | G270  | A276  | U279  | A280  | U284  | G287  | U295  | U296  | G297  | U298  | A299  |       |       |       |       |       |
| G300  | U304  | A309  | U310  | G311  | U312  | G313  | A315  | C316  | U317  | U318  | G319  | A322  | A323  | G324  | G325  | A333  | C336  | U337  | G338  | U340  | G341  | G342  | A343  | A344  | A345  | G353  | C354  | A355  | A356  | G363  | A364  | U365  | A374  | A381  | U382  | U386  | U387  | U388  | C389  | A392  | G397  | C398  | G401  | A402  |       |       |       |       |       |       |       |
| G408  | A409  | G410  | U411  | A412  | G413  | G418  | A420  | A421  | A422  | G423  | U424  | A425  | U426  | A427  | G432  | A436  | A437  | C440  | G447  | A448  | C449  | C450  | A451  | G454  | G455  | G456  | A459  | G460  | U463  | A464  | A465  | U470  | A471  | U474  | A475  | G476  | U477  | G478  | A483  | C487  | G488  | A489  | A490  | G499  |       |       |       |       |       |       |       |
| A502  | G512  | A515  | A516  | G517  | A518  | A519  | C520  | G524  | A527  | U528  | G529  | G530  | G531  | A532  | U539  | A540  | A548  | A549  | C558  | G562  | C565  | G566  | G567  | G568  | U569  | C570  | A573  | G574  | C575  | A581  | A582  | U583  | G584  | U585  | G586  | G586  | C587  | U588  | U589  | U600  | G603  | A604  | A605  | G606  |       |       |       |       |       |       |       |
| U607  | A608  | U609  | G610  | A611  | G614  | G615  | U619  | G620  | U621  | U622  | A623  | A628  | G629  | G630  | A631  | A632  | U636  | U637  | A638  | G648  | A649  | G650  | A651  | U652  | G653  | G656  | A657  | U660  | A663  | G664  | G665  | G666  | A667  | A668  | A669  | G670  | C671  | G672  | A673  | G674  | U675  | U676  | U677  | A680  | A681  | A682  | A684  |       |       |       |       |
| U689  | U690  | G691  | G695  | A698  | U699  | U700  | A701  | U702  | G703  | G704  | A705  | A712  | G713  | G714  | G715  | G716  | A720  | G721  | C722  | A728  | C733  | G739  | A740  | A741  | U749  | C752  | G755  | A756  | A757  | G761  | G764  | A765  | G766  | G767  | G768  | C769  | G775  | U776  | C777  | G780  | U781  | U782  | A784  |       |       |       |       |       |       |       |       |
| G788  | A789  | U790  | G792  | U797  | G798  | U799  | C800  | G810  | G811  | A817  | A818  | U819  | U820  | G824  | A828  | A829  | A830  | U831  | C832  | G840  | G844  | U845  | U846  | U848  | C847  | U849  | C852  | G853  | A854  | A855  | A858  | G859  | C860  | U861  | U862  | U863  | G866  | C867  | C868  | U869  | A870  | C871  | U874  | G875  | U879  |       |       |       |       |       |       |
| C880  | A881  | C882  | A883  | A884  | A887  | G888  | G889  | G891  | G892  | A893  | G894  | A897  | A898  | A899  | G900  | C901  | U902  | A903  | C904  | U905  | G906  | U909  | G910  | U916  | G917  | C922  | A923  | C924  | C925  | U926  | A927  | G928  | G929  | C930  | G931  | U932  | A933  | C934  | U935  | G936  | U944  | A947  | A948  | U949  | U950  | C951  | U952  | G953  | G957  |       |       |
| U963  | A964  | U965  | U968  | A969  | U970  | A981  | G982  | A983  | A984  | A985  | G988  | U994  | A995  | A996  | G997  | A1080 | U1081 | A1082 | A1083 | C1084 | A1002 | U1003 | G1005 | U1006 | C1007 | A1008 | U1009 | G1010 | A1016 | A1019 | A1026 | A1029 | U1030 | U1031 | A1032 | A1033 | A1036 | U1037 | G1038 | G1039 | A1045 | U1048 | U1049 | C951  | U1054 | A1055 |       |       |       |       |       |
| U1058 | G1059 | G1060 | A1061 | A1062 | A1064 | U1068 | U1069 | U1070 | A1071 | A1072 | A1073 | G1074 | G1075 | U1076 | U1077 | C1078 | U1079 | A1143 | A1144 | A1145 | A1146 | U1147 | U1148 | G1149 | G1155 | U1156 | U1157 | A1168 | U1169 | G1170 | U1176 | A1177 | A1178 | A1183 | U1184 | C1188 | A1201 | A1202 | G1203 | A1204 | A1208 | U1209 | A1210 | U1211 | U1212 | G1215 | U1219 |       |       |       |       |
| C1227 | G1228 | U1229 | U1230 | G1231 | U1232 | A1233 | U1234 | U1235 | G1236 | G1239 | U1240 | U1241 | G1242 | G1245 | U1246 | G1247 | A1248 | A1249 | A1250 | G1251 | G1252 | G1253 | U1254 | G1255 | A1256 | G1257 | U1264 | G1265 | G1266 | A1267 | U1268 | G1269 | C1270 | A1271 | U1279 | G1280 | A1281 | G1282 | A1283 | A1284 | U1285 | G1286 | A1292 | U1293 | G1294 | U1295 | G1296 | G1301 | U1304 | G1305 | G1306 |
| G1307 | A1308 | G1309 | U1310 | G1313 | C1317 | U1318 | C1321 | A1322 | A1323 | A1324 | C1325 | A1328 | U1329 | U1330 | U1334 | A1335 | A1336 | A1337 | G1344 | U1345 | U1346 | C1347 | U1348 | U1349 | U1351 | U1352 | U1353 | U1354 | U1355 | U1369 | C1378 | C1379 | U1380 | A1381 | U1385 | G1386 | A1387 | G1388 | C1389 | U1391 | G1392 | U1393 | A1401 | U1404 | U1405 | U1406 | G1407 |       |       |       |       |
| A1412 | A1413 | C1414 | A1415 | A1420 | A1421 | U1422 | U1423 | U1424 | A1431 | A1432 | U1433 | U1434 | A1435 | C1436 | A1437 | G1438 | U1439 | U1440 | A1441 | G1442 | A1443 | U1444 | U1445 | G1446 | A1451 | G1452 | C1456 | A1457 | A1458 | U1459 | G1460 | A1461 | A1462 | G1463 | G1464 | U1467 | C1470 | A1471 | C1472 | C1473 | C1474 | A1479 | A1480 | U1481 | U1482 | G1483 | G1485 | A1486 | U1487 |       |       |
| U1487 | U1488 | A1493 | U1494 | A1495 | A1496 | A1497 | A1502 | A1503 | G1504 | G1508 | U1509 | C1511 | A1512 | A1513 | U1514 | C1518 | A1519 | A1520 | A1521 | U1522 | C1523 | C1524 | G1525 | U1529 | G1530 | A1534 | A1535 | C1536 | A1537 | A1541 | G1542 | U1543 | G1544 | A1545 | U1546 | G1550 | G1557 | A1558 | U1559 | U1560 | G1561 | A1562 | G1563 | U1564 | G1565 | A1566 | U1567 | C1568 |       |       |       |

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| U2845 | A1569 | A1648 | C1771 | C1886 | U2009 | U2088 | A2171 | C2266 | U2352 | G2437 | G2540 | U2644 | G2752 | U2846 |
| A2846 | A1570 | C1649 | A1780 | U1889 | A2010 | A2089 | G2174 | G2267 | G2353 | A2438 | C2541 | U2645 | G2756 | A2847 |
| C2847 | U1571 | C1650 | U1786 | U1890 | G2011 | A2095 | U2175 | A2274 | A2354 | A2443 | G2542 | G2653 | A2755 | A2848 |
| U2853 | A1572 | C1651 | U1789 | C1893 | A2012 | A2094 | G2180 | A2275 | U2355 | U2449 | G2557 | U2654 | C2760 | U2853 |
| A2854 | A1573 | A1652 | C1789 | U1894 | G2017 | A2098 | A2181 | A2276 | U2356 | G2452 | G2558 | U2655 | C2763 | A2854 |
| A2855 | C1574 | A1661 | U1790 | C1906 | U2018 | U2099 | G2186 | G2279 | U2357 | U2456 | G2559 | U2656 | U2764 | A2855 |
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| U2858 | G1579 | U1581 | A1798 | G1910 | U2023 | A2107 | G2194 | A2287 | C2372 | U2459 | C2566 | C2666 | G2771 | U2858 |
| U2862 | U1582 | U1670 | U1801 | G1913 | C2024 | C2108 | U2195 | G2287 | G2376 | A2460 | C2567 | G2667 | A2772 | U2862 |
| G2863 | G1583 | C1671 | C1802 | G1914 | C2025 | A2109 | G2196 | U2291 | A2377 | A2461 | U2568 | A2668 | A2773 | G2863 |
| A2864 | U1584 | U1672 | U1803 | G1915 | A2026 | U2110 | U2197 | A2292 | C2377 | G2462 | U2569 | G2669 | C2774 | A2864 |
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| U2900 | G1614 | A1703 | U1833 | G1955 | G2058 | G2140 | A2224 | U2313 | G2406 | G2493 | G2605 | U2703 | A2806 | U2900 |
| U     | G1615 | C1704 | G1833 | G1956 | G2059 | A2141 | G2225 | A2319 | U2407 | U2499 | U2610 | U2704 | A2807 | U     |
| A     | U1616 | U1705 | U1836 | G1957 | A2060 | A2145 | U2227 | U2320 | G2407 | G2502 | G2611 | U2705 | U2811 | A     |
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| U     | A1618 | A1715 | C1837 | U1962 | C2062 | A2147 | C2229 | U2325 | C2410 | G2510 | C2618 | U2707 | A2813 | U     |
| G     | U1621 | U1727 | C1839 | U1963 | G2063 | G2148 | A2233 | U2326 | C2411 | U2511 | U2619 | G2710 | A2814 | G     |
| G     | A1624 | U1737 | U1848 | U1963 | G2068 | U2148 | U2239 | G2327 | U2414 | A2512 | U2621 | A2713 | G2820 | G     |
| A     | G1635 | G1737 | G1849 | A1977 | C2069 | G2151 | G2243 | U2328 | G2418 | U2513 | U2622 | G2722 | U2821 | A     |
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| A1644 | U1767 | U1767 | A1854 | U1998 | A2079 | C2157 | U2252 | U2337 | U2432 | A2527 | G2636 | A2741 | U2830 | A1644 |
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|       |       |       |       | G2004 | U2083 | U2161 | C2256 | A2344 | G2435 | A2539 | A2640 | A2751 | G2843 |       |
|       |       |       |       |       | A2084 | U2163 | G2260 |       | G2436 |       |       |       | U2844 |       |
|       |       |       |       |       |       | A2165 |       |       |       |       |       |       |       |       |
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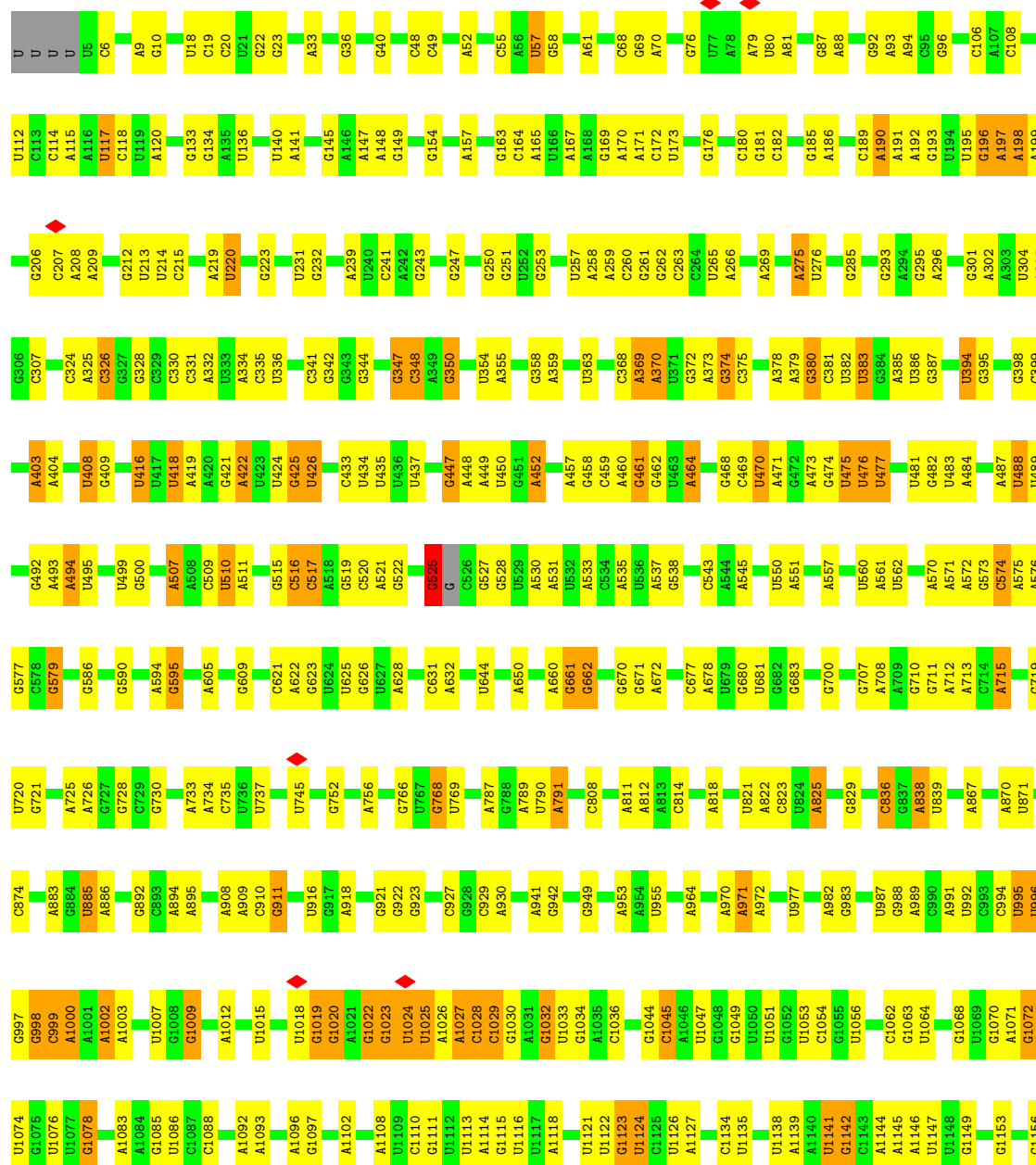
• Molecule 9: 5S ribosomal RNA

Chain 4:  50% 39% 11%



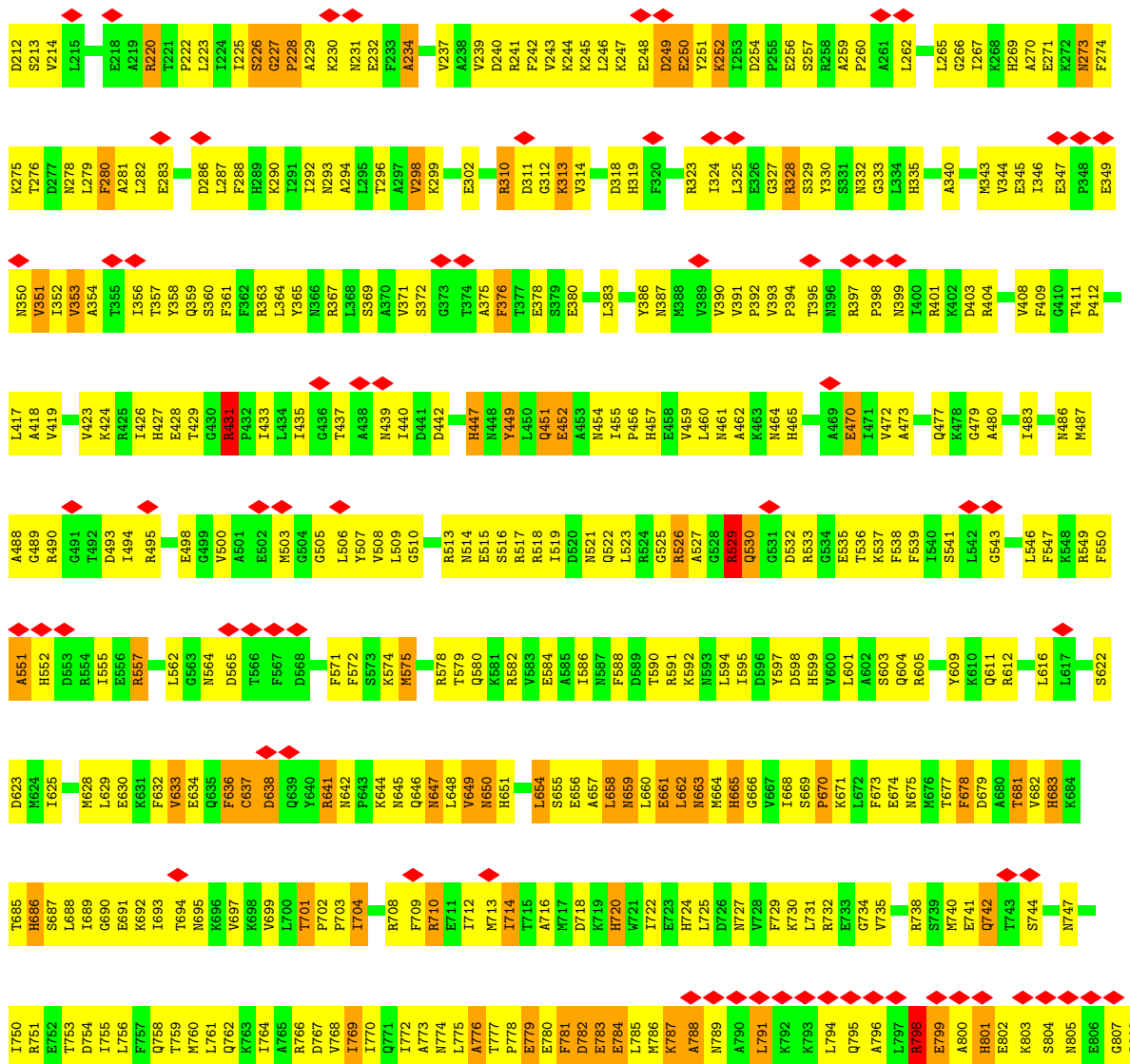
• Molecule 10: 16S ribosomal RNA

Chain 5:  62% 31% 6%

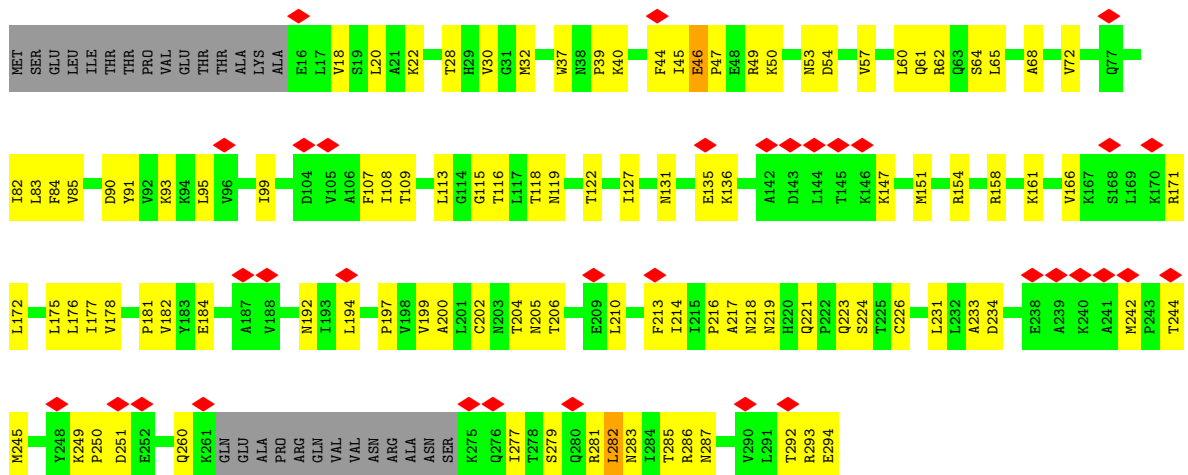




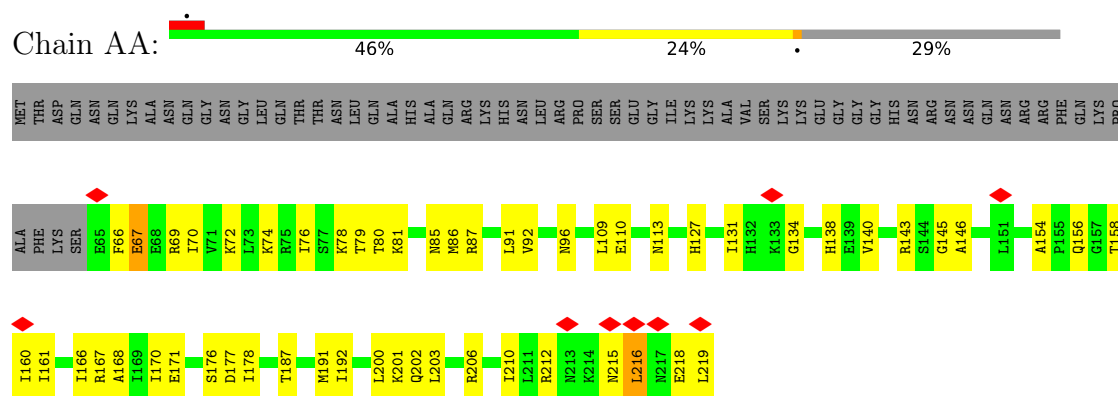




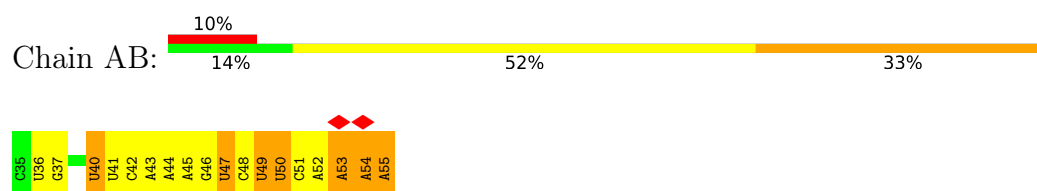
### • Molecule 15: 30S ribosomal protein S2



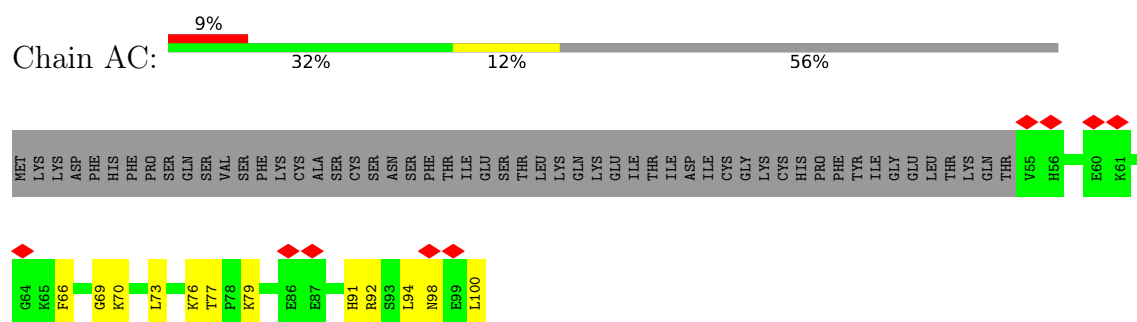
- Molecule 16: 30S ribosomal protein S5



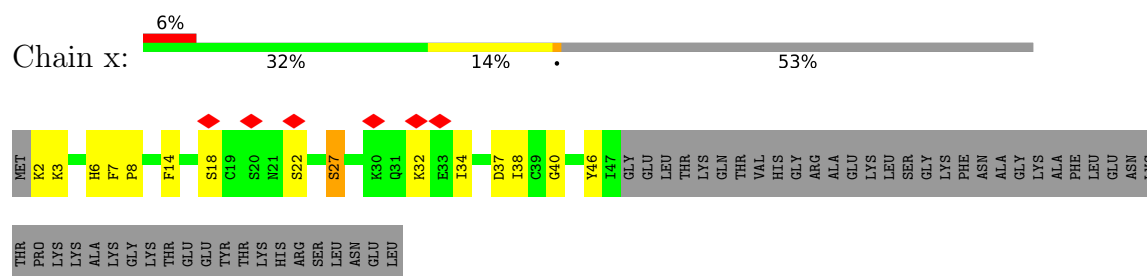
- Molecule 17: mRNA



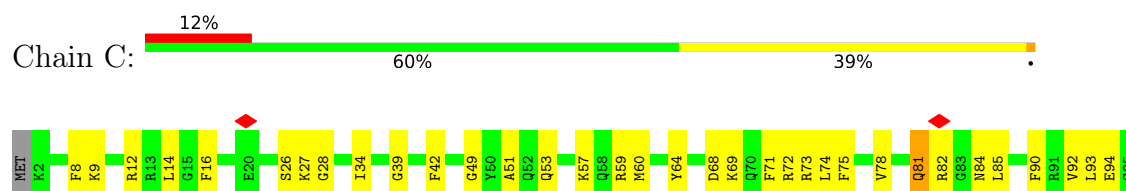
- Molecule 18: 50S ribosomal protein L31

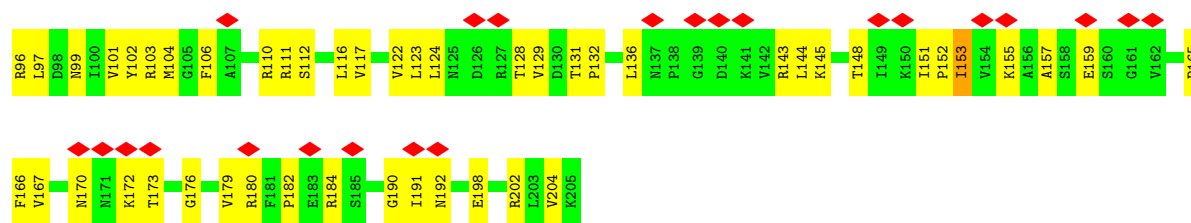


- Molecule 18: 50S ribosomal protein L31

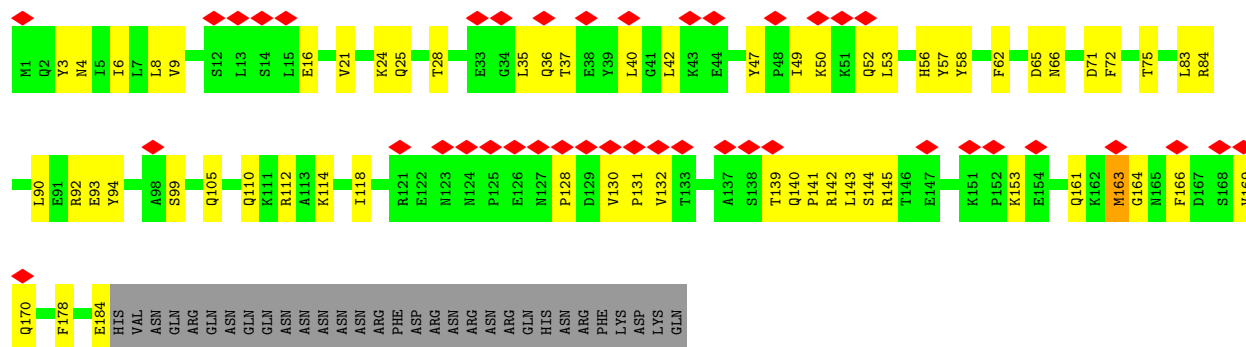


- Molecule 19: 30S ribosomal protein S4

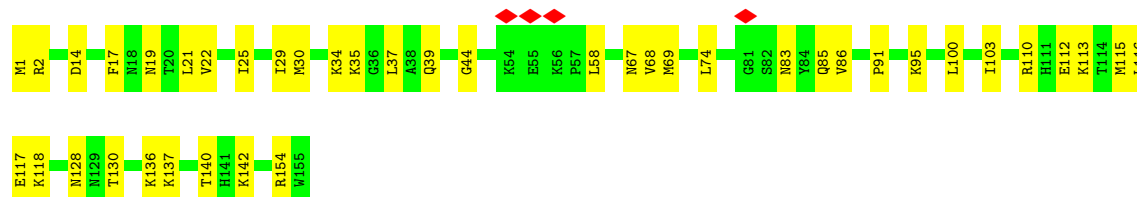
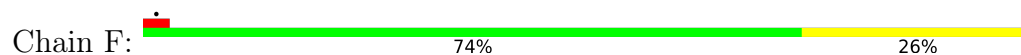




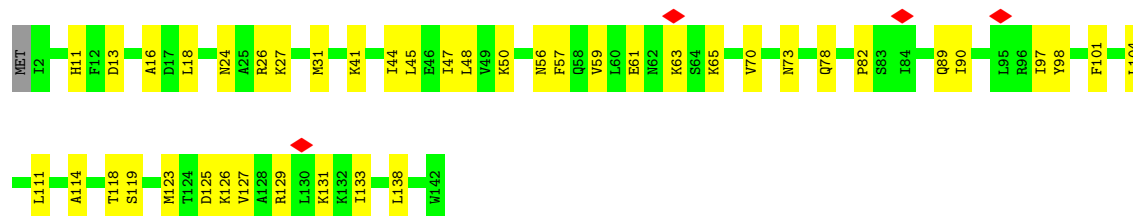
• Molecule 20: 30S ribosomal protein S6



• Molecule 21: 30S ribosomal protein S7

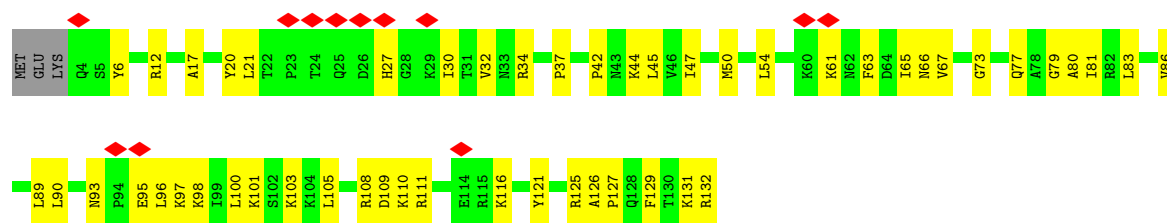


• Molecule 22: 30S ribosomal protein S8

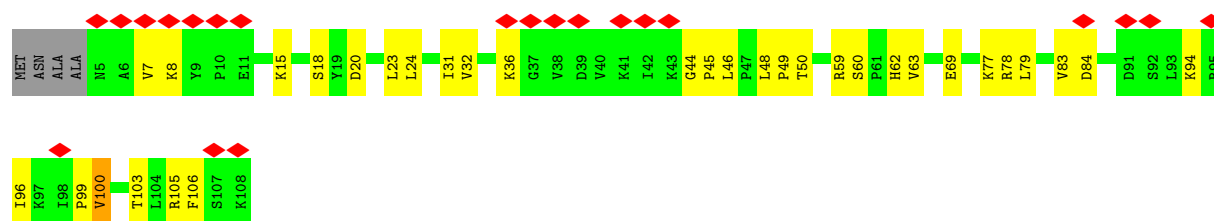


• Molecule 23: Small ribosomal subunit protein uS9

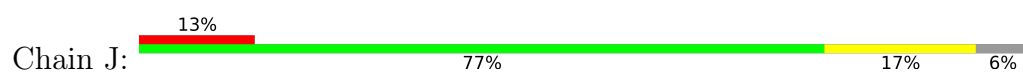




• Molecule 24: 30S ribosomal protein S10



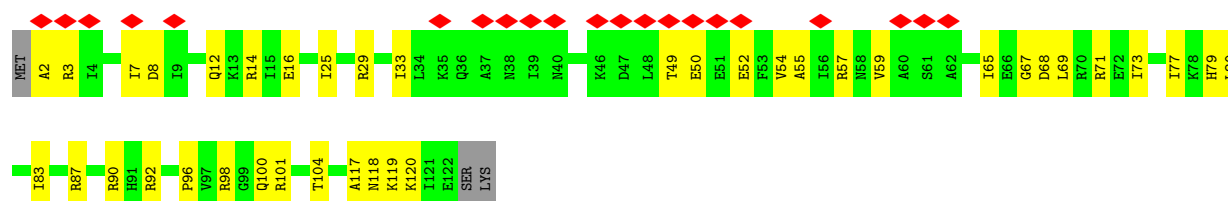
• Molecule 25: 30S ribosomal protein S11



• Molecule 26: 30S ribosomal protein S12



• Molecule 27: 30S ribosomal protein S13



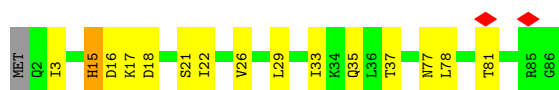
• Molecule 28: 30S ribosomal protein S14 type Z

Chain M:  79% 20% .



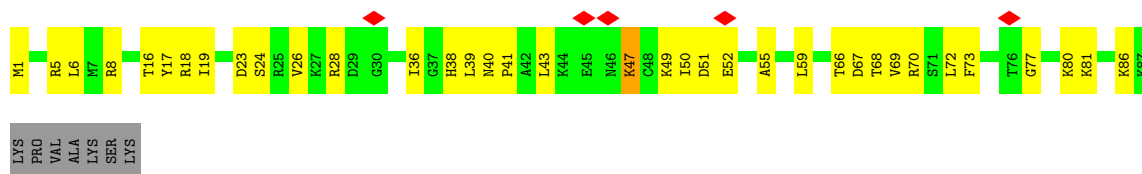
- Molecule 29: 30S ribosomal protein S15

Chain N:  81% 16% ..



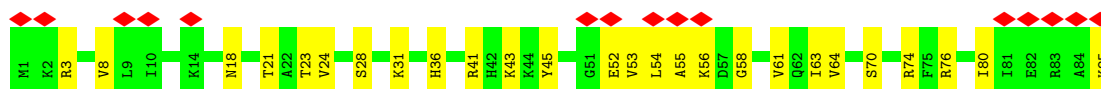
- Molecule 30: 30S ribosomal protein S16

Chain O:  5% 54% 37% 7% .

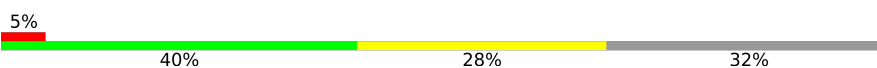


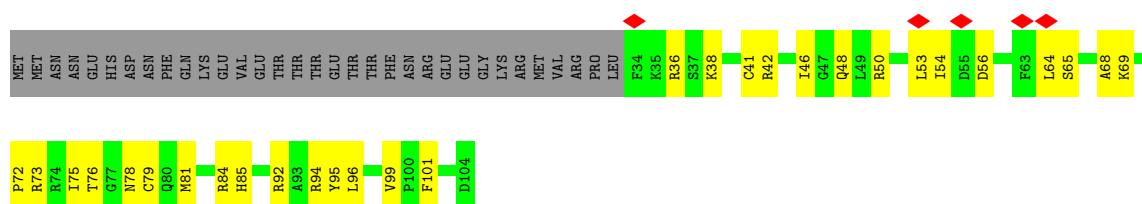
- Molecule 31: 30S ribosomal protein S17

Chain P:  18% 69% 31%



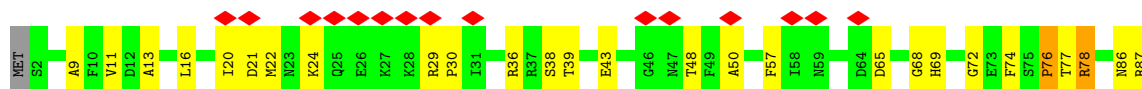
- Molecule 32: 30S ribosomal protein S18

Chain Q:  5% 40% 28% 32%

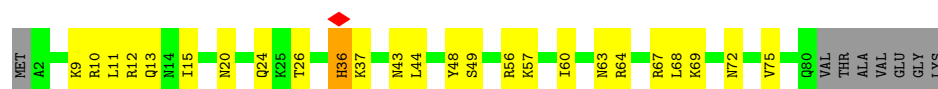


- Molecule 33: 30S ribosomal protein S19

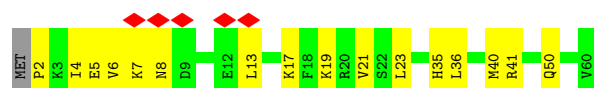
Chain R:  17% 68% 29% ..



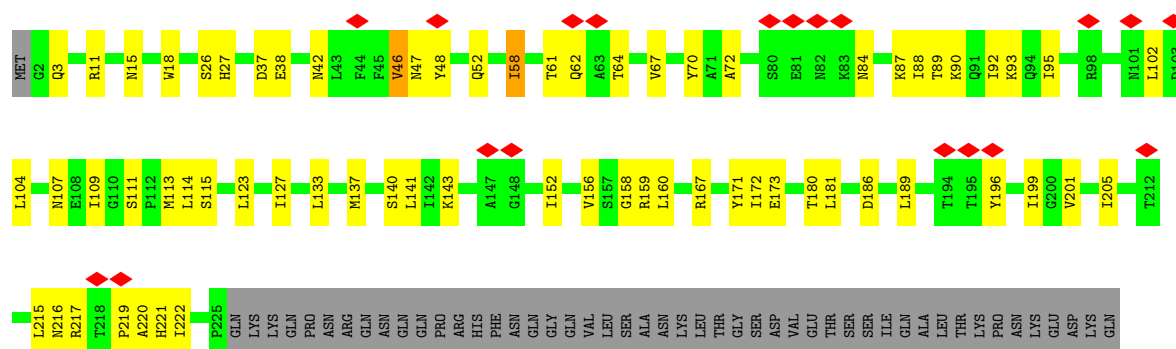
- Molecule 34: 30S ribosomal protein S20



- Molecule 35: 30S ribosomal protein S21



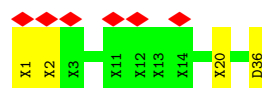
- Molecule 36: 30S ribosomal protein S3



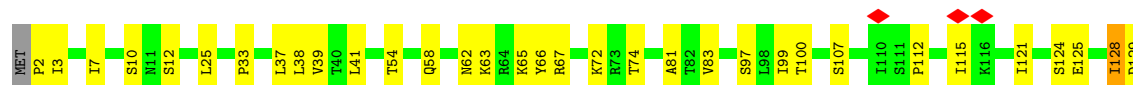
- Molecule 37: mRNA

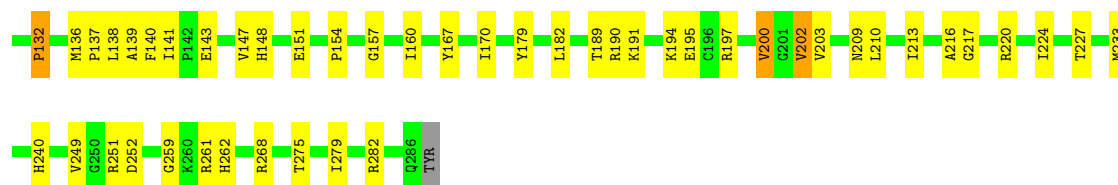


- Molecule 38: Nascent peptide

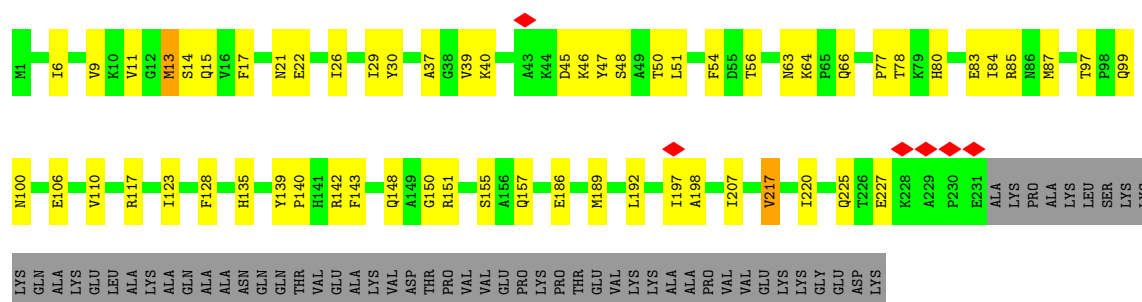


- Molecule 39: 50S ribosomal protein L2

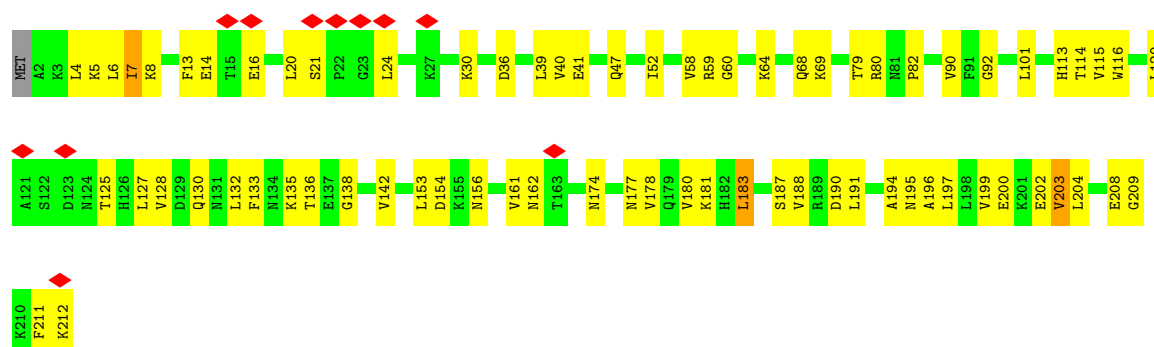




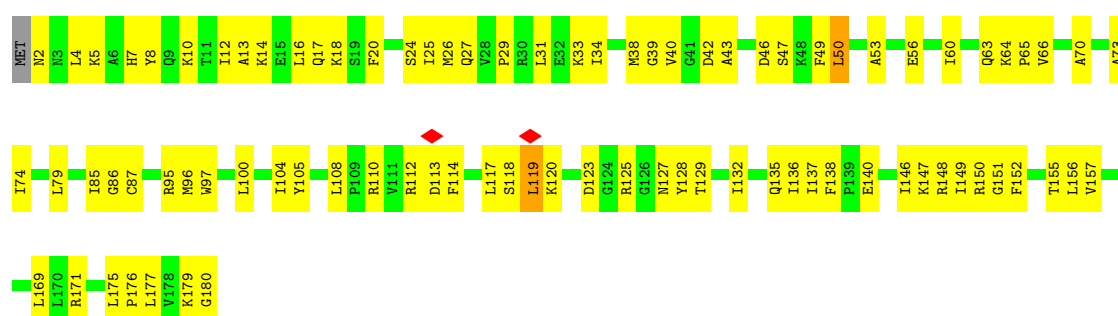
• Molecule 40: 50S ribosomal protein L3



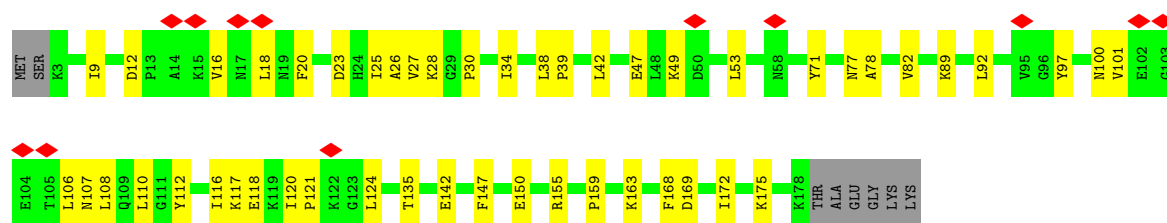
• Molecule 41: 50S ribosomal protein L4



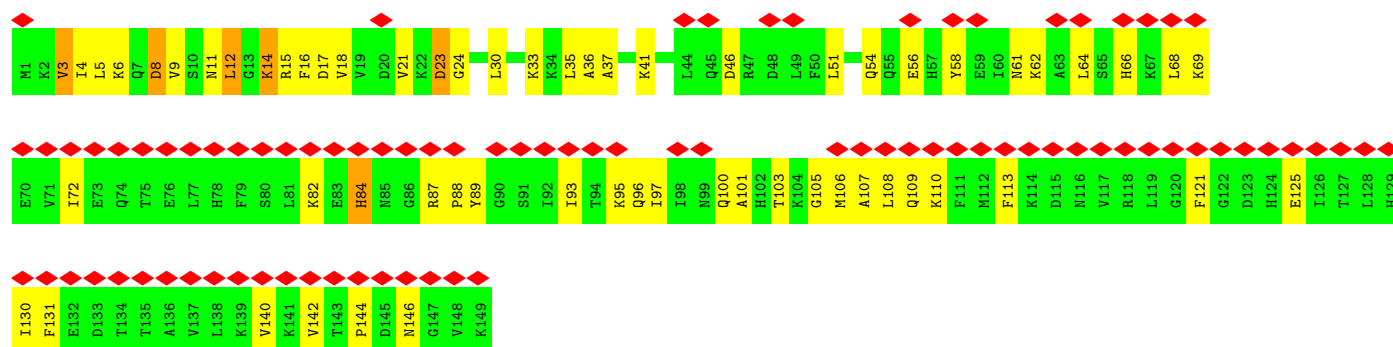
• Molecule 42: 50S ribosomal protein L5



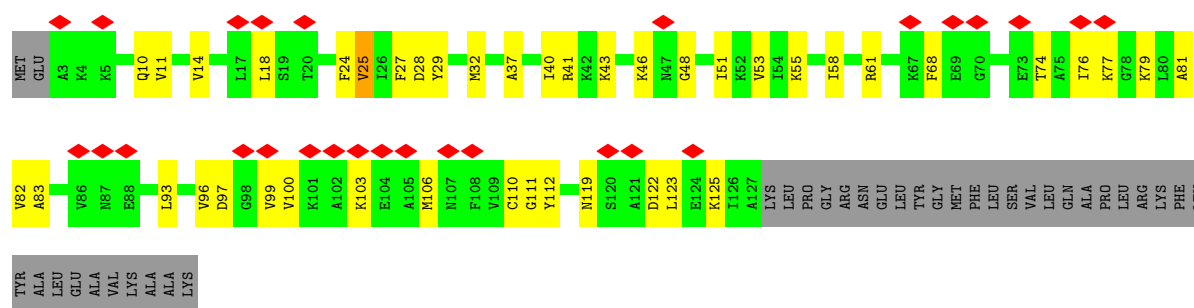
• Molecule 43: 50S ribosomal protein L6



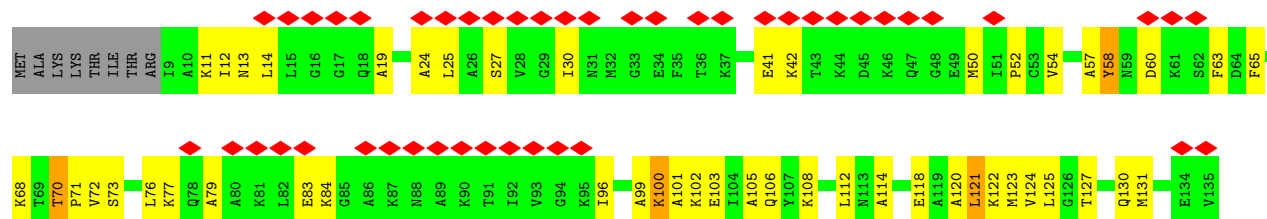
• Molecule 44: 50S ribosomal protein L9



• Molecule 45: 50S ribosomal protein L10



• Molecule 46: 50S ribosomal protein L11





- Molecule 47: 50S ribosomal protein L13

Chain i: 78% 18% ..



- Molecule 48: 50S ribosomal protein L14

Chain j: 70% 28% .



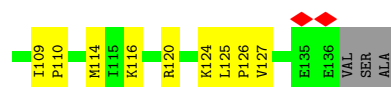
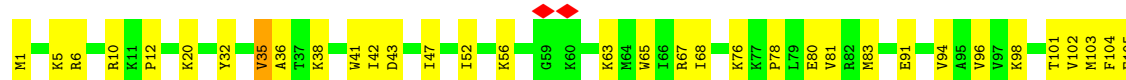
- Molecule 49: 50S ribosomal protein L15

Chain k: 71% 26% ..



- Molecule 50: 50S ribosomal protein L16

Chain l: 67% 30% ..

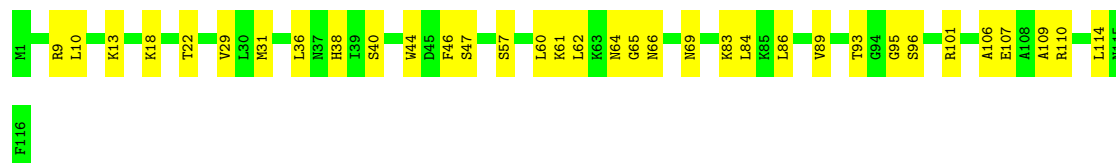


- Molecule 51: 50S ribosomal protein L17

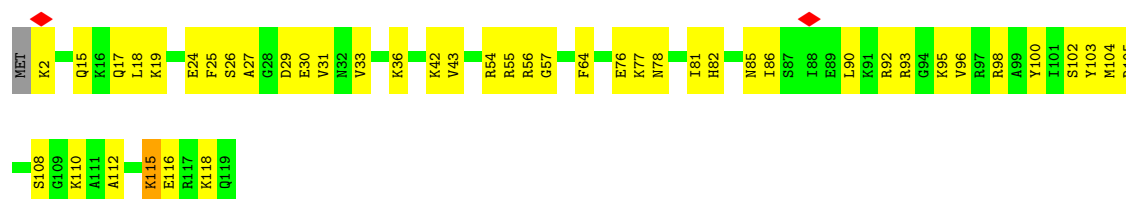
Chain m: 73% 22% ..



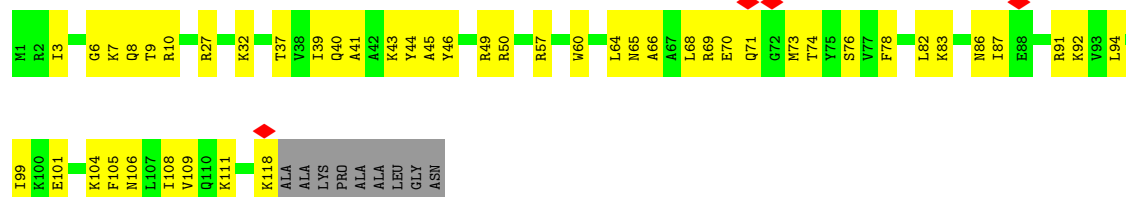
- Molecule 52: Large ribosomal subunit protein uL18



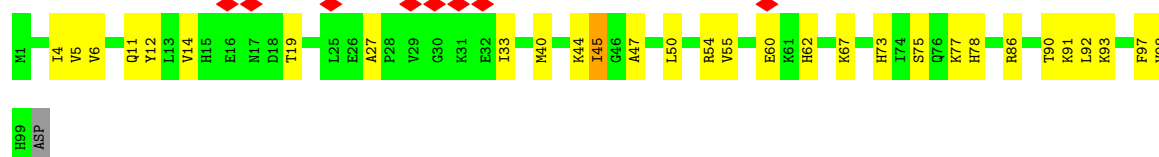
- Molecule 53: 50S ribosomal protein L19



- Molecule 54: 50S ribosomal protein L20

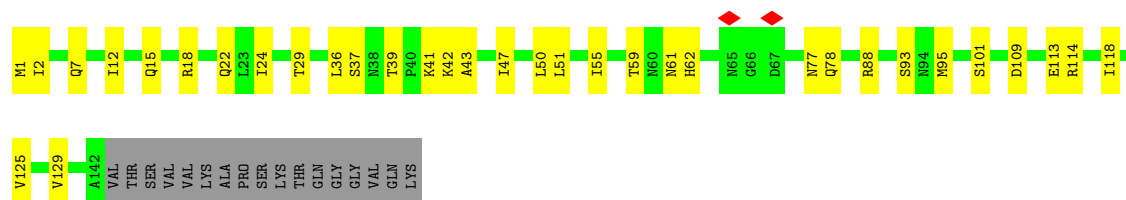


- Molecule 55: 50S ribosomal protein L21

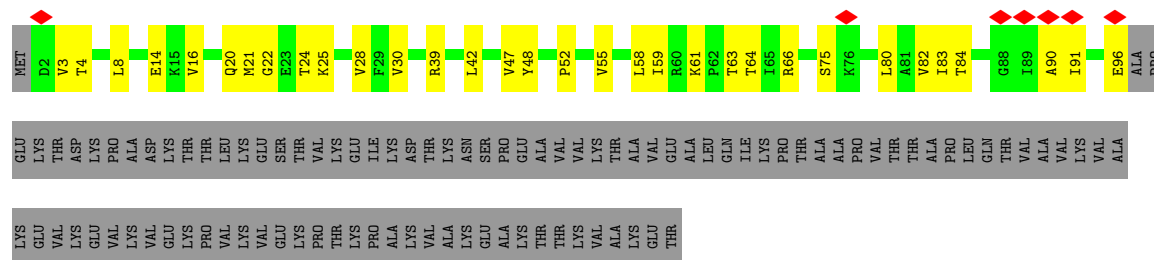
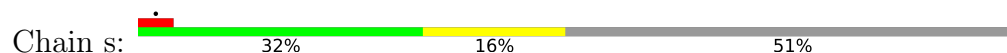


- Molecule 56: 50S ribosomal protein L22

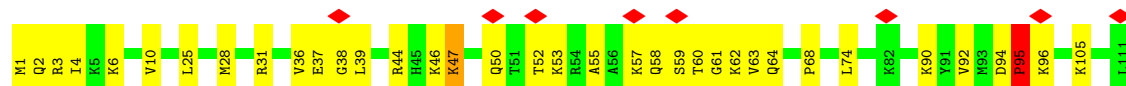




• Molecule 57: Large ribosomal subunit protein uL23



• Molecule 58: 50S ribosomal protein L24



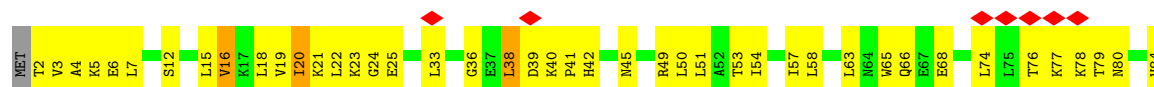
• Molecule 59: 50S ribosomal protein L27



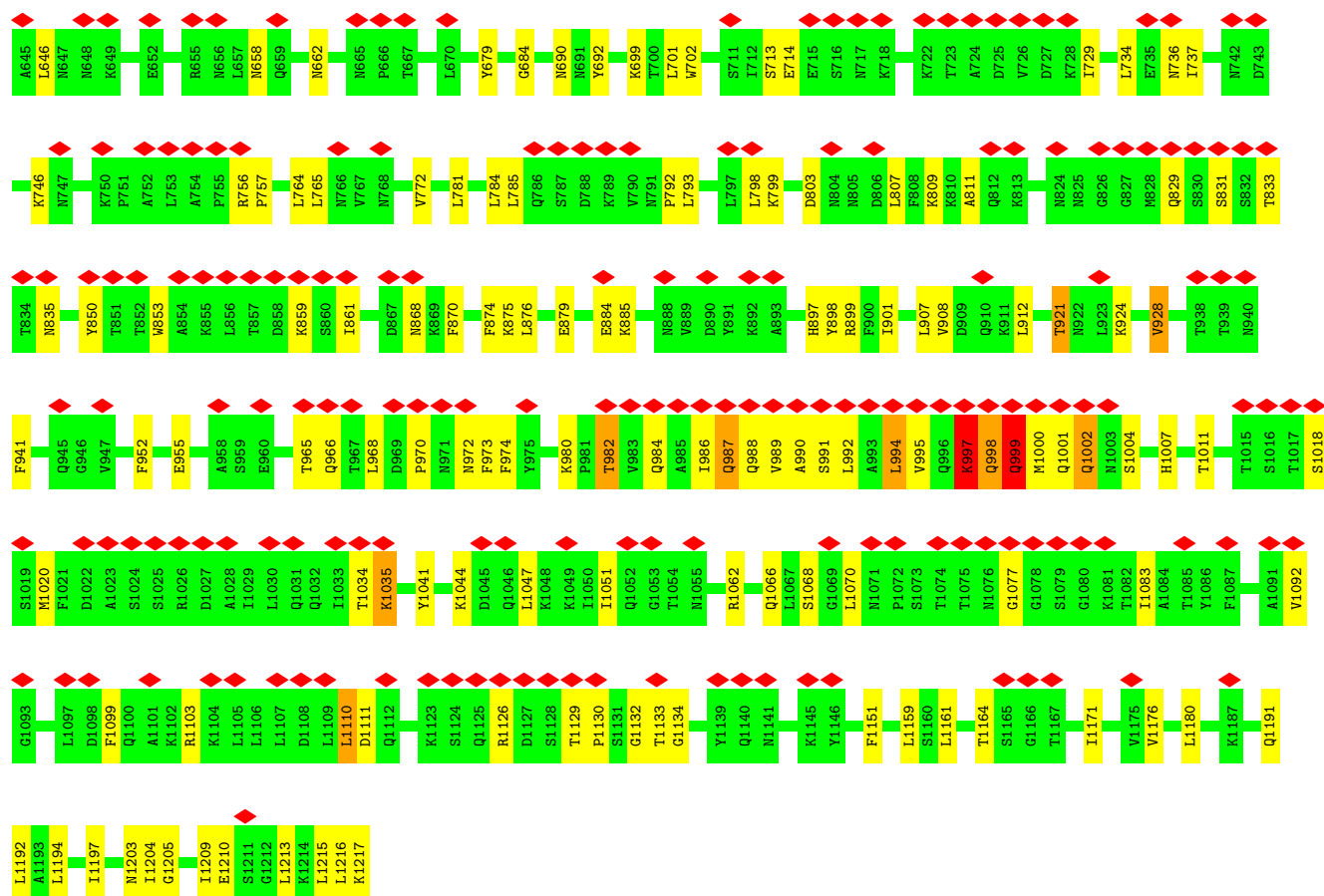
• Molecule 60: 50S ribosomal protein L28



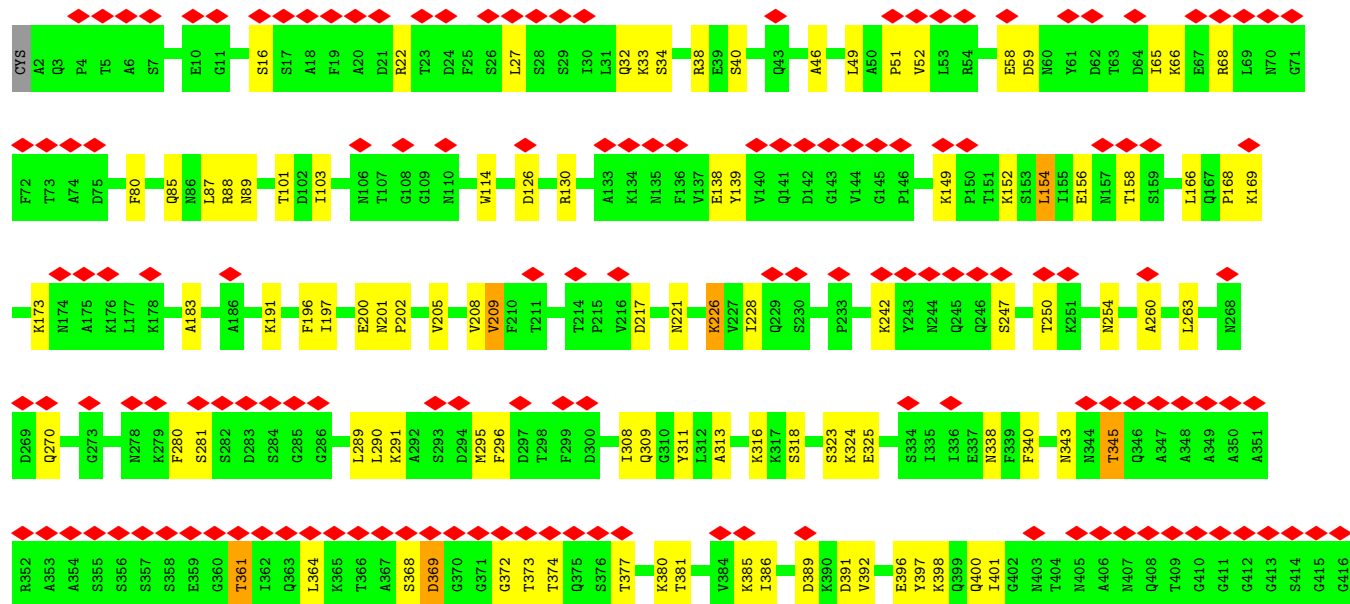
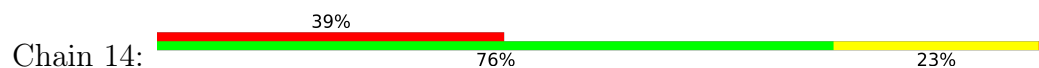
• Molecule 61: 50S ribosomal protein L29

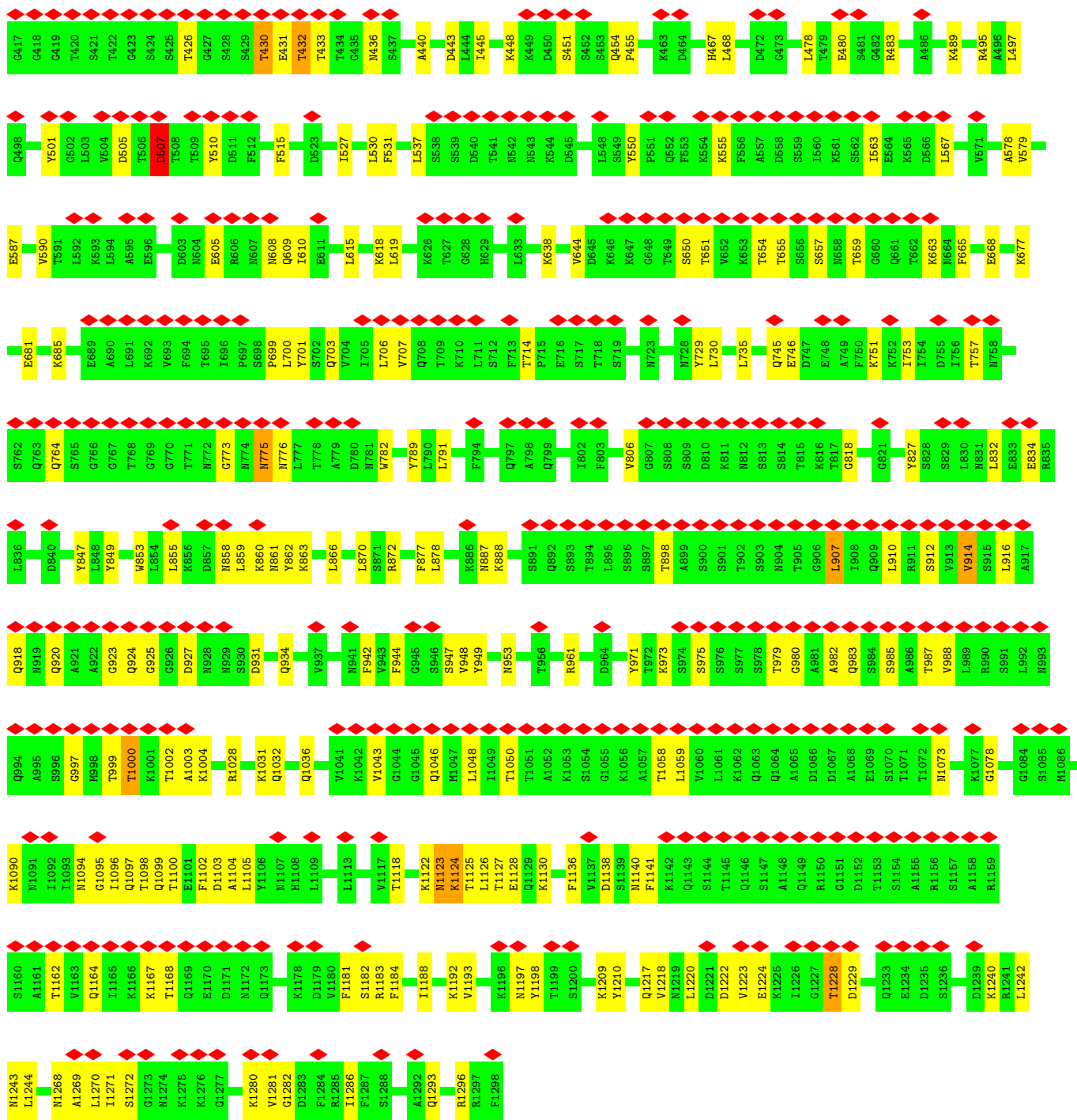




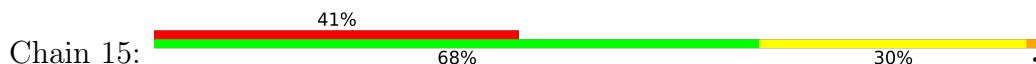


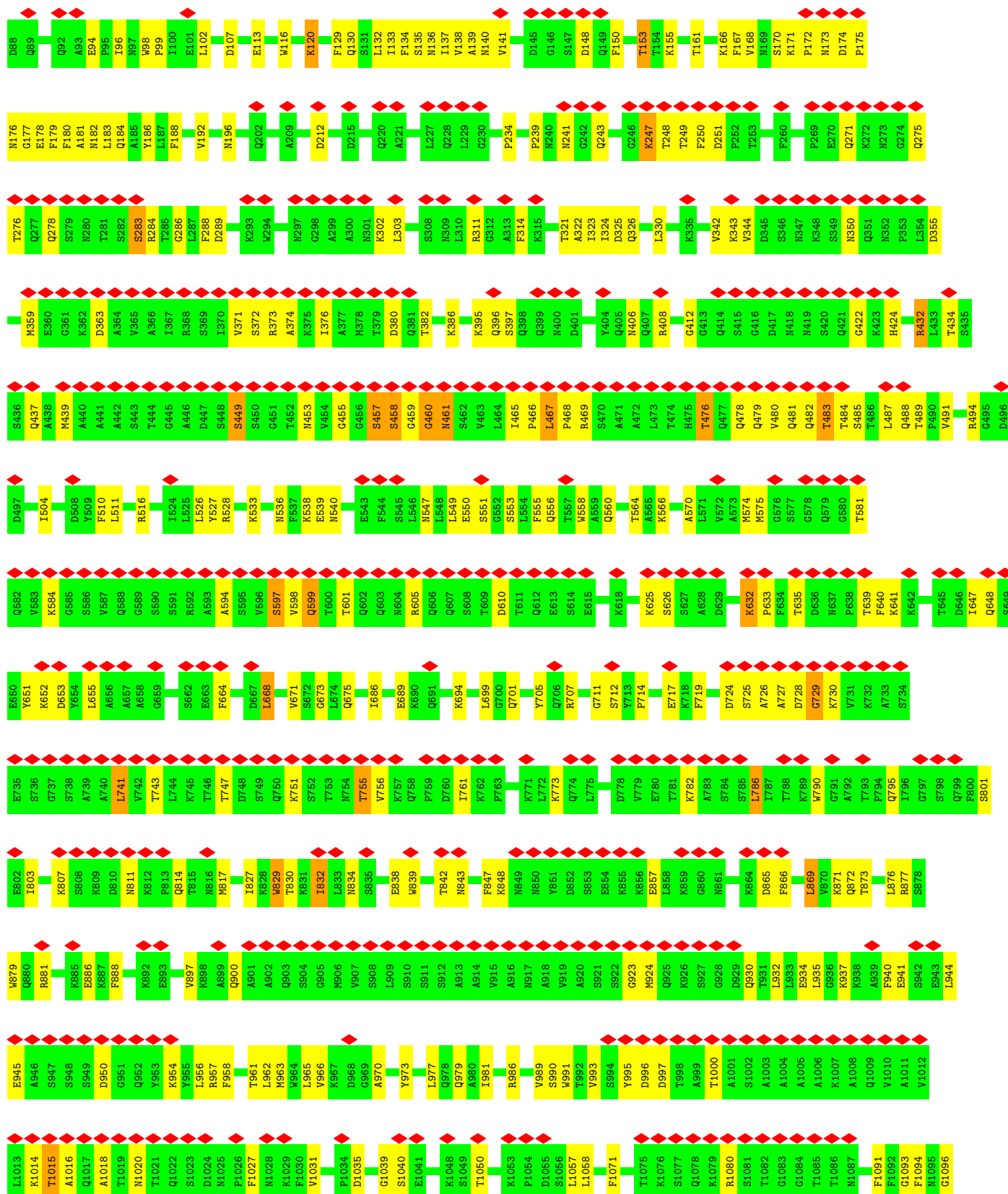
• Molecule 65: Uncharacterized lipoprotein MG309 homolog

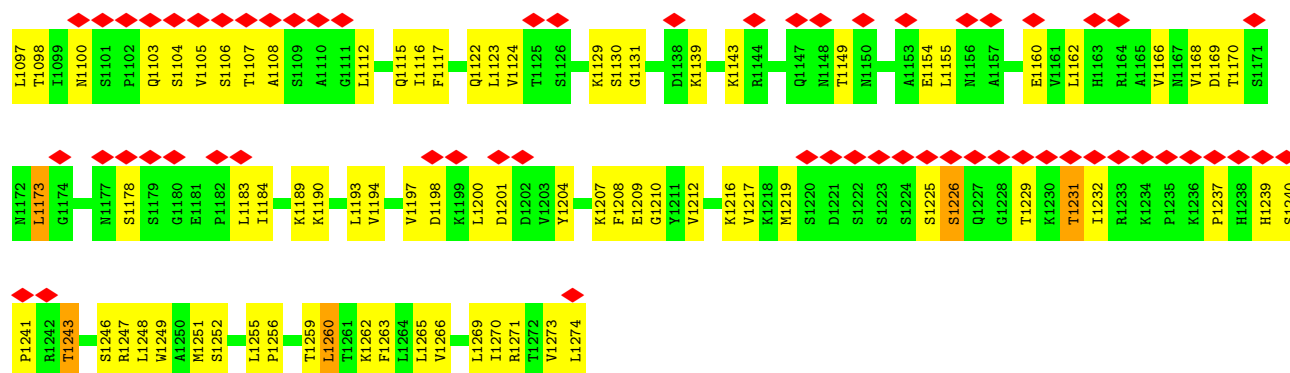




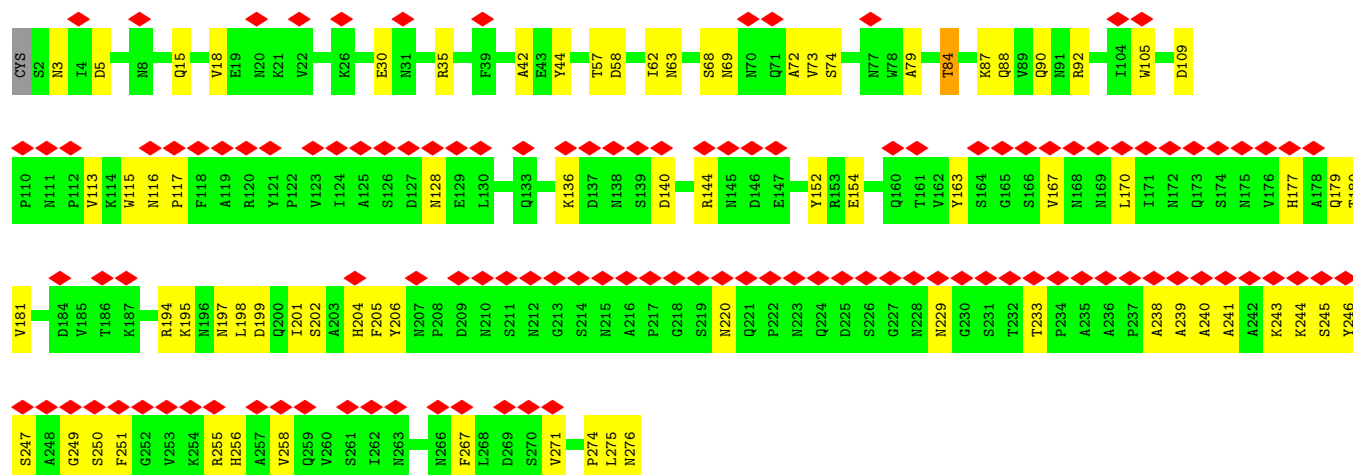
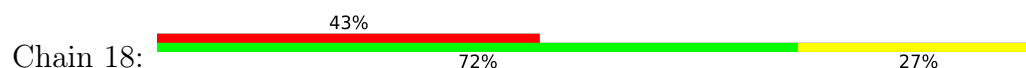
• Molecule 66: Uncharacterized lipoprotein MG338 homolog



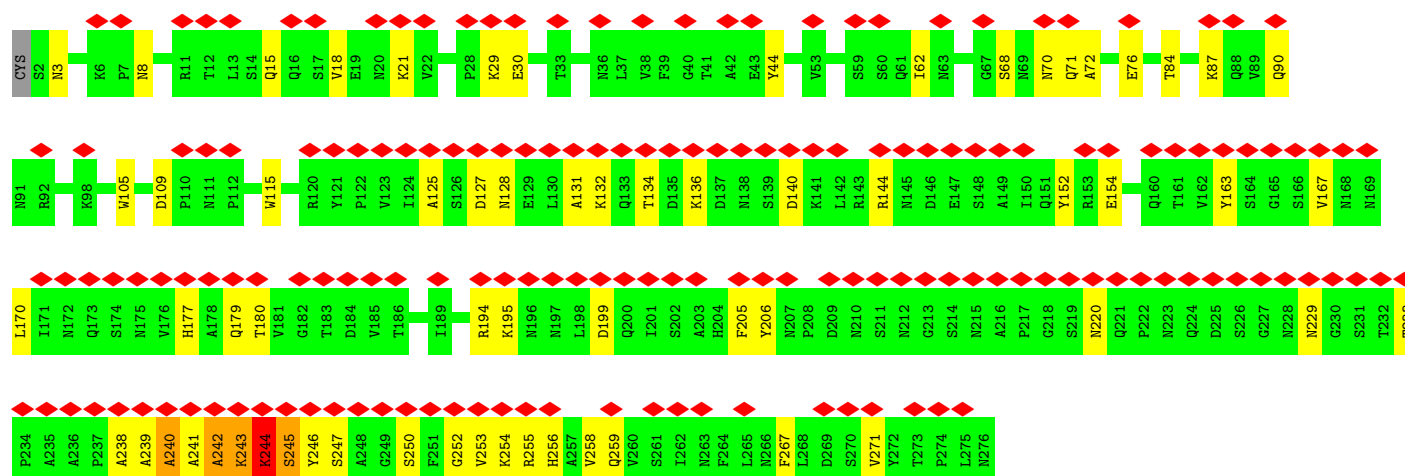




• Molecule 67: Uncharacterized lipoprotein MG348 homolog



• Molecule 67: Uncharacterized lipoprotein MG348 homolog



## 4 Experimental information

| Property                             | Value                                                    | Source    |
|--------------------------------------|----------------------------------------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING                                    | Depositor |
| Imposed symmetry                     | POINT, C1                                                | Depositor |
| Number of subtomograms used          | 2304                                                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                        | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY                                      | Depositor |
| Microscope                           | TFS KRIOS                                                | Depositor |
| Voltage (kV)                         | 300                                                      | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 130, 137                                                 | Depositor |
| Minimum defocus (nm)                 | 1000                                                     | Depositor |
| Maximum defocus (nm)                 | 4000                                                     | Depositor |
| Magnification                        | Not provided                                             |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 3.152                                                    | Depositor |
| Minimum map value                    | -1.126                                                   | Depositor |
| Average map value                    | 0.012                                                    | Depositor |
| Map value standard deviation         | 0.137                                                    | Depositor |
| Recommended contour level            | 0.62                                                     | Depositor |
| Map size (Å)                         | 742.4, 742.4, 742.4                                      | wwPDB     |
| Map dimensions                       | 256, 256, 256                                            | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                         | wwPDB     |
| Pixel spacing (Å)                    | 2.9, 2.9, 2.9                                            | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, K, PUT, PSU, 4SU, U8U, ZN, MA6, MIA, G7M, 3AU, MG, 5MU

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   | 0     | 0.12         | 0/383           | 0.25        | 0/504           |
| 2   | 1     | 0.12         | 0/484           | 0.31        | 0/637           |
| 3   | 10    | 2.25         | 120/3556 (3.4%) | 2.54        | 249/4839 (5.1%) |
| 4   | 11    | 2.30         | 24/592 (4.1%)   | 2.66        | 48/795 (6.0%)   |
| 5   | 12    | 2.17         | 24/864 (2.8%)   | 2.53        | 74/1154 (6.4%)  |
| 6   | 17    | 0.75         | 0/7779          | 1.29        | 16/10551 (0.2%) |
| 7   | 2     | 0.13         | 0/306           | 0.36        | 0/401           |
| 8   | 3     | 0.12         | 0/69441         | 0.26        | 0/108286        |
| 9   | 4     | 0.15         | 0/2578          | 0.28        | 0/4016          |
| 10  | 5     | 0.10         | 0/36037         | 0.21        | 0/56183         |
| 11  | 6     | 0.07         | 0/46            | 0.14        | 0/69            |
| 12  | 7     | 0.19         | 0/1650          | 0.33        | 0/2565          |
| 13  | 8     | 0.58         | 9/1665 (0.5%)   | 0.33        | 0/2588          |
| 14  | 9     | 2.57         | 261/6575 (4.0%) | 2.50        | 469/8870 (5.3%) |
| 15  | A     | 0.15         | 0/2172          | 0.42        | 0/2934          |
| 16  | AA    | 0.13         | 0/1206          | 0.37        | 0/1616          |
| 17  | AB    | 0.15         | 0/490           | 0.37        | 0/759           |
| 18  | AC    | 0.14         | 0/347           | 0.54        | 0/457           |
| 18  | x     | 0.15         | 0/375           | 0.38        | 0/502           |
| 19  | C     | 0.15         | 0/1700          | 0.46        | 1/2278 (0.0%)   |
| 20  | E     | 0.37         | 2/1536 (0.1%)   | 0.93        | 5/2072 (0.2%)   |
| 21  | F     | 0.14         | 0/1274          | 0.40        | 0/1710          |
| 22  | G     | 0.13         | 0/1126          | 0.37        | 0/1517          |
| 23  | H     | 0.17         | 0/1058          | 0.49        | 0/1413          |
| 24  | I     | 0.14         | 0/843           | 0.37        | 0/1132          |
| 25  | J     | 0.13         | 0/844           | 0.36        | 0/1136          |
| 26  | K     | 0.12         | 0/1089          | 0.40        | 0/1461          |
| 27  | L     | 0.14         | 0/986           | 0.39        | 0/1321          |
| 28  | M     | 0.11         | 0/483           | 0.29        | 0/643           |
| 29  | N     | 0.14         | 0/695           | 0.41        | 0/926           |
| 30  | O     | 0.22         | 0/718           | 0.62        | 1/962 (0.1%)    |
| 31  | P     | 0.13         | 0/702           | 0.37        | 0/934           |

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5           |
| 32  | Q     | 0.15         | 0/601             | 0.37        | 0/801             |
| 33  | R     | 0.19         | 0/716             | 0.55        | 1/958 (0.1%)      |
| 34  | S     | 0.14         | 0/645             | 0.38        | 0/857             |
| 35  | T     | 0.14         | 0/524             | 0.37        | 0/685             |
| 36  | W     | 0.16         | 0/1791            | 0.45        | 0/2421            |
| 37  | Y     | 0.09         | 0/140             | 0.24        | 0/215             |
| 38  | Z     | 0.09         | 0/26              | 0.33        | 0/33              |
| 39  | a     | 0.54         | 1/2267 (0.0%)     | 0.48        | 2/3044 (0.1%)     |
| 40  | b     | 0.29         | 1/1811 (0.1%)     | 0.40        | 0/2432            |
| 41  | c     | 0.17         | 0/1681            | 0.42        | 0/2257            |
| 42  | d     | 0.28         | 0/1437            | 0.56        | 0/1931            |
| 43  | e     | 0.43         | 2/1420 (0.1%)     | 0.90        | 5/1912 (0.3%)     |
| 44  | f     | 0.26         | 0/1231            | 0.55        | 0/1650            |
| 45  | g     | 0.22         | 0/960             | 0.42        | 0/1284            |
| 46  | h     | 0.30         | 0/968             | 0.51        | 0/1298            |
| 47  | i     | 0.16         | 0/1186            | 0.36        | 0/1592            |
| 48  | j     | 0.32         | 0/953             | 0.48        | 0/1275            |
| 49  | k     | 0.16         | 0/1187            | 0.99        | 3/1581 (0.2%)     |
| 50  | l     | 0.22         | 0/1104            | 0.45        | 0/1481            |
| 51  | m     | 0.15         | 0/973             | 0.34        | 0/1309            |
| 52  | n     | 0.15         | 0/927             | 0.38        | 0/1239            |
| 53  | o     | 0.19         | 0/976             | 0.44        | 0/1296            |
| 54  | p     | 0.20         | 0/996             | 0.42        | 0/1325            |
| 55  | q     | 0.15         | 0/828             | 0.41        | 0/1111            |
| 56  | r     | 0.15         | 0/1100            | 0.42        | 2/1471 (0.1%)     |
| 57  | s     | 0.27         | 0/752             | 0.51        | 0/1015            |
| 58  | t     | 0.53         | 2/878 (0.2%)      | 0.84        | 5/1165 (0.4%)     |
| 59  | u     | 0.26         | 0/678             | 0.50        | 0/902             |
| 60  | v     | 0.13         | 0/526             | 0.33        | 0/703             |
| 61  | w     | 0.16         | 0/916             | 0.39        | 0/1222            |
| 62  | y     | 0.13         | 0/457             | 0.37        | 0/601             |
| 63  | z     | 0.13         | 0/412             | 0.36        | 0/547             |
| 64  | 13    | 0.85         | 4/9772 (0.0%)     | 1.05        | 3/13211 (0.0%)    |
| 65  | 14    | 0.88         | 9/10260 (0.1%)    | 1.06        | 4/13850 (0.0%)    |
| 66  | 15    | 0.91         | 9/10076 (0.1%)    | 1.10        | 9/13621 (0.1%)    |
| 67  | 16    | 0.90         | 3/2184 (0.1%)     | 1.08        | 1/2975 (0.0%)     |
| 67  | 18    | 0.78         | 0/2184            | 1.04        | 0/2975            |
| All | All   | 0.70         | 471/215143 (0.2%) | 0.79        | 898/313476 (0.3%) |

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 |
|-----|-------|---------------------|---------------------|
| 3   | 10    | 0                   | 10                  |
| 5   | 12    | 0                   | 1                   |
| 6   | 17    | 0                   | 10                  |
| 14  | 9     | 0                   | 16                  |
| 64  | 13    | 0                   | 6                   |
| 65  | 14    | 0                   | 1                   |
| 66  | 15    | 0                   | 16                  |
| 67  | 16    | 0                   | 1                   |
| All | All   | 0                   | 61                  |

All (471) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 14  | 9     | 13   | ARG  | CZ-NH2  | 65.18  | 2.18        | 1.33     |
| 14  | 9     | 376  | PHE  | CG-CD2  | 31.25  | 2.04        | 1.38     |
| 14  | 9     | 376  | PHE  | CG-CD1  | 30.33  | 2.02        | 1.38     |
| 39  | a     | 132  | PRO  | N-CD    | 24.41  | 1.81        | 1.47     |
| 14  | 9     | 376  | PHE  | CD2-CE2 | 23.05  | 2.07        | 1.38     |
| 14  | 9     | 376  | PHE  | CD1-CE1 | 21.38  | 2.02        | 1.38     |
| 14  | 9     | 376  | PHE  | CE1-CZ  | 21.09  | 2.02        | 1.38     |
| 14  | 9     | 376  | PHE  | CE2-CZ  | 20.00  | 1.98        | 1.38     |
| 65  | 14    | 1031 | LYS  | CE-NZ   | -17.78 | 0.96        | 1.49     |
| 64  | 13    | 1035 | LYS  | CE-NZ   | -17.33 | 0.97        | 1.49     |
| 66  | 15    | 1015 | THR  | CB-OG1  | -16.84 | 1.16        | 1.43     |
| 67  | 16    | 132  | LYS  | CE-NZ   | -16.34 | 1.00        | 1.49     |
| 66  | 15    | 694  | LYS  | CE-NZ   | -16.11 | 1.01        | 1.49     |
| 65  | 14    | 149  | LYS  | CE-NZ   | -15.78 | 1.02        | 1.49     |
| 66  | 15    | 120  | LYS  | CE-NZ   | -15.32 | 1.03        | 1.49     |
| 65  | 14    | 226  | LYS  | CE-NZ   | -14.49 | 1.05        | 1.49     |
| 66  | 15    | 395  | LYS  | CE-NZ   | -13.59 | 1.08        | 1.49     |
| 66  | 15    | 247  | LYS  | CE-NZ   | -13.47 | 1.08        | 1.49     |
| 65  | 14    | 1124 | LYS  | CE-NZ   | -13.06 | 1.10        | 1.49     |
| 65  | 14    | 860  | LYS  | CE-NZ   | -12.89 | 1.10        | 1.49     |
| 64  | 13    | 281  | LYS  | CE-NZ   | -12.72 | 1.11        | 1.49     |
| 65  | 14    | 385  | LYS  | CE-NZ   | -12.39 | 1.12        | 1.49     |
| 64  | 13    | 250  | LYS  | CE-NZ   | -12.38 | 1.12        | 1.49     |
| 58  | t     | 95   | PRO  | CG-CD   | -12.08 | 1.09        | 1.50     |
| 43  | e     | 30   | PRO  | CG-CD   | -11.49 | 1.11        | 1.50     |
| 64  | 13    | 71   | LYS  | CE-NZ   | -11.13 | 1.16        | 1.49     |
| 3   | 10    | 416  | GLY  | N-CA    | 11.11  | 1.56        | 1.44     |
| 14  | 9     | 509  | LEU  | C-N     | -10.64 | 1.28        | 1.33     |
| 66  | 15    | 1015 | THR  | CB-CG2  | -10.39 | 1.18        | 1.52     |
| 14  | 9     | 329  | SER  | C-N     | 9.86   | 1.46        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 9     | 514  | ASN  | N-CA    | -9.81 | 1.32        | 1.45     |
| 66  | 15    | 632  | LYS  | CE-NZ   | -9.73 | 1.20        | 1.49     |
| 40  | b     | 77   | PRO  | N-CD    | -9.72 | 1.34        | 1.47     |
| 3   | 10    | 206  | LEU  | N-CA    | -9.51 | 1.34        | 1.46     |
| 3   | 10    | 228  | ASN  | N-CA    | -9.44 | 1.35        | 1.46     |
| 14  | 9     | 591  | ARG  | CD-NE   | 9.16  | 1.59        | 1.46     |
| 3   | 10    | 259  | ARG  | NE-CZ   | 9.12  | 1.43        | 1.33     |
| 20  | E     | 128  | PRO  | CB-CG   | -9.04 | 1.04        | 1.49     |
| 14  | 9     | 755  | ILE  | CA-C    | -8.96 | 1.42        | 1.52     |
| 67  | 16    | 132  | LYS  | C-N     | -8.94 | 1.22        | 1.33     |
| 3   | 10    | 130  | ILE  | C-N     | 8.84  | 1.43        | 1.34     |
| 14  | 9     | 483  | ILE  | CA-C    | -8.73 | 1.42        | 1.52     |
| 14  | 9     | 90   | GLY  | CA-C    | -8.72 | 1.42        | 1.52     |
| 14  | 9     | 324  | ILE  | N-CA    | -8.70 | 1.35        | 1.46     |
| 14  | 9     | 516  | SER  | CA-C    | -8.69 | 1.42        | 1.52     |
| 14  | 9     | 351  | VAL  | C-N     | 8.62  | 1.43        | 1.33     |
| 14  | 9     | 83   | ALA  | N-CA    | -8.56 | 1.35        | 1.46     |
| 4   | 11    | 40   | GLU  | CA-C    | -8.56 | 1.42        | 1.52     |
| 14  | 9     | 369  | SER  | CA-C    | -8.48 | 1.42        | 1.52     |
| 14  | 9     | 783  | GLU  | C-N     | 8.42  | 1.45        | 1.33     |
| 3   | 10    | 244  | PHE  | CA-CB   | 8.34  | 1.66        | 1.53     |
| 14  | 9     | 17   | TYR  | CA-C    | -8.30 | 1.42        | 1.52     |
| 14  | 9     | 708  | ARG  | NE-CZ   | 8.30  | 1.42        | 1.33     |
| 5   | 12    | 103  | ALA  | CA-C    | 8.28  | 1.63        | 1.52     |
| 3   | 10    | 314  | SER  | N-CA    | -8.10 | 1.36        | 1.46     |
| 3   | 10    | 317  | PHE  | CA-C    | -8.06 | 1.42        | 1.52     |
| 20  | E     | 128  | PRO  | CG-CD   | -8.03 | 1.23        | 1.50     |
| 14  | 9     | 345  | GLU  | C-N     | 8.00  | 1.43        | 1.33     |
| 14  | 9     | 724  | HIS  | ND1-CE1 | 7.97  | 1.40        | 1.32     |
| 14  | 9     | 49   | LEU  | CA-C    | -7.96 | 1.42        | 1.52     |
| 14  | 9     | 408  | VAL  | N-CA    | -7.96 | 1.36        | 1.46     |
| 14  | 9     | 776  | ALA  | N-CA    | -7.95 | 1.36        | 1.46     |
| 14  | 9     | 214  | VAL  | CA-CB   | -7.93 | 1.45        | 1.54     |
| 14  | 9     | 686  | HIS  | CA-C    | -7.93 | 1.42        | 1.52     |
| 14  | 9     | 259  | ALA  | CA-C    | 7.90  | 1.62        | 1.52     |
| 14  | 9     | 498  | GLU  | CA-CB   | 7.87  | 1.63        | 1.52     |
| 5   | 12    | 100  | LEU  | C-N     | 7.81  | 1.43        | 1.33     |
| 3   | 10    | 163  | GLY  | CA-C    | -7.80 | 1.44        | 1.52     |
| 66  | 15    | 1015 | THR  | N-CA    | -7.77 | 1.36        | 1.46     |
| 43  | e     | 30   | PRO  | CB-CG   | -7.75 | 1.10        | 1.49     |
| 14  | 9     | 718  | ASP  | CA-CB   | 7.69  | 1.65        | 1.53     |
| 13  | 8     | 16   | U    | C5-C6   | 7.64  | 1.49        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 10    | 195 | ASN  | CA-CB   | 7.61  | 1.62        | 1.53     |
| 14  | 9     | 62  | ASP  | CA-C    | -7.60 | 1.46        | 1.52     |
| 13  | 8     | 17  | U    | C5-C6   | 7.59  | 1.49        | 1.34     |
| 14  | 9     | 714 | ILE  | N-CA    | -7.57 | 1.37        | 1.46     |
| 13  | 8     | 20  | U    | C5-C6   | 7.50  | 1.49        | 1.34     |
| 3   | 10    | 466 | LEU  | CA-CB   | 7.45  | 1.65        | 1.53     |
| 14  | 9     | 262 | LEU  | CA-CB   | 7.40  | 1.65        | 1.53     |
| 14  | 9     | 294 | ALA  | CA-C    | -7.36 | 1.43        | 1.52     |
| 14  | 9     | 164 | HIS  | ND1-CE1 | 7.35  | 1.39        | 1.32     |
| 14  | 9     | 503 | MET  | CA-C    | -7.33 | 1.43        | 1.52     |
| 14  | 9     | 22  | LYS  | CA-C    | -7.26 | 1.43        | 1.52     |
| 14  | 9     | 208 | VAL  | CA-C    | -7.24 | 1.43        | 1.52     |
| 14  | 9     | 798 | ARG  | NE-CZ   | 7.23  | 1.41        | 1.33     |
| 3   | 10    | 403 | VAL  | C-N     | 7.23  | 1.43        | 1.33     |
| 3   | 10    | 417 | GLY  | C-N     | 7.21  | 1.43        | 1.33     |
| 14  | 9     | 103 | MET  | CA-C    | -7.21 | 1.44        | 1.52     |
| 14  | 9     | 408 | VAL  | C-N     | 7.18  | 1.43        | 1.33     |
| 14  | 9     | 88  | ILE  | CA-C    | -7.15 | 1.43        | 1.52     |
| 14  | 9     | 784 | GLU  | N-CA    | -7.14 | 1.37        | 1.46     |
| 3   | 10    | 162 | ASN  | C-N     | 7.13  | 1.39        | 1.33     |
| 3   | 10    | 334 | GLY  | N-CA    | -7.12 | 1.37        | 1.45     |
| 14  | 9     | 575 | MET  | CG-SD   | 7.12  | 1.98        | 1.80     |
| 14  | 9     | 609 | TYR  | CA-CB   | 7.06  | 1.64        | 1.53     |
| 14  | 9     | 539 | PHE  | C-N     | 7.06  | 1.42        | 1.33     |
| 3   | 10    | 181 | SER  | CA-C    | -7.01 | 1.43        | 1.52     |
| 14  | 9     | 708 | ARG  | CA-C    | -6.98 | 1.43        | 1.52     |
| 14  | 9     | 108 | LYS  | CA-C    | 6.96  | 1.61        | 1.52     |
| 14  | 9     | 480 | ALA  | C-N     | 6.96  | 1.42        | 1.33     |
| 14  | 9     | 2   | GLY  | CA-C    | -6.95 | 1.43        | 1.52     |
| 14  | 9     | 776 | ALA  | C-N     | 6.93  | 1.42        | 1.33     |
| 14  | 9     | 681 | THR  | N-CA    | 6.93  | 1.54        | 1.46     |
| 5   | 12    | 99  | VAL  | CA-C    | -6.93 | 1.44        | 1.52     |
| 14  | 9     | 666 | GLY  | CA-C    | -6.90 | 1.43        | 1.51     |
| 14  | 9     | 473 | ALA  | CA-C    | -6.87 | 1.43        | 1.52     |
| 14  | 9     | 314 | VAL  | N-CA    | -6.83 | 1.38        | 1.46     |
| 14  | 9     | 455 | ILE  | CA-C    | -6.83 | 1.47        | 1.52     |
| 3   | 10    | 293 | ILE  | N-CA    | -6.82 | 1.38        | 1.46     |
| 14  | 9     | 599 | HIS  | CB-CG   | 6.80  | 1.59        | 1.50     |
| 14  | 9     | 529 | ARG  | CA-CB   | 6.80  | 1.64        | 1.53     |
| 3   | 10    | 394 | THR  | N-CA    | -6.79 | 1.38        | 1.46     |
| 14  | 9     | 60  | ILE  | C-N     | 6.77  | 1.42        | 1.33     |
| 14  | 9     | 49  | LEU  | N-CA    | 6.77  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | 9     | 525 | GLY  | C-O     | -6.76 | 1.16        | 1.24     |
| 4   | 11    | 43  | ARG  | N-CA    | -6.75 | 1.37        | 1.46     |
| 14  | 9     | 231 | ASN  | CA-C    | 6.75  | 1.61        | 1.52     |
| 14  | 9     | 518 | ARG  | NE-CZ   | 6.74  | 1.40        | 1.33     |
| 4   | 11    | 46  | LYS  | CA-CB   | 6.74  | 1.64        | 1.53     |
| 5   | 12    | 104 | ILE  | CA-CB   | -6.74 | 1.46        | 1.54     |
| 14  | 9     | 140 | ALA  | C-N     | 6.73  | 1.42        | 1.33     |
| 14  | 9     | 557 | ARG  | CZ-NH2  | 6.71  | 1.42        | 1.33     |
| 14  | 9     | 730 | LYS  | N-CA    | -6.71 | 1.38        | 1.46     |
| 5   | 12    | 36  | GLU  | C-N     | 6.69  | 1.42        | 1.33     |
| 3   | 10    | 212 | GLY  | C-N     | 6.69  | 1.43        | 1.33     |
| 3   | 10    | 196 | GLY  | CA-C    | -6.67 | 1.44        | 1.52     |
| 14  | 9     | 273 | ASN  | CA-CB   | 6.66  | 1.63        | 1.53     |
| 5   | 12    | 119 | LEU  | N-CA    | -6.65 | 1.37        | 1.46     |
| 14  | 9     | 426 | ILE  | C-N     | 6.65  | 1.42        | 1.33     |
| 14  | 9     | 695 | ASN  | CA-C    | -6.65 | 1.44        | 1.52     |
| 3   | 10    | 82  | LEU  | C-N     | 6.65  | 1.41        | 1.33     |
| 14  | 9     | 611 | GLN  | N-CA    | 6.62  | 1.54        | 1.46     |
| 14  | 9     | 363 | ARG  | NE-CZ   | 6.61  | 1.40        | 1.33     |
| 14  | 9     | 393 | VAL  | CA-C    | -6.58 | 1.47        | 1.53     |
| 14  | 9     | 751 | ARG  | CD-NE   | 6.58  | 1.55        | 1.46     |
| 4   | 11    | 3   | ALA  | C-N     | 6.58  | 1.42        | 1.33     |
| 3   | 10    | 159 | LEU  | CA-C    | -6.55 | 1.44        | 1.52     |
| 3   | 10    | 295 | ALA  | CA-C    | -6.55 | 1.44        | 1.52     |
| 14  | 9     | 537 | LYS  | N-CA    | 6.54  | 1.54        | 1.46     |
| 14  | 9     | 579 | THR  | N-CA    | -6.54 | 1.38        | 1.46     |
| 14  | 9     | 729 | PHE  | CA-C    | -6.53 | 1.44        | 1.52     |
| 14  | 9     | 533 | ARG  | CA-CB   | 6.52  | 1.63        | 1.53     |
| 14  | 9     | 787 | LYS  | C-N     | 6.52  | 1.42        | 1.33     |
| 14  | 9     | 365 | TYR  | CA-C    | -6.52 | 1.44        | 1.52     |
| 14  | 9     | 55  | LYS  | CA-C    | -6.51 | 1.44        | 1.52     |
| 14  | 9     | 720 | HIS  | CD2-NE2 | 6.51  | 1.45        | 1.37     |
| 14  | 9     | 260 | PRO  | CA-C    | -6.51 | 1.45        | 1.52     |
| 3   | 10    | 450 | LEU  | CA-CB   | 6.51  | 1.63        | 1.53     |
| 14  | 9     | 283 | GLU  | CA-CB   | 6.47  | 1.63        | 1.53     |
| 14  | 9     | 167 | GLN  | CA-CB   | 6.46  | 1.63        | 1.53     |
| 14  | 9     | 543 | GLY  | CA-C    | -6.46 | 1.42        | 1.51     |
| 14  | 9     | 750 | ILE  | C-N     | 6.46  | 1.42        | 1.33     |
| 14  | 9     | 102 | MET  | C-N     | 6.44  | 1.42        | 1.33     |
| 3   | 10    | 209 | LEU  | C-N     | 6.44  | 1.42        | 1.34     |
| 3   | 10    | 285 | ASN  | N-CA    | -6.43 | 1.38        | 1.46     |
| 3   | 10    | 274 | SER  | N-CA    | -6.42 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 14  | 9     | 393 | VAL  | N-CA   | -6.42 | 1.40        | 1.46     |
| 14  | 9     | 387 | ASN  | CA-CB  | 6.41  | 1.63        | 1.53     |
| 66  | 15    | 632 | LYS  | C-O    | -6.41 | 1.18        | 1.24     |
| 14  | 9     | 369 | SER  | N-CA   | -6.41 | 1.37        | 1.45     |
| 4   | 11    | 17  | ILE  | CA-CB  | -6.39 | 1.47        | 1.54     |
| 14  | 9     | 770 | ILE  | CA-CB  | 6.38  | 1.62        | 1.54     |
| 14  | 9     | 729 | PHE  | N-CA   | 6.35  | 1.53        | 1.46     |
| 14  | 9     | 139 | ASP  | C-N    | 6.34  | 1.42        | 1.33     |
| 14  | 9     | 800 | ALA  | CA-C   | -6.34 | 1.44        | 1.52     |
| 14  | 9     | 356 | ILE  | CA-CB  | -6.33 | 1.46        | 1.54     |
| 14  | 9     | 678 | PHE  | CA-C   | -6.32 | 1.44        | 1.52     |
| 3   | 10    | 24  | ARG  | NE-CZ  | 6.31  | 1.40        | 1.33     |
| 14  | 9     | 390 | VAL  | CA-CB  | -6.31 | 1.46        | 1.54     |
| 14  | 9     | 15  | ARG  | CD-NE  | 6.30  | 1.55        | 1.46     |
| 14  | 9     | 8   | LYS  | CA-C   | -6.29 | 1.44        | 1.52     |
| 14  | 9     | 708 | ARG  | CA-CB  | 6.27  | 1.63        | 1.53     |
| 3   | 10    | 122 | ARG  | CZ-NH1 | 6.26  | 1.41        | 1.32     |
| 3   | 10    | 364 | PHE  | CA-C   | -6.26 | 1.44        | 1.52     |
| 14  | 9     | 418 | ALA  | CA-C   | 6.26  | 1.60        | 1.52     |
| 4   | 11    | 54  | LEU  | CA-C   | -6.26 | 1.44        | 1.52     |
| 14  | 9     | 597 | TYR  | CA-C   | -6.25 | 1.45        | 1.52     |
| 14  | 9     | 343 | MET  | CA-C   | -6.24 | 1.43        | 1.52     |
| 14  | 9     | 401 | ARG  | CD-NE  | 6.23  | 1.54        | 1.46     |
| 3   | 10    | 62  | GLN  | C-N    | 6.23  | 1.42        | 1.33     |
| 14  | 9     | 226 | SER  | CA-C   | -6.22 | 1.45        | 1.52     |
| 3   | 10    | 182 | VAL  | N-CA   | -6.21 | 1.38        | 1.46     |
| 14  | 9     | 228 | PRO  | N-CA   | -6.20 | 1.39        | 1.47     |
| 14  | 9     | 240 | ASP  | CA-CB  | 6.20  | 1.63        | 1.53     |
| 3   | 10    | 183 | PHE  | N-CA   | -6.20 | 1.38        | 1.46     |
| 3   | 10    | 467 | ARG  | CA-CB  | 6.20  | 1.63        | 1.53     |
| 14  | 9     | 649 | VAL  | N-CA   | -6.20 | 1.39        | 1.46     |
| 14  | 9     | 532 | ASP  | C-N    | 6.19  | 1.41        | 1.33     |
| 14  | 9     | 312 | GLY  | C-N    | 6.18  | 1.42        | 1.33     |
| 14  | 9     | 518 | ARG  | C-N    | 6.18  | 1.41        | 1.33     |
| 14  | 9     | 47  | ASN  | CA-C   | -6.17 | 1.44        | 1.52     |
| 5   | 12    | 82  | LYS  | N-CA   | 6.16  | 1.53        | 1.46     |
| 3   | 10    | 133 | LEU  | N-CA   | 6.16  | 1.51        | 1.46     |
| 4   | 11    | 57  | THR  | N-CA   | -6.16 | 1.39        | 1.46     |
| 14  | 9     | 252 | LYS  | CA-C   | -6.15 | 1.45        | 1.52     |
| 3   | 10    | 143 | VAL  | CA-CB  | 6.15  | 1.62        | 1.54     |
| 3   | 10    | 283 | LYS  | CA-C   | -6.13 | 1.45        | 1.52     |
| 14  | 9     | 440 | ILE  | C-N    | 6.12  | 1.42        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 14  | 9     | 423  | VAL  | N-CA   | -6.11 | 1.39        | 1.46     |
| 14  | 9     | 226  | SER  | N-CA   | -6.11 | 1.38        | 1.45     |
| 14  | 9     | 124  | ARG  | CZ-NH2 | 6.11  | 1.41        | 1.33     |
| 3   | 10    | 286  | SER  | CA-C   | -6.10 | 1.44        | 1.52     |
| 14  | 9     | 99   | PHE  | CA-C   | 6.10  | 1.60        | 1.52     |
| 3   | 10    | 157  | ILE  | CA-CB  | 6.08  | 1.62        | 1.54     |
| 5   | 12    | 29   | ARG  | CD-NE  | 6.08  | 1.54        | 1.46     |
| 14  | 9     | 193  | HIS  | CB-CG  | 6.08  | 1.58        | 1.50     |
| 3   | 10    | 290  | ILE  | CA-CB  | 6.07  | 1.58        | 1.53     |
| 3   | 10    | 435  | ARG  | NE-CZ  | 6.07  | 1.39        | 1.33     |
| 3   | 10    | 458  | ALA  | C-N    | 6.06  | 1.42        | 1.33     |
| 14  | 9     | 393  | VAL  | CA-CB  | -6.06 | 1.46        | 1.54     |
| 14  | 9     | 628  | MET  | CG-SD  | 6.05  | 1.95        | 1.80     |
| 14  | 9     | 1    | MET  | CA-C   | -6.04 | 1.40        | 1.52     |
| 14  | 9     | 323  | ARG  | NE-CZ  | 6.04  | 1.39        | 1.33     |
| 3   | 10    | 183  | PHE  | CA-CB  | 6.02  | 1.62        | 1.53     |
| 14  | 9     | 487  | MET  | N-CA   | -6.02 | 1.37        | 1.46     |
| 3   | 10    | 297  | SER  | CA-C   | -6.01 | 1.44        | 1.52     |
| 3   | 10    | 144  | ILE  | CA-C   | -6.00 | 1.45        | 1.52     |
| 14  | 9     | 505  | GLY  | CA-C   | -5.99 | 1.43        | 1.51     |
| 3   | 10    | 259  | ARG  | N-CA   | -5.99 | 1.38        | 1.46     |
| 5   | 12    | 37   | ALA  | C-N    | 5.98  | 1.41        | 1.33     |
| 14  | 9     | 517  | ARG  | NE-CZ  | 5.98  | 1.39        | 1.33     |
| 14  | 9     | 533  | ARG  | CD-NE  | 5.96  | 1.54        | 1.46     |
| 3   | 10    | 153  | GLY  | CA-C   | -5.95 | 1.44        | 1.51     |
| 14  | 9     | 586  | ILE  | CA-CB  | -5.94 | 1.47        | 1.54     |
| 14  | 9     | 6    | PHE  | N-CA   | -5.94 | 1.39        | 1.46     |
| 14  | 9     | 365  | TYR  | C-N    | 5.94  | 1.42        | 1.33     |
| 13  | 8     | 17   | U    | C2-N3  | 5.93  | 1.49        | 1.37     |
| 3   | 10    | 302  | PRO  | N-CA   | -5.93 | 1.40        | 1.47     |
| 14  | 9     | 95   | LEU  | C-N    | 5.93  | 1.41        | 1.33     |
| 14  | 9     | 62   | ASP  | C-N    | 5.92  | 1.40        | 1.34     |
| 14  | 9     | 514  | ASN  | CA-CB  | 5.92  | 1.62        | 1.53     |
| 13  | 8     | 20   | U    | C2-N3  | 5.92  | 1.49        | 1.37     |
| 14  | 9     | 493  | ASP  | C-N    | 5.89  | 1.40        | 1.33     |
| 65  | 14    | 1124 | LYS  | C-N    | -5.89 | 1.25        | 1.33     |
| 14  | 9     | 288  | PHE  | CA-CB  | 5.88  | 1.62        | 1.53     |
| 3   | 10    | 442  | ASN  | C-N    | 5.87  | 1.41        | 1.33     |
| 3   | 10    | 237  | PHE  | CA-CB  | 5.87  | 1.62        | 1.53     |
| 14  | 9     | 660  | LEU  | CA-C   | -5.86 | 1.45        | 1.53     |
| 3   | 10    | 227  | ILE  | CB-CG1 | 5.85  | 1.65        | 1.53     |
| 13  | 8     | 16   | U    | C2-N3  | 5.84  | 1.49        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 67  | 16    | 132 | LYS  | C-O    | -5.84 | 1.17        | 1.23     |
| 14  | 9     | 513 | ARG  | N-CA   | -5.84 | 1.38        | 1.46     |
| 4   | 11    | 38  | ASP  | C-N    | 5.84  | 1.42        | 1.33     |
| 14  | 9     | 177 | THR  | C-N    | 5.84  | 1.41        | 1.33     |
| 14  | 9     | 58  | TYR  | C-N    | 5.84  | 1.40        | 1.33     |
| 14  | 9     | 85  | ARG  | CD-NE  | 5.83  | 1.54        | 1.46     |
| 5   | 12    | 98  | ILE  | N-CA   | 5.83  | 1.53        | 1.46     |
| 3   | 10    | 326 | LYS  | CA-CB  | 5.82  | 1.61        | 1.53     |
| 5   | 12    | 62  | LYS  | C-N    | 5.82  | 1.40        | 1.33     |
| 14  | 9     | 514 | ASN  | CA-C   | -5.81 | 1.44        | 1.53     |
| 14  | 9     | 490 | ARG  | NE-CZ  | 5.80  | 1.39        | 1.33     |
| 14  | 9     | 663 | ASN  | CA-C   | -5.79 | 1.45        | 1.52     |
| 4   | 11    | 61  | LEU  | C-N    | 5.77  | 1.41        | 1.33     |
| 14  | 9     | 349 | GLU  | CA-C   | 5.77  | 1.60        | 1.52     |
| 3   | 10    | 43  | ARG  | CZ-NH2 | 5.77  | 1.41        | 1.33     |
| 58  | t     | 95  | PRO  | N-CD   | 5.77  | 1.55        | 1.47     |
| 14  | 9     | 582 | ARG  | NE-CZ  | 5.76  | 1.39        | 1.33     |
| 14  | 9     | 380 | GLU  | CA-CB  | 5.76  | 1.62        | 1.53     |
| 3   | 10    | 42  | PHE  | C-O    | -5.75 | 1.17        | 1.24     |
| 14  | 9     | 650 | ASN  | N-CA   | -5.75 | 1.39        | 1.46     |
| 14  | 9     | 494 | ILE  | C-O    | -5.75 | 1.17        | 1.24     |
| 3   | 10    | 341 | SER  | N-CA   | -5.74 | 1.39        | 1.46     |
| 14  | 9     | 72  | ARG  | NE-CZ  | 5.74  | 1.39        | 1.33     |
| 5   | 12    | 32  | LYS  | C-N    | 5.73  | 1.41        | 1.33     |
| 14  | 9     | 641 | ARG  | CD-NE  | 5.72  | 1.54        | 1.46     |
| 14  | 9     | 766 | ARG  | CD-NE  | 5.72  | 1.54        | 1.46     |
| 5   | 12    | 98  | ILE  | CA-C   | -5.72 | 1.45        | 1.52     |
| 3   | 10    | 463 | GLU  | CA-CB  | 5.72  | 1.62        | 1.53     |
| 14  | 9     | 244 | LYS  | C-N    | 5.72  | 1.41        | 1.33     |
| 14  | 9     | 731 | LEU  | CA-C   | -5.71 | 1.45        | 1.52     |
| 3   | 10    | 249 | PHE  | C-N    | 5.71  | 1.41        | 1.33     |
| 14  | 9     | 51  | ASP  | C-N    | 5.70  | 1.41        | 1.33     |
| 3   | 10    | 92  | TYR  | CA-C   | -5.69 | 1.45        | 1.52     |
| 3   | 10    | 447 | ARG  | CD-NE  | 5.69  | 1.54        | 1.46     |
| 3   | 10    | 117 | GLY  | C-N    | 5.69  | 1.41        | 1.34     |
| 3   | 10    | 447 | ARG  | N-CA   | -5.68 | 1.39        | 1.46     |
| 14  | 9     | 428 | GLU  | CA-C   | 5.68  | 1.60        | 1.52     |
| 3   | 10    | 338 | ILE  | CA-C   | -5.68 | 1.46        | 1.52     |
| 14  | 9     | 562 | LEU  | CB-CG  | 5.68  | 1.64        | 1.53     |
| 14  | 9     | 562 | LEU  | CA-C   | 5.67  | 1.60        | 1.52     |
| 3   | 10    | 205 | ILE  | CA-C   | -5.67 | 1.45        | 1.52     |
| 4   | 11    | 66  | LEU  | CA-C   | -5.67 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | 9     | 681 | THR  | CA-C    | 5.67  | 1.60        | 1.52     |
| 3   | 10    | 61  | ASP  | CA-CB   | 5.66  | 1.62        | 1.53     |
| 3   | 10    | 33  | LEU  | C-N     | 5.65  | 1.41        | 1.33     |
| 14  | 9     | 199 | LYS  | CA-CB   | 5.65  | 1.62        | 1.53     |
| 14  | 9     | 440 | ILE  | N-CA    | -5.64 | 1.39        | 1.46     |
| 3   | 10    | 166 | PHE  | C-O     | -5.64 | 1.17        | 1.24     |
| 14  | 9     | 313 | LYS  | CA-C    | -5.64 | 1.46        | 1.52     |
| 3   | 10    | 234 | ALA  | C-O     | -5.63 | 1.17        | 1.24     |
| 14  | 9     | 480 | ALA  | CA-CB   | 5.63  | 1.62        | 1.53     |
| 14  | 9     | 383 | LEU  | N-CA    | -5.63 | 1.39        | 1.46     |
| 14  | 9     | 538 | PHE  | N-CA    | -5.63 | 1.39        | 1.46     |
| 14  | 9     | 327 | GLY  | CA-C    | -5.62 | 1.44        | 1.51     |
| 14  | 9     | 691 | GLU  | C-N     | 5.62  | 1.41        | 1.33     |
| 14  | 9     | 506 | LEU  | CB-CG   | 5.61  | 1.64        | 1.53     |
| 14  | 9     | 128 | VAL  | CA-C    | -5.61 | 1.45        | 1.52     |
| 3   | 10    | 90  | SER  | N-CA    | -5.61 | 1.40        | 1.46     |
| 5   | 12    | 45  | ASP  | CA-CB   | 5.60  | 1.62        | 1.53     |
| 3   | 10    | 58  | THR  | CA-C    | -5.59 | 1.45        | 1.52     |
| 14  | 9     | 493 | ASP  | CA-CB   | 5.59  | 1.60        | 1.53     |
| 4   | 11    | 25  | HIS  | C-N     | 5.59  | 1.41        | 1.33     |
| 14  | 9     | 351 | VAL  | CA-C    | -5.58 | 1.45        | 1.52     |
| 14  | 9     | 657 | ALA  | CA-C    | -5.56 | 1.45        | 1.52     |
| 3   | 10    | 84  | LEU  | CA-CB   | 5.55  | 1.62        | 1.53     |
| 3   | 10    | 363 | ARG  | CA-CB   | 5.55  | 1.62        | 1.53     |
| 14  | 9     | 126 | VAL  | CA-C    | -5.55 | 1.45        | 1.52     |
| 5   | 12    | 29  | ARG  | NE-CZ   | 5.55  | 1.39        | 1.33     |
| 14  | 9     | 465 | HIS  | ND1-CE1 | 5.54  | 1.38        | 1.32     |
| 14  | 9     | 716 | ALA  | C-N     | 5.54  | 1.40        | 1.33     |
| 14  | 9     | 43  | LEU  | CA-CB   | 5.53  | 1.62        | 1.53     |
| 3   | 10    | 67  | PHE  | CA-CB   | 5.53  | 1.61        | 1.53     |
| 3   | 10    | 263 | ILE  | CA-CB   | -5.52 | 1.47        | 1.54     |
| 3   | 10    | 321 | TYR  | CE2-CZ  | 5.52  | 1.51        | 1.38     |
| 14  | 9     | 282 | LEU  | N-CA    | -5.52 | 1.39        | 1.46     |
| 14  | 9     | 750 | ILE  | N-CA    | 5.51  | 1.53        | 1.46     |
| 14  | 9     | 13  | ARG  | N-CA    | -5.50 | 1.39        | 1.46     |
| 14  | 9     | 290 | LYS  | CA-C    | -5.49 | 1.45        | 1.52     |
| 3   | 10    | 268 | GLN  | CA-C    | -5.49 | 1.45        | 1.52     |
| 14  | 9     | 431 | ARG  | CD-NE   | 5.48  | 1.53        | 1.46     |
| 14  | 9     | 349 | GLU  | CA-CB   | 5.47  | 1.62        | 1.53     |
| 14  | 9     | 494 | ILE  | C-N     | 5.47  | 1.40        | 1.33     |
| 14  | 9     | 148 | LYS  | N-CA    | 5.46  | 1.53        | 1.46     |
| 14  | 9     | 462 | ALA  | C-N     | 5.46  | 1.41        | 1.34     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 14  | 9     | 470 | GLU  | CA-CB  | 5.45  | 1.61        | 1.53     |
| 14  | 9     | 310 | ARG  | C-N    | 5.45  | 1.41        | 1.33     |
| 14  | 9     | 318 | ASP  | CA-C   | -5.45 | 1.46        | 1.52     |
| 3   | 10    | 243 | ALA  | CA-CB  | 5.43  | 1.61        | 1.53     |
| 3   | 10    | 331 | VAL  | C-O    | -5.43 | 1.17        | 1.24     |
| 3   | 10    | 53  | ILE  | C-N    | 5.43  | 1.40        | 1.33     |
| 14  | 9     | 574 | LYS  | CA-C   | -5.43 | 1.45        | 1.52     |
| 3   | 10    | 392 | PHE  | C-O    | -5.42 | 1.17        | 1.24     |
| 3   | 10    | 462 | LYS  | N-CA   | -5.42 | 1.39        | 1.46     |
| 4   | 11    | 48  | ARG  | CZ-NH2 | 5.42  | 1.40        | 1.33     |
| 3   | 10    | 141 | PHE  | C-N    | 5.41  | 1.40        | 1.33     |
| 14  | 9     | 206 | ALA  | CA-C   | -5.41 | 1.46        | 1.52     |
| 14  | 9     | 500 | VAL  | CA-C   | 5.41  | 1.60        | 1.52     |
| 5   | 12    | 36  | GLU  | CA-C   | 5.41  | 1.59        | 1.52     |
| 14  | 9     | 74  | VAL  | CA-CB  | -5.40 | 1.47        | 1.54     |
| 14  | 9     | 160 | ASN  | CA-C   | -5.40 | 1.46        | 1.52     |
| 14  | 9     | 761 | LEU  | CA-C   | -5.39 | 1.45        | 1.52     |
| 3   | 10    | 420 | ILE  | CA-C   | 5.38  | 1.59        | 1.52     |
| 4   | 11    | 45  | THR  | N-CA   | -5.38 | 1.39        | 1.46     |
| 4   | 11    | 69  | GLY  | C-N    | 5.38  | 1.41        | 1.33     |
| 3   | 10    | 191 | LYS  | CA-C   | -5.38 | 1.45        | 1.52     |
| 14  | 9     | 778 | PRO  | CA-C   | -5.37 | 1.43        | 1.52     |
| 14  | 9     | 720 | HIS  | CA-CB  | 5.37  | 1.62        | 1.53     |
| 3   | 10    | 63  | ASN  | CA-C   | -5.37 | 1.46        | 1.52     |
| 13  | 8     | 17  | U    | N1-C2  | 5.37  | 1.49        | 1.38     |
| 14  | 9     | 755 | ILE  | C-N    | 5.37  | 1.40        | 1.33     |
| 3   | 10    | 111 | SER  | CA-C   | -5.36 | 1.46        | 1.52     |
| 14  | 9     | 754 | ASP  | N-CA   | -5.36 | 1.39        | 1.46     |
| 3   | 10    | 333 | TYR  | CA-C   | 5.36  | 1.59        | 1.52     |
| 14  | 9     | 582 | ARG  | CA-C   | -5.36 | 1.45        | 1.52     |
| 3   | 10    | 472 | GLY  | CA-C   | -5.36 | 1.44        | 1.51     |
| 14  | 9     | 239 | VAL  | CA-C   | -5.36 | 1.45        | 1.52     |
| 14  | 9     | 633 | VAL  | CA-CB  | -5.35 | 1.47        | 1.54     |
| 14  | 9     | 594 | LEU  | CA-C   | -5.35 | 1.45        | 1.52     |
| 3   | 10    | 180 | LEU  | C-N    | 5.34  | 1.41        | 1.33     |
| 14  | 9     | 452 | GLU  | CA-C   | 5.34  | 1.59        | 1.52     |
| 3   | 10    | 354 | LEU  | CA-C   | -5.33 | 1.45        | 1.52     |
| 14  | 9     | 588 | PHE  | CA-CB  | 5.33  | 1.61        | 1.53     |
| 3   | 10    | 50  | LEU  | CA-C   | 5.33  | 1.58        | 1.53     |
| 4   | 11    | 43  | ARG  | NE-CZ  | 5.32  | 1.39        | 1.33     |
| 14  | 9     | 423 | VAL  | CA-CB  | -5.32 | 1.48        | 1.54     |
| 3   | 10    | 325 | SER  | CA-CB  | 5.32  | 1.62        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 13  | 8     | 16   | U    | N1-C2 | 5.30  | 1.49        | 1.38     |
| 14  | 9     | 46   | SER  | C-N   | 5.30  | 1.41        | 1.33     |
| 5   | 12    | 106  | ILE  | C-N   | 5.29  | 1.40        | 1.33     |
| 14  | 9     | 714  | ILE  | CA-C  | -5.29 | 1.46        | 1.52     |
| 14  | 9     | 404  | ARG  | NE-CZ | 5.29  | 1.38        | 1.33     |
| 13  | 8     | 20   | U    | N1-C2 | 5.29  | 1.49        | 1.38     |
| 14  | 9     | 378  | GLU  | CA-CB | 5.29  | 1.61        | 1.53     |
| 14  | 9     | 113  | VAL  | C-N   | 5.29  | 1.40        | 1.33     |
| 5   | 12    | 117  | ILE  | CA-C  | -5.28 | 1.46        | 1.52     |
| 14  | 9     | 633  | VAL  | N-CA  | -5.27 | 1.40        | 1.46     |
| 14  | 9     | 152  | MET  | CA-C  | -5.27 | 1.46        | 1.52     |
| 14  | 9     | 333  | GLY  | N-CA  | -5.27 | 1.36        | 1.45     |
| 14  | 9     | 535  | GLU  | CA-C  | -5.27 | 1.46        | 1.52     |
| 3   | 10    | 28   | PHE  | CA-C  | -5.27 | 1.46        | 1.52     |
| 14  | 9     | 325  | LEU  | CA-C  | -5.27 | 1.47        | 1.53     |
| 14  | 9     | 265  | LEU  | N-CA  | -5.27 | 1.40        | 1.46     |
| 14  | 9     | 418  | ALA  | C-N   | 5.26  | 1.40        | 1.33     |
| 3   | 10    | 455  | GLN  | CA-CB | 5.26  | 1.61        | 1.53     |
| 3   | 10    | 85   | PHE  | N-CA  | 5.25  | 1.52        | 1.46     |
| 14  | 9     | 242  | PHE  | CA-CB | 5.25  | 1.61        | 1.53     |
| 14  | 9     | 391  | VAL  | CA-CB | -5.24 | 1.48        | 1.53     |
| 14  | 9     | 267  | ILE  | CA-C  | -5.24 | 1.46        | 1.52     |
| 3   | 10    | 274  | SER  | C-N   | 5.24  | 1.41        | 1.33     |
| 3   | 10    | 460  | GLN  | C-N   | 5.23  | 1.40        | 1.33     |
| 14  | 9     | 461  | ASN  | C-N   | 5.22  | 1.41        | 1.33     |
| 14  | 9     | 88   | ILE  | CA-CB | 5.22  | 1.60        | 1.54     |
| 14  | 9     | 269  | HIS  | C-N   | 5.22  | 1.40        | 1.33     |
| 14  | 9     | 369  | SER  | C-N   | -5.20 | 1.27        | 1.33     |
| 4   | 11    | 54   | LEU  | C-N   | 5.20  | 1.40        | 1.33     |
| 65  | 14    | 1123 | ASN  | C-N   | -5.20 | 1.25        | 1.33     |
| 14  | 9     | 459  | VAL  | CA-C  | -5.19 | 1.46        | 1.52     |
| 4   | 11    | 16   | LEU  | N-CA  | 5.19  | 1.52        | 1.46     |
| 3   | 10    | 31   | SER  | CA-C  | -5.18 | 1.46        | 1.52     |
| 5   | 12    | 26   | GLU  | CA-CB | 5.18  | 1.61        | 1.53     |
| 14  | 9     | 526  | ARG  | N-CA  | 5.18  | 1.53        | 1.46     |
| 14  | 9     | 4    | PHE  | N-CA  | -5.18 | 1.40        | 1.46     |
| 14  | 9     | 367  | ARG  | NE-CZ | 5.18  | 1.38        | 1.33     |
| 5   | 12    | 81   | ASN  | CA-C  | -5.17 | 1.45        | 1.52     |
| 3   | 10    | 226  | THR  | C-N   | 5.16  | 1.39        | 1.33     |
| 4   | 11    | 36   | GLY  | C-N   | 5.16  | 1.39        | 1.33     |
| 14  | 9     | 329  | SER  | N-CA  | -5.16 | 1.38        | 1.46     |
| 65  | 14    | 860  | LYS  | C-O   | -5.16 | 1.18        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | 10    | 471 | PRO  | N-CA   | 5.16  | 1.52        | 1.47     |
| 4   | 11    | 29  | GLY  | CA-C   | 5.16  | 1.59        | 1.51     |
| 14  | 9     | 546 | LEU  | CA-CB  | 5.15  | 1.61        | 1.53     |
| 14  | 9     | 637 | CYS  | CA-C   | -5.14 | 1.45        | 1.52     |
| 4   | 11    | 31  | LEU  | C-N    | 5.14  | 1.41        | 1.33     |
| 14  | 9     | 663 | ASN  | N-CA   | 5.13  | 1.52        | 1.46     |
| 3   | 10    | 452 | ILE  | CA-CB  | -5.12 | 1.47        | 1.54     |
| 3   | 10    | 61  | ASP  | N-CA   | -5.12 | 1.40        | 1.46     |
| 14  | 9     | 742 | GLN  | CA-CB  | 5.12  | 1.62        | 1.53     |
| 4   | 11    | 23  | SER  | N-CA   | -5.12 | 1.39        | 1.46     |
| 14  | 9     | 173 | ASP  | CA-C   | -5.12 | 1.45        | 1.52     |
| 14  | 9     | 690 | GLY  | CA-C   | 5.12  | 1.57        | 1.52     |
| 3   | 10    | 271 | VAL  | N-CA   | -5.12 | 1.39        | 1.46     |
| 3   | 10    | 363 | ARG  | CZ-NH2 | 5.12  | 1.40        | 1.33     |
| 3   | 10    | 398 | ILE  | CA-C   | -5.11 | 1.45        | 1.52     |
| 14  | 9     | 772 | ILE  | CA-C   | 5.11  | 1.59        | 1.52     |
| 3   | 10    | 467 | ARG  | C-N    | 5.10  | 1.40        | 1.33     |
| 14  | 9     | 661 | GLU  | CA-C   | -5.10 | 1.45        | 1.52     |
| 3   | 10    | 168 | ALA  | C-N    | 5.10  | 1.40        | 1.33     |
| 3   | 10    | 351 | PRO  | C-N    | 5.10  | 1.40        | 1.33     |
| 5   | 12    | 115 | LEU  | CA-C   | -5.10 | 1.46        | 1.52     |
| 3   | 10    | 377 | HIS  | CG-CD2 | 5.10  | 1.41        | 1.35     |
| 14  | 9     | 93  | ILE  | N-CA   | -5.10 | 1.40        | 1.46     |
| 14  | 9     | 94  | VAL  | CA-C   | -5.10 | 1.46        | 1.52     |
| 3   | 10    | 86  | ALA  | C-N    | 5.09  | 1.40        | 1.33     |
| 5   | 12    | 61  | VAL  | CA-CB  | 5.09  | 1.61        | 1.54     |
| 14  | 9     | 455 | ILE  | CA-CB  | 5.09  | 1.58        | 1.54     |
| 14  | 9     | 670 | PRO  | CA-C   | 5.09  | 1.60        | 1.52     |
| 3   | 10    | 330 | ILE  | CA-CB  | 5.08  | 1.60        | 1.54     |
| 14  | 9     | 514 | ASN  | CG-ND2 | 5.08  | 1.44        | 1.33     |
| 4   | 11    | 43  | ARG  | CD-NE  | 5.08  | 1.53        | 1.46     |
| 14  | 9     | 269 | HIS  | CG-ND1 | -5.08 | 1.32        | 1.38     |
| 14  | 9     | 398 | PRO  | CA-CB  | -5.08 | 1.46        | 1.53     |
| 14  | 9     | 550 | PHE  | CA-C   | -5.08 | 1.46        | 1.52     |
| 5   | 12    | 75  | GLY  | C-N    | 5.08  | 1.40        | 1.33     |
| 14  | 9     | 403 | ASP  | C-N    | 5.08  | 1.40        | 1.33     |
| 3   | 10    | 459 | GLN  | N-CA   | -5.07 | 1.39        | 1.46     |
| 14  | 9     | 220 | ARG  | NE-CZ  | 5.07  | 1.38        | 1.33     |
| 14  | 9     | 13  | ARG  | NE-CZ  | 5.07  | 1.38        | 1.33     |
| 3   | 10    | 328 | THR  | C-N    | 5.06  | 1.40        | 1.33     |
| 14  | 9     | 759 | THR  | CA-C   | -5.06 | 1.46        | 1.52     |
| 5   | 12    | 26  | GLU  | CA-C   | -5.06 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 10    | 46  | ALA  | N-CA    | -5.06 | 1.39        | 1.46     |
| 14  | 9     | 139 | ASP  | CA-CB   | 5.06  | 1.61        | 1.53     |
| 14  | 9     | 727 | ASN  | CG-ND2  | 5.06  | 1.43        | 1.33     |
| 4   | 11    | 49  | GLY  | CA-C    | -5.06 | 1.45        | 1.52     |
| 3   | 10    | 305 | ILE  | CA-C    | 5.05  | 1.59        | 1.52     |
| 14  | 9     | 35  | ARG  | CD-NE   | 5.05  | 1.53        | 1.46     |
| 3   | 10    | 369 | ARG  | CD-NE   | 5.05  | 1.53        | 1.46     |
| 3   | 10    | 340 | PHE  | N-CA    | -5.05 | 1.40        | 1.46     |
| 14  | 9     | 629 | LEU  | CA-C    | -5.04 | 1.46        | 1.52     |
| 14  | 9     | 92  | TYR  | C-N     | 5.04  | 1.40        | 1.33     |
| 14  | 9     | 530 | GLN  | C-N     | 5.04  | 1.40        | 1.33     |
| 14  | 9     | 14  | HIS  | ND1-CE1 | 5.04  | 1.37        | 1.32     |
| 4   | 11    | 41  | ILE  | N-CA    | -5.04 | 1.40        | 1.46     |
| 14  | 9     | 612 | ARG  | CA-CB   | 5.04  | 1.61        | 1.53     |
| 3   | 10    | 353 | ARG  | N-CA    | -5.03 | 1.40        | 1.46     |
| 3   | 10    | 157 | ILE  | N-CA    | -5.03 | 1.39        | 1.46     |
| 14  | 9     | 146 | ILE  | CA-CB   | 5.03  | 1.60        | 1.54     |
| 14  | 9     | 688 | LEU  | C-N     | 5.01  | 1.40        | 1.33     |
| 3   | 10    | 26  | ARG  | CD-NE   | 5.01  | 1.53        | 1.46     |
| 3   | 10    | 421 | ILE  | CA-CB   | -5.01 | 1.48        | 1.54     |
| 14  | 9     | 447 | HIS  | ND1-CE1 | 5.01  | 1.37        | 1.32     |

All (898) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 49  | k     | 37  | LYS  | N-CA-C     | 29.97  | 149.63      | 112.47   |
| 14  | 9     | 13  | ARG  | NE-CZ-NH1  | -27.67 | 93.83       | 121.50   |
| 43  | e     | 30  | PRO  | CB-CG-CD   | 23.05  | 179.86      | 106.10   |
| 20  | E     | 128 | PRO  | CA-CB-CG   | -20.56 | 65.43       | 104.50   |
| 20  | E     | 128 | PRO  | N-CD-CG    | -20.32 | 72.71       | 103.20   |
| 20  | E     | 128 | PRO  | CB-CG-CD   | 18.90  | 166.58      | 106.10   |
| 43  | e     | 30  | PRO  | N-CD-CG    | -18.68 | 75.18       | 103.20   |
| 49  | k     | 37  | LYS  | CB-CA-C    | -17.64 | 83.44       | 111.48   |
| 43  | e     | 30  | PRO  | CA-CB-CG   | -16.78 | 72.61       | 104.50   |
| 58  | t     | 95  | PRO  | N-CD-CG    | -13.97 | 82.24       | 103.20   |
| 14  | 9     | 13  | ARG  | NH1-CZ-NH2 | 12.61  | 135.69      | 119.30   |
| 58  | t     | 95  | PRO  | N-CA-CB    | -12.56 | 91.61       | 103.41   |
| 14  | 9     | 13  | ARG  | NE-CZ-NH2  | 12.44  | 130.40      | 119.20   |
| 58  | t     | 95  | PRO  | CA-CB-CG   | -11.81 | 82.06       | 104.50   |
| 39  | a     | 132 | PRO  | N-CD-CG    | -11.76 | 85.56       | 103.20   |
| 3   | 10    | 289 | VAL  | CA-C-N     | 11.74  | 127.63      | 120.24   |
| 3   | 10    | 289 | VAL  | C-N-CA     | 11.74  | 127.63      | 120.24   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 39  | a     | 132 | PRO  | CA-N-CD   | -11.72 | 95.59       | 112.00   |
| 14  | 9     | 347 | GLU  | CA-C-N    | 11.27  | 131.40      | 119.90   |
| 14  | 9     | 347 | GLU  | C-N-CA    | 11.27  | 131.40      | 119.90   |
| 14  | 9     | 160 | ASN  | CA-CB-CG  | -10.71 | 101.89      | 112.60   |
| 3   | 10    | 163 | GLY  | CA-C-N    | 10.43  | 134.67      | 120.38   |
| 3   | 10    | 163 | GLY  | C-N-CA    | 10.43  | 134.67      | 120.38   |
| 20  | E     | 128 | PRO  | CA-N-CD   | -10.17 | 97.76       | 112.00   |
| 3   | 10    | 203 | SER  | CA-C-N    | 10.07  | 131.12      | 119.94   |
| 3   | 10    | 203 | SER  | C-N-CA    | 10.07  | 131.12      | 119.94   |
| 3   | 10    | 108 | PRO  | N-CA-C    | 10.05  | 122.97      | 110.70   |
| 3   | 10    | 304 | THR  | CA-C-N    | 9.77   | 133.84      | 120.46   |
| 3   | 10    | 304 | THR  | C-N-CA    | 9.77   | 133.84      | 120.46   |
| 14  | 9     | 227 | GLY  | CA-C-N    | 9.69   | 130.08      | 119.90   |
| 14  | 9     | 227 | GLY  | C-N-CA    | 9.69   | 130.08      | 119.90   |
| 14  | 9     | 63  | VAL  | CA-C-N    | 9.64   | 133.59      | 120.38   |
| 14  | 9     | 63  | VAL  | C-N-CA    | 9.64   | 133.59      | 120.38   |
| 14  | 9     | 740 | MET  | CA-C-N    | 9.63   | 133.58      | 120.38   |
| 14  | 9     | 740 | MET  | C-N-CA    | 9.63   | 133.58      | 120.38   |
| 4   | 11    | 61  | LEU  | CA-C-N    | 9.58   | 132.63      | 120.56   |
| 4   | 11    | 61  | LEU  | C-N-CA    | 9.58   | 132.63      | 120.56   |
| 14  | 9     | 280 | PHE  | CA-CB-CG  | -9.49  | 104.31      | 113.80   |
| 4   | 11    | 9   | PHE  | CA-C-N    | 9.30   | 133.20      | 120.46   |
| 4   | 11    | 9   | PHE  | C-N-CA    | 9.30   | 133.20      | 120.46   |
| 3   | 10    | 358 | PHE  | CA-C-N    | 9.24   | 133.02      | 120.54   |
| 3   | 10    | 358 | PHE  | C-N-CA    | 9.24   | 133.02      | 120.54   |
| 3   | 10    | 227 | ILE  | CA-C-O    | 9.21   | 129.35      | 120.14   |
| 14  | 9     | 702 | PRO  | N-CA-C    | 9.20   | 121.93      | 110.70   |
| 14  | 9     | 313 | LYS  | CA-C-O    | -9.20  | 110.71      | 121.11   |
| 33  | R     | 76  | PRO  | CA-N-CD   | -9.04  | 99.34       | 112.00   |
| 14  | 9     | 409 | PHE  | CA-CB-CG  | -9.01  | 104.79      | 113.80   |
| 14  | 9     | 372 | SER  | CA-C-N    | 8.96   | 130.12      | 119.99   |
| 14  | 9     | 372 | SER  | C-N-CA    | 8.96   | 130.12      | 119.99   |
| 14  | 9     | 638 | ASP  | CA-CB-CG  | 8.94   | 121.54      | 112.60   |
| 14  | 9     | 564 | ASN  | N-CA-C    | -8.91  | 102.56      | 112.72   |
| 4   | 11    | 50  | ILE  | N-CA-C    | 8.88   | 119.67      | 110.62   |
| 49  | k     | 38  | GLY  | N-CA-C    | -8.86  | 100.59      | 112.81   |
| 3   | 10    | 327 | PRO  | CA-C-N    | 8.84   | 131.94      | 120.44   |
| 3   | 10    | 327 | PRO  | C-N-CA    | 8.84   | 131.94      | 120.44   |
| 14  | 9     | 35  | ARG  | NE-CZ-NH2 | 8.77   | 127.09      | 119.20   |
| 30  | O     | 41  | PRO  | CA-N-CD   | -8.70  | 99.83       | 112.00   |
| 4   | 11    | 18  | ILE  | CA-C-N    | 8.69   | 129.58      | 119.94   |
| 4   | 11    | 18  | ILE  | C-N-CA    | 8.69   | 129.58      | 119.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 10    | 65  | ASN  | CA-C-N      | 8.64  | 132.99      | 120.38   |
| 3   | 10    | 65  | ASN  | C-N-CA      | 8.64  | 132.99      | 120.38   |
| 14  | 9     | 287 | LEU  | CA-C-N      | 8.60  | 131.81      | 120.28   |
| 14  | 9     | 287 | LEU  | C-N-CA      | 8.60  | 131.81      | 120.28   |
| 4   | 11    | 44  | LYS  | CA-C-N      | 8.60  | 132.94      | 120.82   |
| 4   | 11    | 44  | LYS  | C-N-CA      | 8.60  | 132.94      | 120.82   |
| 14  | 9     | 220 | ARG  | NE-CZ-NH2   | 8.48  | 126.83      | 119.20   |
| 3   | 10    | 374 | THR  | CA-C-N      | 8.48  | 131.46      | 120.44   |
| 3   | 10    | 374 | THR  | C-N-CA      | 8.48  | 131.46      | 120.44   |
| 14  | 9     | 591 | ARG  | NE-CZ-NH2   | 8.45  | 126.81      | 119.20   |
| 3   | 10    | 377 | HIS  | ND1-CE1-NE2 | 8.39  | 116.79      | 108.40   |
| 14  | 9     | 514 | ASN  | CA-C-N      | 8.33  | 131.44      | 120.28   |
| 14  | 9     | 514 | ASN  | C-N-CA      | 8.33  | 131.44      | 120.28   |
| 14  | 9     | 637 | CYS  | CA-C-N      | 8.32  | 131.43      | 120.28   |
| 14  | 9     | 637 | CYS  | C-N-CA      | 8.32  | 131.43      | 120.28   |
| 3   | 10    | 52  | GLY  | CA-C-N      | 8.31  | 133.09      | 122.37   |
| 3   | 10    | 52  | GLY  | C-N-CA      | 8.31  | 133.09      | 122.37   |
| 3   | 10    | 183 | PHE  | N-CA-C      | 8.30  | 120.33      | 111.28   |
| 6   | 17    | 42  | LEU  | CA-C-N      | 8.30  | 137.67      | 121.41   |
| 6   | 17    | 42  | LEU  | C-N-CA      | 8.30  | 137.67      | 121.41   |
| 14  | 9     | 713 | MET  | CA-C-N      | 8.27  | 131.15      | 120.56   |
| 14  | 9     | 713 | MET  | C-N-CA      | 8.27  | 131.15      | 120.56   |
| 14  | 9     | 65  | VAL  | N-CA-C      | -8.24 | 102.51      | 110.42   |
| 5   | 12    | 69  | PHE  | CA-CB-CG    | 8.22  | 122.02      | 113.80   |
| 14  | 9     | 712 | ILE  | O-C-N       | 8.22  | 129.84      | 121.87   |
| 3   | 10    | 384 | ARG  | NE-CZ-NH1   | 8.22  | 129.72      | 121.50   |
| 14  | 9     | 399 | ASN  | N-CA-C      | -8.13 | 96.04       | 108.96   |
| 4   | 11    | 62  | VAL  | CA-C-N      | 8.12  | 131.94      | 120.42   |
| 4   | 11    | 62  | VAL  | C-N-CA      | 8.12  | 131.94      | 120.42   |
| 14  | 9     | 599 | HIS  | CA-CB-CG    | 8.11  | 121.91      | 113.80   |
| 3   | 10    | 418 | THR  | CA-C-N      | 8.10  | 128.97      | 119.98   |
| 3   | 10    | 418 | THR  | C-N-CA      | 8.10  | 128.97      | 119.98   |
| 14  | 9     | 658 | LEU  | O-C-N       | 8.10  | 131.39      | 122.15   |
| 3   | 10    | 373 | ASP  | CA-C-N      | 8.10  | 130.97      | 120.44   |
| 3   | 10    | 373 | ASP  | C-N-CA      | 8.10  | 130.97      | 120.44   |
| 3   | 10    | 249 | PHE  | CA-CB-CG    | 7.99  | 121.79      | 113.80   |
| 4   | 11    | 12  | ALA  | CA-C-O      | -7.97 | 112.45      | 120.82   |
| 5   | 12    | 114 | HIS  | CE1-NE2-CD2 | -7.96 | 101.04      | 109.00   |
| 3   | 10    | 305 | ILE  | CA-C-N      | 7.96  | 131.74      | 120.28   |
| 3   | 10    | 305 | ILE  | C-N-CA      | 7.96  | 131.74      | 120.28   |
| 14  | 9     | 198 | LYS  | CA-C-N      | 7.95  | 131.58      | 120.29   |
| 14  | 9     | 198 | LYS  | C-N-CA      | 7.95  | 131.58      | 120.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | 9     | 649 | VAL  | N-CA-C      | -7.95 | 95.71       | 108.90   |
| 14  | 9     | 437 | THR  | CA-C-N      | 7.92  | 130.73      | 120.44   |
| 14  | 9     | 437 | THR  | C-N-CA      | 7.92  | 130.73      | 120.44   |
| 14  | 9     | 552 | HIS  | CA-C-N      | 7.89  | 131.18      | 120.38   |
| 14  | 9     | 552 | HIS  | C-N-CA      | 7.89  | 131.18      | 120.38   |
| 14  | 9     | 519 | ILE  | CA-C-N      | 7.86  | 130.81      | 120.28   |
| 14  | 9     | 519 | ILE  | C-N-CA      | 7.86  | 130.81      | 120.28   |
| 14  | 9     | 659 | ASN  | CB-CA-C     | -7.84 | 97.77       | 110.79   |
| 3   | 10    | 312 | THR  | CA-C-N      | 7.83  | 131.10      | 120.38   |
| 3   | 10    | 312 | THR  | C-N-CA      | 7.83  | 131.10      | 120.38   |
| 4   | 11    | 70  | LEU  | CA-C-O      | -7.81 | 112.15      | 120.42   |
| 14  | 9     | 278 | ASN  | CA-CB-CG    | -7.80 | 104.80      | 112.60   |
| 14  | 9     | 472 | VAL  | N-CA-C      | 7.80  | 118.57      | 110.62   |
| 14  | 9     | 801 | HIS  | ND1-CE1-NE2 | 7.77  | 116.17      | 108.40   |
| 14  | 9     | 658 | LEU  | CA-C-O      | -7.76 | 112.19      | 120.42   |
| 4   | 11    | 67  | ILE  | N-CA-C      | 7.74  | 117.85      | 110.42   |
| 14  | 9     | 508 | VAL  | CA-C-O      | 7.70  | 128.77      | 120.53   |
| 14  | 9     | 350 | ASN  | CA-CB-CG    | 7.69  | 120.29      | 112.60   |
| 3   | 10    | 471 | PRO  | N-CA-C      | -7.69 | 103.75      | 114.98   |
| 3   | 10    | 89  | ILE  | N-CA-C      | -7.65 | 104.00      | 112.80   |
| 3   | 10    | 261 | ILE  | CA-C-N      | 7.64  | 127.63      | 119.76   |
| 3   | 10    | 261 | ILE  | C-N-CA      | 7.64  | 127.63      | 119.76   |
| 3   | 10    | 473 | ILE  | CA-C-N      | 7.58  | 129.90      | 120.34   |
| 3   | 10    | 473 | ILE  | C-N-CA      | 7.58  | 129.90      | 120.34   |
| 14  | 9     | 783 | GLU  | CA-C-N      | 7.58  | 130.44      | 120.28   |
| 14  | 9     | 783 | GLU  | C-N-CA      | 7.58  | 130.44      | 120.28   |
| 3   | 10    | 399 | ILE  | CA-C-N      | 7.57  | 127.45      | 119.05   |
| 3   | 10    | 399 | ILE  | C-N-CA      | 7.57  | 127.45      | 119.05   |
| 4   | 11    | 73  | HIS  | CE1-NE2-CD2 | -7.57 | 101.44      | 109.00   |
| 3   | 10    | 93  | ILE  | CA-C-N      | 7.56  | 130.27      | 120.44   |
| 3   | 10    | 93  | ILE  | C-N-CA      | 7.56  | 130.27      | 120.44   |
| 14  | 9     | 171 | ALA  | CA-C-N      | 7.56  | 132.16      | 120.75   |
| 14  | 9     | 171 | ALA  | C-N-CA      | 7.56  | 132.16      | 120.75   |
| 14  | 9     | 751 | ARG  | N-CA-C      | -7.55 | 102.98      | 111.14   |
| 14  | 9     | 411 | THR  | CA-C-N      | 7.51  | 127.39      | 119.05   |
| 14  | 9     | 411 | THR  | C-N-CA      | 7.51  | 127.39      | 119.05   |
| 14  | 9     | 451 | GLN  | CA-C-N      | 7.50  | 131.08      | 120.28   |
| 14  | 9     | 451 | GLN  | C-N-CA      | 7.50  | 131.08      | 120.28   |
| 3   | 10    | 317 | PHE  | CA-CB-CG    | 7.49  | 121.29      | 113.80   |
| 14  | 9     | 521 | ASN  | OD1-CG-ND2  | 7.49  | 130.09      | 122.60   |
| 3   | 10    | 32  | PHE  | CA-CB-CG    | 7.48  | 121.28      | 113.80   |
| 14  | 9     | 250 | GLU  | N-CA-C      | -7.47 | 104.16      | 113.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 10    | 388 | ILE  | N-CA-C     | -7.47 | 105.14      | 111.56   |
| 14  | 9     | 195 | PHE  | N-CA-C     | -7.46 | 103.22      | 111.36   |
| 3   | 10    | 109 | PRO  | CA-C-N     | 7.46  | 133.33      | 120.58   |
| 3   | 10    | 109 | PRO  | C-N-CA     | 7.46  | 133.33      | 120.58   |
| 14  | 9     | 433 | ILE  | N-CA-C     | -7.45 | 96.74       | 107.77   |
| 3   | 10    | 87  | VAL  | N-CA-C     | -7.45 | 102.06      | 113.16   |
| 14  | 9     | 200 | ILE  | CB-CA-C    | 7.43  | 119.26      | 111.23   |
| 14  | 9     | 572 | PHE  | CA-CB-CG   | 7.43  | 121.23      | 113.80   |
| 14  | 9     | 332 | ASN  | OD1-CG-ND2 | 7.40  | 130.00      | 122.60   |
| 14  | 9     | 328 | ARG  | N-CA-C     | -7.38 | 97.30       | 108.52   |
| 4   | 11    | 26  | GLY  | CA-C-N     | 7.38  | 135.63      | 121.54   |
| 4   | 11    | 26  | GLY  | C-N-CA     | 7.38  | 135.63      | 121.54   |
| 3   | 10    | 287 | ALA  | N-CA-C     | -7.37 | 104.54      | 113.97   |
| 14  | 9     | 279 | LEU  | N-CA-C     | -7.36 | 104.69      | 112.93   |
| 14  | 9     | 130 | THR  | N-CA-C     | -7.35 | 99.11       | 109.69   |
| 3   | 10    | 184 | LEU  | CA-C-N     | 7.35  | 128.10      | 119.94   |
| 3   | 10    | 184 | LEU  | C-N-CA     | 7.35  | 128.10      | 119.94   |
| 14  | 9     | 404 | ARG  | NE-CZ-NH2  | 7.35  | 125.81      | 119.20   |
| 3   | 10    | 167 | VAL  | N-CA-CB    | 7.33  | 119.13      | 110.55   |
| 14  | 9     | 270 | ALA  | CA-C-N     | 7.29  | 130.39      | 120.54   |
| 14  | 9     | 270 | ALA  | C-N-CA     | 7.29  | 130.39      | 120.54   |
| 14  | 9     | 40  | VAL  | CA-C-N     | 7.27  | 131.36      | 120.31   |
| 14  | 9     | 40  | VAL  | C-N-CA     | 7.27  | 131.36      | 120.31   |
| 66  | 15    | 461 | ASN  | N-CA-C     | 7.25  | 121.88      | 112.89   |
| 65  | 14    | 369 | ASP  | N-CA-C     | 7.25  | 119.86      | 111.02   |
| 5   | 12    | 33  | ALA  | N-CA-C     | 7.24  | 119.17      | 111.28   |
| 3   | 10    | 423 | ILE  | O-C-N      | 7.23  | 129.17      | 121.94   |
| 14  | 9     | 603 | SER  | CA-C-N     | 7.23  | 130.56      | 120.29   |
| 14  | 9     | 603 | SER  | C-N-CA     | 7.23  | 130.56      | 120.29   |
| 3   | 10    | 390 | ALA  | CA-C-O     | -7.22 | 111.86      | 118.79   |
| 4   | 11    | 52  | LYS  | CA-C-N     | 7.21  | 129.65      | 120.56   |
| 4   | 11    | 52  | LYS  | C-N-CA     | 7.21  | 129.65      | 120.56   |
| 3   | 10    | 26  | ARG  | N-CA-C     | 7.21  | 119.76      | 111.11   |
| 14  | 9     | 229 | ALA  | CA-C-N     | 7.20  | 133.04      | 120.87   |
| 14  | 9     | 229 | ALA  | C-N-CA     | 7.20  | 133.04      | 120.87   |
| 14  | 9     | 604 | GLN  | CA-C-N     | 7.17  | 129.77      | 120.44   |
| 14  | 9     | 604 | GLN  | C-N-CA     | 7.17  | 129.77      | 120.44   |
| 65  | 14    | 507 | ASP  | CA-CB-CG   | 7.16  | 119.76      | 112.60   |
| 14  | 9     | 549 | ARG  | CB-CA-C    | -7.16 | 98.91       | 110.79   |
| 5   | 12    | 52  | ASP  | CA-CB-CG   | 7.14  | 119.74      | 112.60   |
| 14  | 9     | 678 | PHE  | N-CA-C     | 7.14  | 119.68      | 111.11   |
| 14  | 9     | 184 | PHE  | CA-CB-CG   | 7.13  | 120.93      | 113.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | 9     | 195 | PHE  | CA-CB-CG    | -7.11 | 106.69      | 113.80   |
| 3   | 10    | 290 | ILE  | O-C-N       | 7.10  | 125.11      | 120.07   |
| 14  | 9     | 801 | HIS  | CE1-NE2-CD2 | -7.09 | 101.91      | 109.00   |
| 4   | 11    | 73  | HIS  | ND1-CE1-NE2 | 7.08  | 115.48      | 108.40   |
| 3   | 10    | 422 | ILE  | CA-C-N      | 7.07  | 129.72      | 120.60   |
| 3   | 10    | 422 | ILE  | C-N-CA      | 7.07  | 129.72      | 120.60   |
| 5   | 12    | 72  | LEU  | CA-C-O      | -7.06 | 113.42      | 120.70   |
| 5   | 12    | 25  | HIS  | N-CA-CB     | 7.04  | 121.19      | 110.28   |
| 14  | 9     | 273 | ASN  | CA-CB-CG    | 7.03  | 119.63      | 112.60   |
| 14  | 9     | 412 | PRO  | CA-C-N      | 7.03  | 130.27      | 120.29   |
| 14  | 9     | 412 | PRO  | C-N-CA      | 7.03  | 130.27      | 120.29   |
| 14  | 9     | 209 | ASP  | CA-CB-CG    | 7.03  | 119.62      | 112.60   |
| 3   | 10    | 460 | GLN  | OE1-CD-NE2  | 7.02  | 129.62      | 122.60   |
| 14  | 9     | 725 | LEU  | N-CA-CB     | 7.00  | 120.17      | 110.01   |
| 5   | 12    | 25  | HIS  | ND1-CE1-NE2 | 7.00  | 115.40      | 108.40   |
| 58  | t     | 95  | PRO  | CB-CA-C     | 6.99  | 122.00      | 111.44   |
| 14  | 9     | 801 | HIS  | CA-CB-CG    | 6.99  | 120.79      | 113.80   |
| 3   | 10    | 170 | TYR  | CA-C-N      | 6.98  | 129.35      | 120.56   |
| 3   | 10    | 170 | TYR  | C-N-CA      | 6.98  | 129.35      | 120.56   |
| 3   | 10    | 43  | ARG  | NE-CZ-NH2   | -6.96 | 112.94      | 119.20   |
| 43  | e     | 30  | PRO  | CA-N-CD     | -6.94 | 102.28      | 112.00   |
| 5   | 12    | 109 | TYR  | CA-C-N      | 6.93  | 130.14      | 120.29   |
| 5   | 12    | 109 | TYR  | C-N-CA      | 6.93  | 130.14      | 120.29   |
| 14  | 9     | 724 | HIS  | CE1-NE2-CD2 | -6.93 | 102.07      | 109.00   |
| 3   | 10    | 267 | GLY  | CA-C-N      | 6.92  | 133.40      | 122.60   |
| 3   | 10    | 267 | GLY  | C-N-CA      | 6.92  | 133.40      | 122.60   |
| 14  | 9     | 214 | VAL  | CA-C-O      | -6.92 | 113.83      | 121.17   |
| 14  | 9     | 718 | ASP  | CA-C-N      | 6.91  | 130.39      | 120.79   |
| 14  | 9     | 718 | ASP  | C-N-CA      | 6.91  | 130.39      | 120.79   |
| 3   | 10    | 424 | VAL  | N-CA-C      | 6.89  | 117.04      | 110.42   |
| 14  | 9     | 754 | ASP  | CA-C-O      | 6.88  | 127.71      | 120.42   |
| 14  | 9     | 508 | VAL  | N-CA-C      | -6.87 | 97.84       | 107.80   |
| 14  | 9     | 599 | HIS  | ND1-CE1-NE2 | 6.83  | 115.23      | 108.40   |
| 3   | 10    | 127 | ILE  | CA-C-N      | 6.82  | 129.72      | 120.38   |
| 3   | 10    | 127 | ILE  | C-N-CA      | 6.82  | 129.72      | 120.38   |
| 5   | 12    | 114 | HIS  | ND1-CE1-NE2 | 6.82  | 115.22      | 108.40   |
| 14  | 9     | 292 | ILE  | N-CA-C      | 6.80  | 117.59      | 110.72   |
| 14  | 9     | 704 | ILE  | CA-C-N      | 6.80  | 129.28      | 120.44   |
| 14  | 9     | 704 | ILE  | C-N-CA      | 6.80  | 129.28      | 120.44   |
| 14  | 9     | 401 | ARG  | NE-CZ-NH1   | 6.80  | 128.30      | 121.50   |
| 3   | 10    | 252 | THR  | N-CA-C      | 6.77  | 118.66      | 111.28   |
| 58  | t     | 95  | PRO  | CA-N-CD     | -6.76 | 102.53      | 112.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | 12    | 114 | HIS  | CA-CB-CG    | -6.76 | 107.04      | 113.80   |
| 14  | 9     | 270 | ALA  | N-CA-C      | 6.76  | 118.30      | 111.07   |
| 3   | 10    | 386 | ASN  | CA-CB-CG    | -6.75 | 105.84      | 112.60   |
| 14  | 9     | 457 | HIS  | ND1-CE1-NE2 | 6.75  | 115.16      | 108.40   |
| 3   | 10    | 160 | LYS  | N-CA-C      | -6.74 | 103.86      | 111.07   |
| 14  | 9     | 709 | PHE  | CA-CB-CG    | 6.74  | 120.54      | 113.80   |
| 14  | 9     | 417 | LEU  | N-CA-C      | 6.73  | 118.62      | 111.28   |
| 14  | 9     | 456 | PRO  | CA-C-O      | -6.73 | 113.46      | 122.08   |
| 3   | 10    | 173 | ALA  | CA-C-N      | 6.73  | 129.29      | 120.28   |
| 3   | 10    | 173 | ALA  | C-N-CA      | 6.73  | 129.29      | 120.28   |
| 3   | 10    | 177 | GLY  | CA-C-N      | 6.72  | 129.18      | 120.44   |
| 3   | 10    | 177 | GLY  | C-N-CA      | 6.72  | 129.18      | 120.44   |
| 14  | 9     | 750 | ILE  | CA-C-N      | 6.72  | 129.58      | 120.44   |
| 14  | 9     | 750 | ILE  | C-N-CA      | 6.72  | 129.58      | 120.44   |
| 3   | 10    | 321 | TYR  | CA-C-O      | 6.72  | 126.16      | 118.97   |
| 5   | 12    | 83  | ILE  | CA-C-N      | 6.71  | 129.50      | 120.50   |
| 5   | 12    | 83  | ILE  | C-N-CA      | 6.71  | 129.50      | 120.50   |
| 5   | 12    | 27  | LEU  | CA-C-O      | 6.71  | 127.66      | 120.55   |
| 14  | 9     | 732 | ARG  | N-CA-C      | 6.70  | 118.58      | 111.28   |
| 5   | 12    | 123 | LYS  | CA-C-N      | 6.69  | 134.53      | 121.41   |
| 5   | 12    | 123 | LYS  | C-N-CA      | 6.69  | 134.53      | 121.41   |
| 3   | 10    | 392 | PHE  | CA-C-N      | 6.69  | 129.24      | 120.28   |
| 3   | 10    | 392 | PHE  | C-N-CA      | 6.69  | 129.24      | 120.28   |
| 5   | 12    | 63  | VAL  | N-CA-C      | -6.68 | 102.81      | 109.02   |
| 3   | 10    | 159 | LEU  | N-CA-CB     | 6.67  | 120.74      | 109.87   |
| 14  | 9     | 169 | ALA  | N-CA-CB     | 6.66  | 120.02      | 110.16   |
| 14  | 9     | 662 | LEU  | CA-C-N      | 6.66  | 134.26      | 121.54   |
| 14  | 9     | 662 | LEU  | C-N-CA      | 6.66  | 134.26      | 121.54   |
| 3   | 10    | 420 | ILE  | CA-C-N      | 6.64  | 129.85      | 120.42   |
| 3   | 10    | 420 | ILE  | C-N-CA      | 6.64  | 129.85      | 120.42   |
| 14  | 9     | 296 | THR  | O-C-N       | 6.64  | 128.91      | 122.07   |
| 14  | 9     | 678 | PHE  | CA-C-O      | -6.64 | 113.80      | 120.90   |
| 14  | 9     | 167 | GLN  | OE1-CD-NE2  | -6.63 | 115.97      | 122.60   |
| 14  | 9     | 650 | ASN  | CA-C-N      | 6.63  | 129.16      | 120.28   |
| 14  | 9     | 650 | ASN  | C-N-CA      | 6.63  | 129.16      | 120.28   |
| 14  | 9     | 734 | GLY  | CA-C-O      | -6.63 | 113.24      | 120.40   |
| 56  | r     | 109 | ASP  | CA-C-N      | 6.59  | 132.11      | 121.83   |
| 56  | r     | 109 | ASP  | C-N-CA      | 6.59  | 132.11      | 121.83   |
| 4   | 11    | 14  | LEU  | CD1-CG-CD2  | 6.58  | 125.28      | 110.80   |
| 3   | 10    | 121 | ARG  | N-CA-CB     | 6.58  | 119.55      | 110.01   |
| 3   | 10    | 138 | VAL  | CA-C-O      | -6.57 | 113.88      | 120.85   |
| 5   | 12    | 116 | PHE  | N-CA-CB     | 6.57  | 120.47      | 110.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | 11    | 14  | LEU  | N-CA-C      | 6.57  | 118.09      | 111.07   |
| 14  | 9     | 788 | ALA  | N-CA-C      | 6.56  | 118.51      | 111.36   |
| 14  | 9     | 371 | VAL  | O-C-N       | -6.56 | 116.08      | 123.10   |
| 14  | 9     | 89  | ILE  | CA-C-N      | 6.55  | 127.21      | 119.94   |
| 14  | 9     | 89  | ILE  | C-N-CA      | 6.55  | 127.21      | 119.94   |
| 5   | 12    | 73  | TRP  | CB-CG-CD1   | 6.53  | 136.69      | 126.90   |
| 14  | 9     | 349 | GLU  | CA-C-O      | -6.53 | 114.63      | 121.55   |
| 14  | 9     | 657 | ALA  | O-C-N       | -6.53 | 114.71      | 122.15   |
| 14  | 9     | 1   | MET  | CB-CA-C     | 6.52  | 122.49      | 110.10   |
| 3   | 10    | 48  | ILE  | CA-C-N      | 6.52  | 126.43      | 119.85   |
| 3   | 10    | 48  | ILE  | C-N-CA      | 6.52  | 126.43      | 119.85   |
| 14  | 9     | 650 | ASN  | CA-CB-CG    | 6.51  | 119.11      | 112.60   |
| 14  | 9     | 121 | LEU  | CA-C-N      | 6.49  | 129.30      | 120.54   |
| 14  | 9     | 121 | LEU  | C-N-CA      | 6.49  | 129.30      | 120.54   |
| 14  | 9     | 599 | HIS  | CE1-NE2-CD2 | -6.47 | 102.53      | 109.00   |
| 14  | 9     | 665 | HIS  | CA-C-N      | 6.45  | 134.22      | 121.06   |
| 14  | 9     | 665 | HIS  | C-N-CA      | 6.45  | 134.22      | 121.06   |
| 14  | 9     | 755 | ILE  | N-CA-C      | 6.43  | 116.59      | 110.42   |
| 4   | 11    | 9   | PHE  | CA-C-O      | 6.42  | 127.56      | 120.82   |
| 14  | 9     | 205 | PHE  | CA-C-O      | 6.42  | 127.44      | 120.32   |
| 4   | 11    | 24  | ASN  | N-CA-C      | -6.42 | 105.41      | 112.72   |
| 14  | 9     | 73  | GLU  | CA-C-O      | 6.42  | 127.36      | 119.79   |
| 5   | 12    | 76  | ILE  | CA-C-O      | -6.41 | 114.06      | 120.85   |
| 3   | 10    | 66  | ASP  | N-CA-C      | 6.41  | 119.95      | 111.75   |
| 14  | 9     | 256 | GLU  | N-CA-C      | -6.39 | 104.97      | 112.89   |
| 14  | 9     | 601 | LEU  | CA-C-N      | 6.38  | 129.47      | 120.28   |
| 14  | 9     | 601 | LEU  | C-N-CA      | 6.38  | 129.47      | 120.28   |
| 14  | 9     | 688 | LEU  | N-CA-CB     | 6.37  | 119.24      | 110.01   |
| 14  | 9     | 199 | LYS  | N-CA-C      | 6.37  | 118.30      | 111.36   |
| 5   | 12    | 28  | HIS  | CA-C-N      | 6.36  | 128.71      | 120.44   |
| 5   | 12    | 28  | HIS  | C-N-CA      | 6.36  | 128.71      | 120.44   |
| 3   | 10    | 297 | SER  | CA-CB-OG    | 6.35  | 123.81      | 111.10   |
| 3   | 10    | 431 | MET  | N-CA-C      | 6.35  | 119.19      | 111.82   |
| 3   | 10    | 453 | GLU  | CA-C-N      | 6.35  | 129.16      | 120.46   |
| 3   | 10    | 453 | GLU  | C-N-CA      | 6.35  | 129.16      | 120.46   |
| 14  | 9     | 591 | ARG  | NH1-CZ-NH2  | -6.34 | 111.05      | 119.30   |
| 3   | 10    | 395 | VAL  | N-CA-C      | 6.34  | 117.09      | 110.62   |
| 3   | 10    | 266 | SER  | CA-C-O      | 6.33  | 127.36      | 120.58   |
| 3   | 10    | 330 | ILE  | N-CA-CB     | 6.33  | 117.96      | 110.55   |
| 14  | 9     | 683 | HIS  | CE1-NE2-CD2 | -6.33 | 102.67      | 109.00   |
| 3   | 10    | 312 | THR  | N-CA-CB     | 6.30  | 122.42      | 111.39   |
| 4   | 11    | 42  | PHE  | CA-CB-CG    | 6.30  | 120.10      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | 12    | 113  | ASN  | CA-C-N      | 6.30  | 129.24      | 120.29   |
| 5   | 12    | 113  | ASN  | C-N-CA      | 6.30  | 129.24      | 120.29   |
| 14  | 9     | 747  | ASN  | N-CA-CB     | 6.30  | 120.05      | 110.28   |
| 14  | 9     | 762  | GLN  | CA-C-N      | 6.30  | 128.63      | 120.44   |
| 14  | 9     | 762  | GLN  | C-N-CA      | 6.30  | 128.63      | 120.44   |
| 14  | 9     | 708  | ARG  | N-CA-C      | 6.28  | 118.20      | 111.36   |
| 14  | 9     | 132  | ASN  | CA-C-N      | 6.28  | 129.32      | 120.28   |
| 14  | 9     | 132  | ASN  | C-N-CA      | 6.28  | 129.32      | 120.28   |
| 14  | 9     | 712  | ILE  | N-CA-C      | 6.28  | 117.02      | 110.62   |
| 14  | 9     | 190  | ASN  | O-C-N       | -6.27 | 114.55      | 122.26   |
| 14  | 9     | 74   | VAL  | CA-C-N      | 6.27  | 128.69      | 120.60   |
| 14  | 9     | 74   | VAL  | C-N-CA      | 6.27  | 128.69      | 120.60   |
| 14  | 9     | 35   | ARG  | N-CA-C      | 6.26  | 118.91      | 111.71   |
| 14  | 9     | 457  | HIS  | CE1-NE2-CD2 | -6.25 | 102.75      | 109.00   |
| 3   | 10    | 246  | THR  | CA-CB-CG2   | 6.25  | 121.12      | 110.50   |
| 14  | 9     | 108  | LYS  | CA-C-N      | 6.25  | 128.97      | 120.54   |
| 14  | 9     | 108  | LYS  | C-N-CA      | 6.25  | 128.97      | 120.54   |
| 14  | 9     | 148  | LYS  | N-CA-C      | 6.25  | 118.89      | 111.71   |
| 14  | 9     | 557  | ARG  | NE-CZ-NH1   | 6.24  | 127.74      | 121.50   |
| 6   | 17    | 43   | GLY  | N-CA-C      | 6.24  | 127.96      | 113.18   |
| 14  | 9     | 470  | GLU  | CA-C-N      | 6.24  | 128.42      | 120.56   |
| 14  | 9     | 470  | GLU  | C-N-CA      | 6.24  | 128.42      | 120.56   |
| 14  | 9     | 622  | SER  | CA-C-O      | 6.23  | 127.36      | 120.82   |
| 14  | 9     | 132  | ASN  | OD1-CG-ND2  | 6.23  | 128.83      | 122.60   |
| 14  | 9     | 361  | PHE  | CA-C-O      | 6.23  | 127.36      | 120.82   |
| 3   | 10    | 46   | ALA  | N-CA-C      | 6.22  | 120.13      | 112.54   |
| 6   | 17    | 509  | LEU  | N-CA-C      | 6.22  | 119.03      | 111.82   |
| 6   | 17    | 155  | GLU  | N-CA-C      | 6.21  | 120.03      | 111.71   |
| 14  | 9     | 565  | ASP  | CA-CB-CG    | -6.21 | 106.39      | 112.60   |
| 14  | 9     | 647  | ASN  | CB-CA-C     | -6.20 | 98.86       | 109.65   |
| 14  | 9     | 398  | PRO  | N-CA-CB     | 6.20  | 109.75      | 103.25   |
| 14  | 9     | 580  | GLN  | OE1-CD-NE2  | 6.20  | 128.80      | 122.60   |
| 6   | 17    | 402  | ASP  | CA-CB-CG    | 6.19  | 118.79      | 112.60   |
| 3   | 10    | 415  | LEU  | O-C-N       | 6.19  | 130.59      | 123.29   |
| 64  | 13    | 1035 | LYS  | CD-CE-NZ    | 6.19  | 131.70      | 111.90   |
| 3   | 10    | 328  | THR  | CA-C-N      | 6.18  | 126.84      | 119.98   |
| 3   | 10    | 328  | THR  | C-N-CA      | 6.18  | 126.84      | 119.98   |
| 14  | 9     | 799  | GLU  | CA-C-O      | -6.18 | 114.00      | 120.55   |
| 14  | 9     | 449  | TYR  | CA-C-O      | 6.17  | 127.08      | 120.10   |
| 14  | 9     | 572  | PHE  | CA-C-N      | 6.17  | 128.54      | 120.28   |
| 14  | 9     | 572  | PHE  | C-N-CA      | 6.17  | 128.54      | 120.28   |
| 14  | 9     | 514  | ASN  | OD1-CG-ND2  | 6.16  | 128.76      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 10    | 295 | ALA  | N-CA-C     | 6.16  | 117.66      | 111.07   |
| 3   | 10    | 247 | LEU  | N-CA-CB    | 6.16  | 119.17      | 110.12   |
| 14  | 9     | 547 | PHE  | CA-C-N     | 6.14  | 128.43      | 120.44   |
| 14  | 9     | 547 | PHE  | C-N-CA     | 6.14  | 128.43      | 120.44   |
| 66  | 15    | 458 | SER  | N-CA-C     | 6.14  | 120.94      | 112.90   |
| 3   | 10    | 195 | ASN  | CA-C-N     | 6.14  | 126.79      | 119.98   |
| 3   | 10    | 195 | ASN  | C-N-CA     | 6.14  | 126.79      | 119.98   |
| 14  | 9     | 232 | GLU  | CA-C-N     | 6.13  | 128.50      | 120.28   |
| 14  | 9     | 232 | GLU  | C-N-CA     | 6.13  | 128.50      | 120.28   |
| 14  | 9     | 759 | THR  | O-C-N      | 6.13  | 128.61      | 122.12   |
| 3   | 10    | 179 | TYR  | CA-C-O     | -6.12 | 112.93      | 119.97   |
| 3   | 10    | 276 | ALA  | CB-CA-C    | -6.12 | 101.61      | 111.28   |
| 14  | 9     | 182 | LEU  | CA-C-N     | 6.12  | 126.73      | 120.00   |
| 14  | 9     | 182 | LEU  | C-N-CA     | 6.12  | 126.73      | 120.00   |
| 14  | 9     | 780 | GLU  | CB-CG-CD   | -6.11 | 102.21      | 112.60   |
| 66  | 15    | 597 | SER  | N-CA-C     | 6.10  | 117.75      | 110.19   |
| 3   | 10    | 412 | SER  | CA-C-O     | -6.08 | 113.40      | 120.20   |
| 3   | 10    | 228 | ASN  | CA-C-N     | 6.06  | 128.72      | 120.54   |
| 3   | 10    | 228 | ASN  | C-N-CA     | 6.06  | 128.72      | 120.54   |
| 5   | 12    | 32  | LYS  | N-CA-C     | -6.06 | 104.75      | 111.36   |
| 14  | 9     | 280 | PHE  | CA-C-O     | 6.06  | 126.63      | 119.48   |
| 14  | 9     | 766 | ARG  | CA-C-N     | 6.05  | 128.39      | 120.28   |
| 14  | 9     | 766 | ARG  | C-N-CA     | 6.05  | 128.39      | 120.28   |
| 14  | 9     | 222 | PRO  | CA-C-N     | 6.05  | 129.46      | 120.87   |
| 14  | 9     | 222 | PRO  | C-N-CA     | 6.05  | 129.46      | 120.87   |
| 14  | 9     | 397 | ARG  | CA-C-N     | 6.04  | 127.39      | 119.84   |
| 14  | 9     | 397 | ARG  | C-N-CA     | 6.04  | 127.39      | 119.84   |
| 14  | 9     | 691 | GLU  | N-CA-C     | 6.04  | 117.86      | 111.28   |
| 14  | 9     | 158 | PHE  | CA-CB-CG   | -6.03 | 107.77      | 113.80   |
| 14  | 9     | 213 | SER  | CA-C-N     | 6.03  | 128.16      | 120.56   |
| 14  | 9     | 213 | SER  | C-N-CA     | 6.03  | 128.16      | 120.56   |
| 3   | 10    | 326 | LYS  | CA-C-O     | -6.03 | 114.59      | 120.19   |
| 14  | 9     | 281 | ALA  | CA-C-N     | 6.02  | 128.35      | 120.28   |
| 14  | 9     | 281 | ALA  | C-N-CA     | 6.02  | 128.35      | 120.28   |
| 14  | 9     | 47  | ASN  | OD1-CG-ND2 | 6.02  | 128.62      | 122.60   |
| 5   | 12    | 47  | LYS  | CA-C-N     | 6.02  | 128.84      | 120.29   |
| 5   | 12    | 47  | LYS  | C-N-CA     | 6.02  | 128.84      | 120.29   |
| 14  | 9     | 584 | GLU  | O-C-N      | -6.02 | 115.74      | 122.12   |
| 14  | 9     | 433 | ILE  | CA-CB-CG1  | 6.02  | 120.63      | 110.40   |
| 3   | 10    | 214 | ILE  | CA-CB-CG2  | 6.01  | 120.72      | 110.50   |
| 3   | 10    | 380 | ARG  | NE-CZ-NH2  | 6.01  | 124.61      | 119.20   |
| 3   | 10    | 337 | VAL  | CB-CA-C    | -6.01 | 104.03      | 112.14   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 14  | 9     | 286 | ASP  | CA-CB-CG   | 6.01  | 118.61      | 112.60   |
| 6   | 17    | 895 | PHE  | CA-CB-CG   | 6.01  | 119.81      | 113.80   |
| 14  | 9     | 779 | GLU  | N-CA-C     | 6.01  | 120.34      | 112.89   |
| 5   | 12    | 73  | TRP  | CB-CG-CD2  | -6.01 | 118.39      | 126.80   |
| 14  | 9     | 204 | HIS  | CG-CD2-NE2 | 6.01  | 113.21      | 107.20   |
| 14  | 9     | 710 | ARG  | CA-C-N     | 6.00  | 128.32      | 120.28   |
| 14  | 9     | 710 | ARG  | C-N-CA     | 6.00  | 128.32      | 120.28   |
| 3   | 10    | 402 | ILE  | N-CA-CB    | 6.00  | 118.70      | 110.54   |
| 5   | 12    | 102 | SER  | CA-C-N     | 6.00  | 128.31      | 120.28   |
| 5   | 12    | 102 | SER  | C-N-CA     | 6.00  | 128.31      | 120.28   |
| 5   | 12    | 117 | ILE  | CA-C-N     | 5.99  | 128.91      | 120.28   |
| 5   | 12    | 117 | ILE  | C-N-CA     | 5.99  | 128.91      | 120.28   |
| 3   | 10    | 126 | MET  | O-C-N      | 5.99  | 128.24      | 122.07   |
| 14  | 9     | 26  | GLU  | CA-C-N     | 5.98  | 128.65      | 120.46   |
| 14  | 9     | 26  | GLU  | C-N-CA     | 5.98  | 128.65      | 120.46   |
| 3   | 10    | 244 | PHE  | CA-C-N     | 5.98  | 128.65      | 120.46   |
| 3   | 10    | 244 | PHE  | C-N-CA     | 5.98  | 128.65      | 120.46   |
| 14  | 9     | 777 | THR  | CA-C-O     | -5.98 | 114.00      | 119.62   |
| 14  | 9     | 404 | ARG  | CA-C-O     | -5.97 | 115.07      | 121.94   |
| 14  | 9     | 636 | PHE  | CA-C-N     | 5.97  | 128.88      | 120.28   |
| 14  | 9     | 636 | PHE  | C-N-CA     | 5.97  | 128.88      | 120.28   |
| 14  | 9     | 521 | ASN  | N-CA-CB    | 5.97  | 119.00      | 110.16   |
| 4   | 11    | 51  | VAL  | CA-C-N     | 5.97  | 128.76      | 120.29   |
| 4   | 11    | 51  | VAL  | C-N-CA     | 5.97  | 128.76      | 120.29   |
| 14  | 9     | 240 | ASP  | CA-C-N     | 5.96  | 128.86      | 120.28   |
| 14  | 9     | 240 | ASP  | C-N-CA     | 5.96  | 128.86      | 120.28   |
| 3   | 10    | 126 | MET  | N-CA-CB    | -5.96 | 101.37      | 110.01   |
| 14  | 9     | 722 | ILE  | CA-C-N     | 5.95  | 128.25      | 120.28   |
| 14  | 9     | 722 | ILE  | C-N-CA     | 5.95  | 128.25      | 120.28   |
| 14  | 9     | 799 | GLU  | N-CA-C     | 5.95  | 117.76      | 111.28   |
| 14  | 9     | 11  | SER  | CA-C-N     | 5.94  | 126.09      | 119.32   |
| 14  | 9     | 11  | SER  | C-N-CA     | 5.94  | 126.09      | 119.32   |
| 14  | 9     | 254 | ASP  | CA-C-O     | -5.94 | 114.37      | 119.36   |
| 3   | 10    | 199 | LEU  | CA-C-N     | 5.94  | 128.72      | 120.29   |
| 3   | 10    | 199 | LEU  | C-N-CA     | 5.94  | 128.72      | 120.29   |
| 14  | 9     | 354 | ALA  | O-C-N      | -5.94 | 116.62      | 123.33   |
| 3   | 10    | 90  | SER  | O-C-N      | -5.92 | 114.84      | 120.70   |
| 5   | 12    | 61  | VAL  | N-CA-C     | -5.92 | 99.87       | 108.87   |
| 5   | 12    | 89  | LYS  | CA-C-N     | 5.92  | 128.69      | 120.29   |
| 5   | 12    | 89  | LYS  | C-N-CA     | 5.92  | 128.69      | 120.29   |
| 14  | 9     | 730 | LYS  | N-CA-C     | 5.92  | 117.40      | 111.07   |
| 4   | 11    | 61  | LEU  | N-CA-CB    | 5.92  | 118.82      | 110.12   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 14  | 9     | 546 | LEU  | CA-C-N     | 5.92  | 130.70      | 120.58   |
| 14  | 9     | 546 | LEU  | C-N-CA     | 5.92  | 130.70      | 120.58   |
| 14  | 9     | 697 | VAL  | O-C-N      | 5.92  | 127.61      | 121.87   |
| 3   | 10    | 89  | ILE  | CA-C-N     | 5.91  | 128.38      | 120.58   |
| 3   | 10    | 89  | ILE  | C-N-CA     | 5.91  | 128.38      | 120.58   |
| 3   | 10    | 189 | SER  | N-CA-C     | 5.91  | 118.50      | 111.71   |
| 5   | 12    | 98  | ILE  | CA-C-N     | 5.91  | 128.00      | 120.56   |
| 5   | 12    | 98  | ILE  | C-N-CA     | 5.91  | 128.00      | 120.56   |
| 3   | 10    | 403 | VAL  | N-CA-C     | 5.90  | 116.64      | 110.62   |
| 14  | 9     | 185 | ASP  | N-CA-CB    | 5.89  | 118.78      | 110.12   |
| 14  | 9     | 477 | GLN  | CA-C-N     | 5.89  | 129.24      | 120.87   |
| 14  | 9     | 477 | GLN  | C-N-CA     | 5.89  | 129.24      | 120.87   |
| 14  | 9     | 138 | ARG  | NE-CZ-NH2  | -5.89 | 113.90      | 119.20   |
| 14  | 9     | 401 | ARG  | CA-C-N     | 5.89  | 131.76      | 122.34   |
| 14  | 9     | 401 | ARG  | C-N-CA     | 5.89  | 131.76      | 122.34   |
| 14  | 9     | 67  | ALA  | CA-C-N     | 5.89  | 128.65      | 120.29   |
| 14  | 9     | 67  | ALA  | C-N-CA     | 5.89  | 128.65      | 120.29   |
| 4   | 11    | 71  | VAL  | CA-C-O     | -5.88 | 114.61      | 120.85   |
| 14  | 9     | 796 | ALA  | CA-C-N     | 5.88  | 128.16      | 120.28   |
| 14  | 9     | 796 | ALA  | C-N-CA     | 5.88  | 128.16      | 120.28   |
| 14  | 9     | 433 | ILE  | CA-C-O     | -5.88 | 114.33      | 120.27   |
| 5   | 12    | 98  | ILE  | N-CA-CB    | 5.88  | 118.54      | 110.54   |
| 14  | 9     | 110 | LEU  | CA-C-N     | 5.88  | 128.16      | 120.28   |
| 14  | 9     | 110 | LEU  | C-N-CA     | 5.88  | 128.16      | 120.28   |
| 14  | 9     | 170 | PHE  | CA-CB-CG   | -5.88 | 107.92      | 113.80   |
| 3   | 10    | 446 | LEU  | CA-C-N     | 5.88  | 128.15      | 120.28   |
| 3   | 10    | 446 | LEU  | C-N-CA     | 5.88  | 128.15      | 120.28   |
| 14  | 9     | 460 | LEU  | N-CA-CB    | 5.87  | 119.04      | 110.58   |
| 3   | 10    | 461 | ASP  | CA-C-N     | 5.86  | 128.61      | 120.29   |
| 3   | 10    | 461 | ASP  | C-N-CA     | 5.86  | 128.61      | 120.29   |
| 14  | 9     | 473 | ALA  | CA-C-N     | 5.86  | 131.40      | 121.14   |
| 14  | 9     | 473 | ALA  | C-N-CA     | 5.86  | 131.40      | 121.14   |
| 14  | 9     | 747 | ASN  | OD1-CG-ND2 | 5.86  | 128.46      | 122.60   |
| 14  | 9     | 598 | ASP  | O-C-N      | -5.86 | 114.78      | 122.39   |
| 14  | 9     | 47  | ASN  | CA-C-N     | 5.85  | 128.12      | 120.28   |
| 14  | 9     | 47  | ASN  | C-N-CA     | 5.85  | 128.12      | 120.28   |
| 5   | 12    | 69  | PHE  | CA-C-N     | 5.84  | 128.11      | 120.28   |
| 5   | 12    | 69  | PHE  | C-N-CA     | 5.84  | 128.11      | 120.28   |
| 3   | 10    | 61  | ASP  | N-CA-C     | 5.84  | 117.64      | 111.28   |
| 3   | 10    | 384 | ARG  | NH1-CZ-NH2 | -5.83 | 111.72      | 119.30   |
| 14  | 9     | 259 | ALA  | CA-C-N     | 5.83  | 127.86      | 120.51   |
| 14  | 9     | 259 | ALA  | C-N-CA     | 5.83  | 127.86      | 120.51   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 14  | 9     | 659  | ASN  | OD1-CG-ND2 | 5.83  | 128.43      | 122.60   |
| 14  | 9     | 33   | TYR  | N-CA-C     | -5.83 | 104.56      | 111.03   |
| 6   | 17    | 369  | HIS  | CB-CG-CD2  | -5.82 | 123.64      | 131.20   |
| 14  | 9     | 100  | ALA  | N-CA-CB    | 5.81  | 119.45      | 110.21   |
| 14  | 9     | 359  | GLN  | OE1-CD-NE2 | -5.81 | 116.79      | 122.60   |
| 14  | 9     | 523  | LEU  | CA-C-N     | 5.81  | 128.06      | 120.28   |
| 14  | 9     | 523  | LEU  | C-N-CA     | 5.81  | 128.06      | 120.28   |
| 3   | 10    | 49   | PRO  | N-CA-CB    | 5.80  | 108.73      | 103.33   |
| 3   | 10    | 186  | ASP  | O-C-N      | 5.80  | 128.27      | 122.12   |
| 14  | 9     | 358  | TYR  | CA-C-N     | 5.80  | 127.98      | 120.44   |
| 14  | 9     | 358  | TYR  | C-N-CA     | 5.80  | 127.98      | 120.44   |
| 3   | 10    | 93   | ILE  | N-CA-CB    | 5.80  | 117.33      | 110.55   |
| 3   | 10    | 27   | ASP  | CA-C-N     | 5.80  | 128.32      | 120.44   |
| 3   | 10    | 27   | ASP  | C-N-CA     | 5.80  | 128.32      | 120.44   |
| 3   | 10    | 301  | ILE  | N-CA-CB    | -5.80 | 105.93      | 110.45   |
| 3   | 10    | 240  | TYR  | CA-C-N     | 5.79  | 128.04      | 120.28   |
| 3   | 10    | 240  | TYR  | C-N-CA     | 5.79  | 128.04      | 120.28   |
| 14  | 9     | 488  | ALA  | CA-C-N     | 5.79  | 130.85      | 120.77   |
| 14  | 9     | 488  | ALA  | C-N-CA     | 5.79  | 130.85      | 120.77   |
| 5   | 12    | 79   | GLU  | CA-C-N     | 5.79  | 128.07      | 120.60   |
| 5   | 12    | 79   | GLU  | C-N-CA     | 5.79  | 128.07      | 120.60   |
| 3   | 10    | 350  | ASN  | CA-C-N     | 5.79  | 125.47      | 119.05   |
| 3   | 10    | 350  | ASN  | C-N-CA     | 5.79  | 125.47      | 119.05   |
| 4   | 11    | 7    | VAL  | CA-C-N     | 5.79  | 129.10      | 120.31   |
| 4   | 11    | 7    | VAL  | C-N-CA     | 5.79  | 129.10      | 120.31   |
| 3   | 10    | 434  | LEU  | CA-C-N     | 5.78  | 127.96      | 120.44   |
| 3   | 10    | 434  | LEU  | C-N-CA     | 5.78  | 127.96      | 120.44   |
| 66  | 15    | 1015 | THR  | CA-CB-OG1  | 5.78  | 118.27      | 109.60   |
| 14  | 9     | 311  | ASP  | CA-CB-CG   | -5.78 | 106.82      | 112.60   |
| 3   | 10    | 204  | GLY  | CA-C-N     | 5.78  | 127.95      | 120.56   |
| 3   | 10    | 204  | GLY  | C-N-CA     | 5.78  | 127.95      | 120.56   |
| 14  | 9     | 212  | ASP  | CA-CB-CG   | 5.78  | 118.38      | 112.60   |
| 14  | 9     | 727  | ASN  | CA-CB-CG   | -5.77 | 106.83      | 112.60   |
| 14  | 9     | 769  | ILE  | CA-C-O     | -5.77 | 114.74      | 120.85   |
| 4   | 11    | 53   | ILE  | N-CA-C     | -5.76 | 104.89      | 110.42   |
| 14  | 9     | 20   | ALA  | N-CA-CB    | 5.76  | 118.59      | 110.12   |
| 3   | 10    | 195  | ASN  | CA-CB-CG   | -5.76 | 106.84      | 112.60   |
| 3   | 10    | 168  | ALA  | CA-C-O     | 5.75  | 126.64      | 120.55   |
| 14  | 9     | 411  | THR  | CA-CB-OG1  | 5.75  | 118.22      | 109.60   |
| 14  | 9     | 694  | THR  | N-CA-C     | -5.75 | 105.02      | 111.28   |
| 14  | 9     | 399  | ASN  | CA-C-O     | 5.74  | 126.86      | 120.43   |
| 4   | 11    | 17   | ILE  | O-C-N      | 5.74  | 127.53      | 121.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 10    | 214 | ILE  | N-CA-CB     | 5.73  | 118.34      | 110.54   |
| 14  | 9     | 457 | HIS  | CG-CD2-NE2  | 5.73  | 112.93      | 107.20   |
| 3   | 10    | 215 | ALA  | CA-C-O      | -5.72 | 114.36      | 120.42   |
| 14  | 9     | 335 | HIS  | CA-C-N      | 5.71  | 128.50      | 120.28   |
| 14  | 9     | 335 | HIS  | C-N-CA      | 5.71  | 128.50      | 120.28   |
| 3   | 10    | 205 | ILE  | CA-C-N      | 5.70  | 128.49      | 120.28   |
| 3   | 10    | 205 | ILE  | C-N-CA      | 5.70  | 128.49      | 120.28   |
| 3   | 10    | 403 | VAL  | CA-C-N      | 5.70  | 128.38      | 120.29   |
| 3   | 10    | 403 | VAL  | C-N-CA      | 5.70  | 128.38      | 120.29   |
| 4   | 11    | 70  | LEU  | O-C-N       | 5.69  | 128.64      | 122.15   |
| 14  | 9     | 32  | ASN  | CA-C-N      | 5.68  | 128.36      | 120.63   |
| 14  | 9     | 32  | ASN  | C-N-CA      | 5.68  | 128.36      | 120.63   |
| 3   | 10    | 458 | ALA  | CA-C-O      | 5.68  | 126.36      | 119.38   |
| 3   | 10    | 154 | SER  | N-CA-CB     | 5.67  | 121.28      | 111.13   |
| 14  | 9     | 162 | ALA  | CA-C-N      | 5.67  | 125.78      | 119.32   |
| 14  | 9     | 162 | ALA  | C-N-CA      | 5.67  | 125.78      | 119.32   |
| 3   | 10    | 238 | PHE  | N-CA-C      | 5.66  | 117.45      | 111.28   |
| 4   | 11    | 48  | ARG  | NE-CZ-NH2   | -5.66 | 114.10      | 119.20   |
| 3   | 10    | 342 | PHE  | O-C-N       | -5.66 | 115.98      | 122.09   |
| 3   | 10    | 429 | GLU  | N-CA-C      | 5.66  | 117.25      | 111.14   |
| 14  | 9     | 588 | PHE  | CA-C-N      | 5.66  | 127.86      | 120.28   |
| 14  | 9     | 588 | PHE  | C-N-CA      | 5.66  | 127.86      | 120.28   |
| 3   | 10    | 143 | VAL  | O-C-N       | 5.66  | 127.36      | 121.87   |
| 14  | 9     | 79  | THR  | CA-C-N      | 5.66  | 131.19      | 121.07   |
| 14  | 9     | 79  | THR  | C-N-CA      | 5.66  | 131.19      | 121.07   |
| 14  | 9     | 551 | ALA  | CA-C-N      | 5.65  | 130.18      | 121.19   |
| 14  | 9     | 551 | ALA  | C-N-CA      | 5.65  | 130.18      | 121.19   |
| 14  | 9     | 77  | ARG  | N-CA-C      | 5.65  | 118.37      | 111.82   |
| 5   | 12    | 31  | LEU  | CA-C-O      | 5.64  | 126.40      | 120.42   |
| 3   | 10    | 102 | LEU  | N-CA-C      | 5.64  | 119.42      | 112.54   |
| 5   | 12    | 60  | LYS  | CA-C-O      | 5.64  | 127.48      | 120.54   |
| 14  | 9     | 170 | PHE  | N-CA-CB     | 5.63  | 119.88      | 110.41   |
| 3   | 10    | 422 | ILE  | N-CA-CB     | 5.63  | 117.14      | 110.55   |
| 14  | 9     | 538 | PHE  | CA-CB-CG    | -5.63 | 108.17      | 113.80   |
| 3   | 10    | 72  | ASN  | OD1-CG-ND2  | 5.63  | 128.23      | 122.60   |
| 3   | 10    | 105 | ASP  | CA-CB-CG    | -5.63 | 106.97      | 112.60   |
| 4   | 11    | 72  | PHE  | CB-CA-C     | -5.63 | 101.28      | 110.85   |
| 3   | 10    | 374 | THR  | N-CA-C      | -5.62 | 105.05      | 111.07   |
| 14  | 9     | 20  | ALA  | CB-CA-C     | -5.62 | 101.46      | 110.79   |
| 3   | 10    | 377 | HIS  | CE1-NE2-CD2 | -5.62 | 103.38      | 109.00   |
| 14  | 9     | 592 | LYS  | CA-C-O      | -5.62 | 114.92      | 120.82   |
| 14  | 9     | 657 | ALA  | CA-C-N      | 5.62  | 128.27      | 120.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | 9     | 657 | ALA  | C-N-CA      | 5.62  | 128.27      | 120.29   |
| 3   | 10    | 468 | ALA  | CA-C-N      | 5.62  | 130.97      | 121.14   |
| 3   | 10    | 468 | ALA  | C-N-CA      | 5.62  | 130.97      | 121.14   |
| 14  | 9     | 429 | THR  | N-CA-C      | -5.62 | 106.31      | 114.12   |
| 14  | 9     | 552 | HIS  | ND1-CE1-NE2 | 5.61  | 114.01      | 108.40   |
| 14  | 9     | 510 | GLY  | O-C-N       | -5.61 | 119.82      | 123.35   |
| 3   | 10    | 290 | ILE  | CA-C-O      | -5.61 | 114.09      | 118.85   |
| 14  | 9     | 456 | PRO  | O-C-N       | 5.60  | 129.84      | 123.00   |
| 14  | 9     | 89  | ILE  | N-CA-CB     | 5.60  | 117.11      | 110.55   |
| 3   | 10    | 235 | ILE  | CA-C-O      | -5.60 | 114.83      | 121.05   |
| 14  | 9     | 768 | VAL  | N-CA-C      | -5.60 | 105.05      | 110.42   |
| 3   | 10    | 433 | ALA  | CA-C-O      | -5.59 | 114.95      | 120.82   |
| 14  | 9     | 293 | ASN  | CA-C-N      | 5.59  | 128.23      | 120.29   |
| 14  | 9     | 293 | ASN  | C-N-CA      | 5.59  | 128.23      | 120.29   |
| 5   | 12    | 106 | ILE  | N-CA-CB     | 5.59  | 117.09      | 110.55   |
| 14  | 9     | 571 | PHE  | N-CA-C      | -5.59 | 105.26      | 111.36   |
| 14  | 9     | 654 | LEU  | N-CA-C      | 5.59  | 117.17      | 111.14   |
| 3   | 10    | 36  | VAL  | CA-C-O      | -5.59 | 115.25      | 121.17   |
| 14  | 9     | 124 | ARG  | CA-C-O      | 5.58  | 125.42      | 119.34   |
| 3   | 10    | 120 | GLY  | CA-C-N      | 5.58  | 127.70      | 120.44   |
| 3   | 10    | 120 | GLY  | C-N-CA      | 5.58  | 127.70      | 120.44   |
| 6   | 17    | 894 | ASN  | CA-CB-CG    | -5.58 | 107.02      | 112.60   |
| 5   | 12    | 62  | LYS  | CA-C-O      | 5.58  | 126.12      | 120.88   |
| 14  | 9     | 687 | SER  | CA-C-O      | -5.57 | 114.64      | 120.55   |
| 14  | 9     | 149 | ARG  | NE-CZ-NH2   | -5.56 | 114.20      | 119.20   |
| 6   | 17    | 867 | ASP  | CA-CB-CG    | 5.55  | 118.15      | 112.60   |
| 5   | 12    | 49  | LYS  | N-CA-CB     | 5.55  | 118.77      | 110.22   |
| 14  | 9     | 395 | THR  | O-C-N       | -5.55 | 116.69      | 122.96   |
| 14  | 9     | 85  | ARG  | NE-CZ-NH1   | 5.55  | 127.05      | 121.50   |
| 3   | 10    | 156 | PRO  | N-CA-C      | -5.55 | 105.97      | 113.40   |
| 14  | 9     | 429 | THR  | N-CA-CB     | 5.54  | 118.53      | 110.88   |
| 3   | 10    | 387 | PHE  | CA-C-O      | -5.54 | 112.79      | 119.49   |
| 3   | 10    | 268 | GLN  | CA-C-O      | 5.54  | 126.12      | 119.59   |
| 20  | E     | 128 | PRO  | N-CA-CB     | -5.54 | 98.49       | 103.36   |
| 3   | 10    | 344 | TYR  | CA-C-N      | 5.54  | 127.70      | 120.28   |
| 3   | 10    | 344 | TYR  | C-N-CA      | 5.54  | 127.70      | 120.28   |
| 5   | 12    | 99  | VAL  | CA-C-O      | -5.54 | 115.30      | 121.17   |
| 14  | 9     | 578 | ARG  | CA-C-N      | 5.54  | 127.97      | 120.44   |
| 14  | 9     | 578 | ARG  | C-N-CA      | 5.54  | 127.97      | 120.44   |
| 3   | 10    | 262 | PRO  | N-CD-CG     | 5.53  | 111.50      | 103.20   |
| 5   | 12    | 37  | ALA  | CB-CA-C     | -5.53 | 101.61      | 110.79   |
| 14  | 9     | 282 | LEU  | N-CA-C      | -5.53 | 105.25      | 111.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | 9     | 252 | LYS  | CA-C-N      | 5.52  | 130.38      | 123.14   |
| 14  | 9     | 252 | LYS  | C-N-CA      | 5.52  | 130.38      | 123.14   |
| 3   | 10    | 100 | GLN  | OE1-CD-NE2  | -5.52 | 117.08      | 122.60   |
| 66  | 15    | 460 | GLY  | CA-C-N      | 5.52  | 130.80      | 121.14   |
| 66  | 15    | 460 | GLY  | C-N-CA      | 5.52  | 130.80      | 121.14   |
| 14  | 9     | 190 | ASN  | N-CA-C      | -5.52 | 105.86      | 112.59   |
| 3   | 10    | 60  | LEU  | N-CA-C      | -5.51 | 104.91      | 111.69   |
| 4   | 11    | 48  | ARG  | CA-C-O      | 5.51  | 127.68      | 121.51   |
| 14  | 9     | 527 | ALA  | N-CA-C      | -5.50 | 100.21      | 109.07   |
| 14  | 9     | 609 | TYR  | CB-CG-CD1   | 5.50  | 129.04      | 120.80   |
| 14  | 9     | 131 | VAL  | CA-C-O      | 5.49  | 125.57      | 119.42   |
| 3   | 10    | 257 | GLU  | N-CA-CB     | 5.49  | 118.46      | 109.95   |
| 4   | 11    | 21  | LEU  | CA-C-N      | 5.49  | 129.89      | 120.72   |
| 4   | 11    | 21  | LEU  | C-N-CA      | 5.49  | 129.89      | 120.72   |
| 6   | 17    | 506 | SER  | N-CA-C      | 5.49  | 120.09      | 113.17   |
| 14  | 9     | 767 | ASP  | CA-C-N      | 5.49  | 127.48      | 120.56   |
| 14  | 9     | 767 | ASP  | C-N-CA      | 5.49  | 127.48      | 120.56   |
| 65  | 14    | 368 | SER  | CA-C-N      | 5.49  | 128.42      | 120.79   |
| 65  | 14    | 368 | SER  | C-N-CA      | 5.49  | 128.42      | 120.79   |
| 3   | 10    | 292 | VAL  | CA-C-N      | 5.48  | 127.97      | 120.46   |
| 3   | 10    | 292 | VAL  | C-N-CA      | 5.48  | 127.97      | 120.46   |
| 14  | 9     | 237 | VAL  | N-CA-CB     | -5.48 | 102.36      | 110.58   |
| 3   | 10    | 112 | LYS  | CA-C-O      | -5.47 | 112.86      | 119.49   |
| 14  | 9     | 8   | LYS  | N-CA-C      | 5.47  | 116.93      | 111.07   |
| 3   | 10    | 471 | PRO  | CB-CA-C     | 5.47  | 116.62      | 109.89   |
| 14  | 9     | 571 | PHE  | CA-CB-CG    | -5.47 | 108.33      | 113.80   |
| 14  | 9     | 495 | ARG  | NE-CZ-NH2   | -5.46 | 114.28      | 119.20   |
| 14  | 9     | 575 | MET  | CG-SD-CE    | -5.46 | 88.89       | 100.90   |
| 14  | 9     | 683 | HIS  | ND1-CE1-NE2 | 5.46  | 113.86      | 108.40   |
| 5   | 12    | 30  | GLN  | CB-CA-C     | -5.46 | 101.73      | 110.79   |
| 14  | 9     | 266 | GLY  | CA-C-N      | 5.45  | 127.43      | 120.56   |
| 14  | 9     | 266 | GLY  | C-N-CA      | 5.45  | 127.43      | 120.56   |
| 14  | 9     | 693 | ILE  | N-CA-C      | 5.45  | 116.18      | 110.62   |
| 19  | C     | 152 | PRO  | CA-N-CD     | -5.45 | 104.37      | 112.00   |
| 3   | 10    | 432 | SER  | O-C-N       | 5.44  | 128.36      | 122.15   |
| 6   | 17    | 563 | VAL  | CA-CB-CG1   | 5.44  | 119.65      | 110.40   |
| 14  | 9     | 109 | THR  | N-CA-CB     | 5.44  | 118.05      | 109.94   |
| 14  | 9     | 536 | THR  | CA-C-O      | 5.44  | 126.91      | 120.66   |
| 14  | 9     | 657 | ALA  | N-CA-CB     | 5.43  | 118.20      | 110.16   |
| 3   | 10    | 149 | ASN  | CA-C-N      | 5.43  | 130.62      | 120.95   |
| 3   | 10    | 149 | ASN  | C-N-CA      | 5.43  | 130.62      | 120.95   |
| 14  | 9     | 353 | VAL  | CB-CA-C     | -5.43 | 105.10      | 111.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 10    | 167 | VAL  | CB-CA-C     | -5.43 | 105.02      | 111.97   |
| 3   | 10    | 45  | LEU  | CB-CA-C     | -5.42 | 98.98       | 110.31   |
| 4   | 11    | 41  | ILE  | O-C-N       | -5.42 | 115.80      | 122.57   |
| 5   | 12    | 51  | THR  | CA-C-N      | 5.42  | 127.54      | 120.28   |
| 5   | 12    | 51  | THR  | C-N-CA      | 5.42  | 127.54      | 120.28   |
| 14  | 9     | 240 | ASP  | CA-C-O      | -5.42 | 115.10      | 120.90   |
| 66  | 15    | 459 | GLY  | N-CA-C      | 5.42  | 119.51      | 112.25   |
| 14  | 9     | 393 | VAL  | CA-C-O      | -5.42 | 114.42      | 119.62   |
| 5   | 12    | 31  | LEU  | N-CA-C      | 5.42  | 117.26      | 111.36   |
| 5   | 12    | 70  | SER  | CA-C-O      | 5.41  | 126.29      | 120.55   |
| 3   | 10    | 343 | PHE  | CB-CA-C     | -5.41 | 102.39      | 110.88   |
| 4   | 11    | 27  | SER  | O-C-N       | -5.41 | 115.40      | 122.59   |
| 3   | 10    | 277 | LEU  | N-CA-CB     | 5.41  | 117.70      | 109.75   |
| 14  | 9     | 442 | ASP  | CA-C-N      | 5.41  | 127.79      | 120.44   |
| 14  | 9     | 442 | ASP  | C-N-CA      | 5.41  | 127.79      | 120.44   |
| 14  | 9     | 500 | VAL  | N-CA-C      | -5.41 | 104.99      | 112.50   |
| 3   | 10    | 354 | LEU  | CA-C-O      | 5.40  | 126.28      | 120.55   |
| 5   | 12    | 42  | GLU  | CA-C-N      | 5.40  | 128.52      | 120.31   |
| 5   | 12    | 42  | GLU  | C-N-CA      | 5.40  | 128.52      | 120.31   |
| 3   | 10    | 81  | GLN  | CA-CB-CG    | -5.40 | 103.30      | 114.10   |
| 3   | 10    | 200 | LEU  | O-C-N       | 5.40  | 128.30      | 122.15   |
| 14  | 9     | 129 | VAL  | N-CA-C      | -5.39 | 99.98       | 107.80   |
| 14  | 9     | 612 | ARG  | CA-C-N      | 5.39  | 127.51      | 120.28   |
| 14  | 9     | 612 | ARG  | C-N-CA      | 5.39  | 127.51      | 120.28   |
| 5   | 12    | 45  | ASP  | CA-C-O      | -5.39 | 114.01      | 120.10   |
| 5   | 12    | 66  | THR  | CA-CB-OG1   | 5.39  | 117.69      | 109.60   |
| 14  | 9     | 18  | HIS  | CE1-NE2-CD2 | -5.39 | 103.61      | 109.00   |
| 14  | 9     | 137 | GLN  | OE1-CD-NE2  | -5.39 | 117.21      | 122.60   |
| 14  | 9     | 278 | ASN  | O-C-N       | 5.39  | 129.61      | 123.31   |
| 14  | 9     | 539 | PHE  | N-CA-C      | -5.39 | 99.74       | 108.52   |
| 14  | 9     | 417 | LEU  | CA-C-O      | -5.38 | 114.84      | 120.55   |
| 14  | 9     | 156 | CYS  | N-CA-C      | -5.38 | 99.16       | 108.69   |
| 14  | 9     | 647 | ASN  | CA-C-O      | 5.38  | 125.29      | 119.15   |
| 14  | 9     | 134 | TYR  | N-CA-C      | 5.38  | 116.83      | 111.07   |
| 14  | 9     | 633 | VAL  | CA-C-N      | 5.38  | 127.75      | 120.38   |
| 14  | 9     | 633 | VAL  | C-N-CA      | 5.38  | 127.75      | 120.38   |
| 14  | 9     | 744 | SER  | CA-C-N      | 5.38  | 125.45      | 119.32   |
| 14  | 9     | 744 | SER  | C-N-CA      | 5.38  | 125.45      | 119.32   |
| 14  | 9     | 394 | PRO  | CB-CA-C     | 5.37  | 119.88      | 110.96   |
| 14  | 9     | 683 | HIS  | CG-CD2-NE2  | 5.37  | 112.57      | 107.20   |
| 3   | 10    | 446 | LEU  | N-CA-C      | 5.37  | 117.13      | 111.28   |
| 14  | 9     | 605 | ARG  | CA-C-N      | 5.37  | 128.01      | 120.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 14  | 9     | 605 | ARG  | C-N-CA     | 5.37  | 128.01      | 120.28   |
| 3   | 10    | 468 | ALA  | O-C-N      | 5.36  | 127.81      | 122.12   |
| 14  | 9     | 701 | THR  | CA-CB-OG1  | 5.36  | 117.65      | 109.60   |
| 43  | e     | 30  | PRO  | N-CA-CB    | -5.36 | 97.44       | 103.33   |
| 14  | 9     | 657 | ALA  | CA-C-O     | 5.35  | 126.09      | 120.42   |
| 14  | 9     | 522 | GLN  | N-CA-CB    | 5.35  | 117.77      | 110.01   |
| 14  | 9     | 464 | ASN  | CB-CA-C    | -5.35 | 102.52      | 111.13   |
| 14  | 9     | 477 | GLN  | N-CA-CB    | 5.35  | 117.90      | 110.04   |
| 3   | 10    | 288 | GLY  | CA-C-O     | 5.35  | 128.57      | 121.83   |
| 14  | 9     | 193 | HIS  | N-CA-C     | -5.35 | 106.69      | 114.12   |
| 3   | 10    | 52  | GLY  | N-CA-C     | -5.34 | 107.94      | 115.32   |
| 3   | 10    | 98  | VAL  | N-CA-CB    | 5.34  | 116.80      | 110.55   |
| 3   | 10    | 324 | LEU  | CA-C-O     | 5.34  | 126.14      | 119.78   |
| 3   | 10    | 347 | ILE  | CA-C-N     | 5.34  | 127.88      | 120.29   |
| 3   | 10    | 347 | ILE  | C-N-CA     | 5.34  | 127.88      | 120.29   |
| 14  | 9     | 791 | LEU  | CA-C-O     | -5.34 | 114.89      | 120.55   |
| 14  | 9     | 344 | VAL  | CA-C-N     | 5.34  | 131.74      | 121.54   |
| 14  | 9     | 344 | VAL  | C-N-CA     | 5.34  | 131.74      | 121.54   |
| 4   | 11    | 11  | MET  | CB-CA-C    | -5.34 | 101.93      | 110.79   |
| 5   | 12    | 37  | ALA  | N-CA-CB    | 5.34  | 117.97      | 110.12   |
| 14  | 9     | 486 | ASN  | CA-C-N     | 5.33  | 129.69      | 122.07   |
| 14  | 9     | 486 | ASN  | C-N-CA     | 5.33  | 129.69      | 122.07   |
| 14  | 9     | 782 | ASP  | N-CA-C     | -5.33 | 100.34      | 109.24   |
| 3   | 10    | 157 | ILE  | N-CA-C     | -5.32 | 98.30       | 107.24   |
| 64  | 13    | 520 | ASN  | CA-C-N     | 5.31  | 129.10      | 120.60   |
| 64  | 13    | 520 | ASN  | C-N-CA     | 5.31  | 129.10      | 120.60   |
| 3   | 10    | 114 | VAL  | CG1-CB-CG2 | -5.31 | 99.12       | 110.80   |
| 14  | 9     | 625 | ILE  | CA-C-N     | 5.31  | 127.39      | 120.28   |
| 14  | 9     | 625 | ILE  | C-N-CA     | 5.31  | 127.39      | 120.28   |
| 3   | 10    | 340 | PHE  | CA-C-N     | 5.31  | 127.39      | 120.28   |
| 3   | 10    | 340 | PHE  | C-N-CA     | 5.31  | 127.39      | 120.28   |
| 3   | 10    | 151 | GLY  | O-C-N      | -5.30 | 115.81      | 122.70   |
| 14  | 9     | 351 | VAL  | CA-C-N     | 5.29  | 129.12      | 121.18   |
| 14  | 9     | 351 | VAL  | C-N-CA     | 5.29  | 129.12      | 121.18   |
| 3   | 10    | 475 | ASN  | OD1-CG-ND2 | 5.29  | 127.89      | 122.60   |
| 14  | 9     | 541 | SER  | N-CA-C     | -5.29 | 101.65      | 110.17   |
| 5   | 12    | 44  | GLN  | CB-CG-CD   | -5.29 | 103.61      | 112.60   |
| 14  | 9     | 449 | TYR  | N-CA-C     | 5.29  | 117.79      | 111.71   |
| 3   | 10    | 473 | ILE  | O-C-N      | -5.29 | 117.01      | 122.14   |
| 4   | 11    | 48  | ARG  | NE-CZ-NH1  | 5.29  | 126.79      | 121.50   |
| 14  | 9     | 538 | PHE  | N-CA-CB    | 5.28  | 119.19      | 110.69   |
| 14  | 9     | 657 | ALA  | CB-CA-C    | -5.28 | 101.88      | 110.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | 12    | 23  | LYS  | CA-C-N      | 5.27  | 128.94      | 120.30   |
| 5   | 12    | 23  | LYS  | C-N-CA      | 5.27  | 128.94      | 120.30   |
| 14  | 9     | 257 | SER  | N-CA-C      | -5.27 | 106.75      | 114.39   |
| 14  | 9     | 638 | ASP  | N-CA-C      | 5.27  | 117.02      | 111.28   |
| 5   | 12    | 31  | LEU  | CA-C-N      | 5.26  | 127.76      | 120.29   |
| 5   | 12    | 31  | LEU  | C-N-CA      | 5.26  | 127.76      | 120.29   |
| 14  | 9     | 127 | HIS  | ND1-CE1-NE2 | 5.26  | 113.66      | 108.40   |
| 3   | 10    | 470 | THR  | N-CA-C      | -5.25 | 97.92       | 109.11   |
| 14  | 9     | 333 | GLY  | N-CA-C      | -5.25 | 108.38      | 115.21   |
| 3   | 10    | 302 | PRO  | O-C-N       | 5.25  | 128.10      | 122.17   |
| 3   | 10    | 241 | PHE  | CB-CG-CD2   | 5.25  | 129.62      | 120.70   |
| 14  | 9     | 781 | PHE  | CA-CB-CG    | 5.25  | 119.05      | 113.80   |
| 14  | 9     | 800 | ALA  | N-CA-C      | 5.24  | 117.07      | 111.36   |
| 3   | 10    | 128 | THR  | N-CA-C      | -5.24 | 104.99      | 111.33   |
| 3   | 10    | 245 | VAL  | CA-C-O      | -5.24 | 115.50      | 120.95   |
| 14  | 9     | 144 | THR  | CA-C-N      | 5.24  | 127.25      | 120.44   |
| 14  | 9     | 144 | THR  | C-N-CA      | 5.24  | 127.25      | 120.44   |
| 14  | 9     | 419 | VAL  | O-C-N       | 5.24  | 127.04      | 121.91   |
| 14  | 9     | 77  | ARG  | NE-CZ-NH1   | 5.24  | 126.74      | 121.50   |
| 14  | 9     | 508 | VAL  | O-C-N       | -5.24 | 116.97      | 123.10   |
| 3   | 10    | 244 | PHE  | O-C-N       | 5.23  | 127.46      | 122.07   |
| 3   | 10    | 386 | ASN  | CA-C-N      | 5.23  | 128.96      | 120.60   |
| 3   | 10    | 386 | ASN  | C-N-CA      | 5.23  | 128.96      | 120.60   |
| 14  | 9     | 758 | GLN  | CA-C-N      | 5.23  | 127.28      | 120.28   |
| 14  | 9     | 758 | GLN  | C-N-CA      | 5.23  | 127.28      | 120.28   |
| 14  | 9     | 729 | PHE  | CA-CB-CG    | -5.23 | 108.57      | 113.80   |
| 3   | 10    | 217 | TYR  | CB-CG-CD2   | -5.22 | 112.97      | 120.80   |
| 14  | 9     | 611 | GLN  | N-CA-C      | -5.22 | 105.67      | 111.36   |
| 5   | 12    | 122 | PHE  | CA-CB-CG    | -5.22 | 108.58      | 113.80   |
| 3   | 10    | 317 | PHE  | O-C-N       | 5.22  | 127.65      | 122.12   |
| 3   | 10    | 420 | ILE  | CB-CA-C     | -5.22 | 105.02      | 112.22   |
| 14  | 9     | 64  | ALA  | CA-C-O      | -5.22 | 115.00      | 120.63   |
| 14  | 9     | 234 | ALA  | CA-C-N      | 5.22  | 127.70      | 120.29   |
| 14  | 9     | 234 | ALA  | C-N-CA      | 5.22  | 127.70      | 120.29   |
| 66  | 15    | 457 | SER  | N-CA-C      | 5.21  | 116.65      | 110.19   |
| 14  | 9     | 249 | ASP  | N-CA-C      | -5.21 | 105.80      | 113.61   |
| 14  | 9     | 781 | PHE  | CA-C-N      | 5.21  | 131.16      | 122.73   |
| 14  | 9     | 781 | PHE  | C-N-CA      | 5.21  | 131.16      | 122.73   |
| 14  | 9     | 127 | HIS  | CE1-NE2-CD2 | -5.20 | 103.80      | 109.00   |
| 3   | 10    | 64  | SER  | CA-C-N      | 5.20  | 132.27      | 123.01   |
| 3   | 10    | 64  | SER  | C-N-CA      | 5.20  | 132.27      | 123.01   |
| 14  | 9     | 630 | GLU  | O-C-N       | -5.20 | 116.68      | 122.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | 9     | 319 | HIS  | CG-CD2-NE2  | 5.20  | 112.40      | 107.20   |
| 14  | 9     | 364 | LEU  | CA-C-N      | 5.20  | 128.25      | 120.87   |
| 14  | 9     | 364 | LEU  | C-N-CA      | 5.20  | 128.25      | 120.87   |
| 3   | 10    | 24  | ARG  | CD-NE-CZ    | -5.19 | 117.13      | 124.40   |
| 4   | 11    | 40  | GLU  | CA-C-N      | 5.19  | 131.31      | 121.97   |
| 4   | 11    | 40  | GLU  | C-N-CA      | 5.19  | 131.31      | 121.97   |
| 14  | 9     | 287 | LEU  | CA-C-O      | 5.19  | 126.27      | 120.82   |
| 14  | 9     | 42  | LEU  | N-CA-C      | 5.19  | 116.93      | 111.28   |
| 3   | 10    | 156 | PRO  | N-CA-CB     | 5.18  | 109.25      | 103.44   |
| 14  | 9     | 332 | ASN  | N-CA-CB     | 5.18  | 120.54      | 112.25   |
| 3   | 10    | 72  | ASN  | CA-CB-CG    | -5.18 | 107.42      | 112.60   |
| 3   | 10    | 435 | ARG  | N-CA-C      | 5.18  | 116.61      | 111.07   |
| 3   | 10    | 442 | ASN  | N-CA-CB     | 5.18  | 117.52      | 110.01   |
| 14  | 9     | 34  | TYR  | CA-CB-CG    | -5.18 | 104.58      | 113.90   |
| 4   | 11    | 74  | PHE  | CB-CG-CD1   | 5.17  | 129.50      | 120.70   |
| 14  | 9     | 214 | VAL  | CA-CB-CG2   | -5.17 | 101.60      | 110.40   |
| 14  | 9     | 727 | ASN  | CA-C-N      | 5.17  | 128.79      | 120.30   |
| 14  | 9     | 727 | ASN  | C-N-CA      | 5.17  | 128.79      | 120.30   |
| 3   | 10    | 285 | ASN  | CA-CB-CG    | 5.17  | 117.77      | 112.60   |
| 14  | 9     | 677 | THR  | CA-C-O      | 5.17  | 127.03      | 121.55   |
| 14  | 9     | 612 | ARG  | N-CA-C      | -5.17 | 105.72      | 111.36   |
| 3   | 10    | 375 | GLU  | O-C-N       | 5.17  | 127.39      | 122.07   |
| 14  | 9     | 565 | ASP  | N-CA-C      | -5.17 | 102.13      | 110.14   |
| 3   | 10    | 138 | VAL  | CB-CA-C     | -5.16 | 105.10      | 112.22   |
| 14  | 9     | 427 | HIS  | O-C-N       | 5.16  | 127.59      | 122.12   |
| 5   | 12    | 105 | MET  | CA-C-N      | 5.16  | 127.06      | 120.56   |
| 5   | 12    | 105 | MET  | C-N-CA      | 5.16  | 127.06      | 120.56   |
| 14  | 9     | 245 | LYS  | CA-C-N      | 5.16  | 128.03      | 120.71   |
| 14  | 9     | 245 | LYS  | C-N-CA      | 5.16  | 128.03      | 120.71   |
| 14  | 9     | 609 | TYR  | O-C-N       | -5.15 | 116.76      | 122.07   |
| 5   | 12    | 104 | ILE  | CA-C-N      | 5.15  | 127.44      | 120.44   |
| 5   | 12    | 104 | ILE  | C-N-CA      | 5.15  | 127.44      | 120.44   |
| 14  | 9     | 18  | HIS  | ND1-CE1-NE2 | 5.15  | 113.55      | 108.40   |
| 14  | 9     | 310 | ARG  | N-CA-C      | -5.14 | 100.31      | 109.06   |
| 3   | 10    | 438 | ALA  | O-C-N       | 5.14  | 127.37      | 122.07   |
| 3   | 10    | 112 | LYS  | N-CA-C      | 5.14  | 118.65      | 112.38   |
| 14  | 9     | 509 | LEU  | CA-C-N      | 5.14  | 126.86      | 122.29   |
| 14  | 9     | 509 | LEU  | C-N-CA      | 5.14  | 126.86      | 122.29   |
| 14  | 9     | 645 | ASN  | CA-CB-CG    | 5.14  | 117.74      | 112.60   |
| 14  | 9     | 780 | GLU  | N-CA-C      | -5.14 | 106.79      | 113.16   |
| 14  | 9     | 584 | GLU  | CA-C-O      | 5.13  | 126.17      | 120.63   |
| 3   | 10    | 307 | GLN  | OE1-CD-NE2  | 5.13  | 127.73      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | 12    | 46  | SER  | CA-C-O     | -5.13 | 114.98      | 120.42   |
| 14  | 9     | 298 | VAL  | CA-C-O     | -5.13 | 114.53      | 119.92   |
| 14  | 9     | 503 | MET  | N-CA-C     | -5.13 | 107.05      | 113.72   |
| 14  | 9     | 44  | GLU  | CA-C-N     | 5.12  | 127.15      | 120.28   |
| 14  | 9     | 44  | GLU  | C-N-CA     | 5.12  | 127.15      | 120.28   |
| 14  | 9     | 190 | ASN  | CA-C-N     | 5.12  | 130.70      | 122.14   |
| 14  | 9     | 190 | ASN  | C-N-CA     | 5.12  | 130.70      | 122.14   |
| 14  | 9     | 515 | GLU  | CA-C-N     | 5.12  | 130.63      | 122.94   |
| 14  | 9     | 515 | GLU  | C-N-CA     | 5.12  | 130.63      | 122.94   |
| 3   | 10    | 68  | PHE  | N-CA-CB    | 5.12  | 117.74      | 110.16   |
| 4   | 11    | 60  | ILE  | CA-C-O     | -5.12 | 115.62      | 120.95   |
| 14  | 9     | 424 | LYS  | N-CA-C     | 5.12  | 117.25      | 111.11   |
| 14  | 9     | 590 | THR  | CA-C-N     | 5.12  | 127.56      | 120.29   |
| 14  | 9     | 590 | THR  | C-N-CA     | 5.12  | 127.56      | 120.29   |
| 14  | 9     | 489 | GLY  | O-C-N      | -5.12 | 117.39      | 122.41   |
| 3   | 10    | 380 | ARG  | CA-C-N     | 5.11  | 127.47      | 120.46   |
| 3   | 10    | 380 | ARG  | C-N-CA     | 5.11  | 127.47      | 120.46   |
| 14  | 9     | 376 | PHE  | CA-C-N     | 5.11  | 131.31      | 121.54   |
| 14  | 9     | 376 | PHE  | C-N-CA     | 5.11  | 131.31      | 121.54   |
| 14  | 9     | 392 | PRO  | N-CA-CB    | 5.11  | 107.86      | 103.36   |
| 3   | 10    | 409 | LEU  | O-C-N      | -5.11 | 116.19      | 121.60   |
| 14  | 9     | 357 | THR  | CA-CB-OG1  | -5.11 | 101.94      | 109.60   |
| 14  | 9     | 427 | HIS  | N-CA-CB    | 5.11  | 117.63      | 110.12   |
| 14  | 9     | 128 | VAL  | O-C-N      | -5.10 | 116.23      | 122.97   |
| 14  | 9     | 756 | LEU  | N-CA-C     | 5.10  | 116.53      | 111.07   |
| 3   | 10    | 58  | THR  | CA-CB-OG1  | 5.10  | 117.25      | 109.60   |
| 3   | 10    | 227 | ILE  | O-C-N      | -5.10 | 116.85      | 122.05   |
| 14  | 9     | 356 | ILE  | N-CA-CB    | 5.10  | 119.72      | 111.36   |
| 14  | 9     | 109 | THR  | CA-CB-OG1  | 5.09  | 117.23      | 109.60   |
| 14  | 9     | 578 | ARG  | CA-C-O     | -5.09 | 113.00      | 119.31   |
| 3   | 10    | 476 | LEU  | CA-C-N     | 5.09  | 130.86      | 121.70   |
| 3   | 10    | 476 | LEU  | C-N-CA     | 5.09  | 130.86      | 121.70   |
| 3   | 10    | 385 | ILE  | CA-CB-CG1  | -5.08 | 101.76      | 110.40   |
| 3   | 10    | 88  | GLY  | O-C-N      | 5.08  | 128.26      | 122.67   |
| 14  | 9     | 623 | ASP  | CA-C-O     | 5.08  | 125.84      | 120.10   |
| 5   | 12    | 30  | GLN  | CA-C-O     | 5.08  | 125.93      | 120.55   |
| 14  | 9     | 768 | VAL  | CB-CA-C    | 5.07  | 118.47      | 111.97   |
| 3   | 10    | 303 | VAL  | N-CA-C     | -5.07 | 105.45      | 110.62   |
| 6   | 17    | 296 | GLN  | OE1-CD-NE2 | -5.07 | 117.53      | 122.60   |
| 14  | 9     | 703 | PRO  | CA-C-N     | 5.07  | 127.41      | 120.46   |
| 14  | 9     | 703 | PRO  | C-N-CA     | 5.07  | 127.41      | 120.46   |
| 66  | 15    | 599 | GLN  | N-CA-C     | 5.07  | 117.25      | 110.35   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 14  | 9     | 33  | TYR  | CB-CG-CD2 | -5.06 | 113.20      | 120.80   |
| 14  | 9     | 132 | ASN  | CB-CG-OD1 | -5.06 | 110.68      | 120.80   |
| 14  | 9     | 734 | GLY  | O-C-N     | 5.06  | 127.60      | 122.24   |
| 14  | 9     | 764 | ILE  | CA-C-O    | -5.06 | 115.81      | 121.17   |
| 14  | 9     | 455 | ILE  | CB-CA-C   | 5.06  | 115.04      | 110.13   |
| 14  | 9     | 191 | MET  | CG-SD-CE  | -5.06 | 89.78       | 100.90   |
| 14  | 9     | 163 | PRO  | N-CA-CB   | 5.05  | 109.01      | 103.26   |
| 14  | 9     | 84  | TYR  | CA-C-O    | -5.04 | 115.31      | 121.36   |
| 14  | 9     | 146 | ILE  | CA-C-N    | 5.04  | 129.26      | 120.68   |
| 14  | 9     | 146 | ILE  | C-N-CA    | 5.04  | 129.26      | 120.68   |
| 14  | 9     | 616 | LEU  | O-C-N     | 5.04  | 127.90      | 122.15   |
| 3   | 10    | 337 | VAL  | CA-C-N    | 5.04  | 126.91      | 120.56   |
| 3   | 10    | 337 | VAL  | C-N-CA    | 5.04  | 126.91      | 120.56   |
| 14  | 9     | 693 | ILE  | CA-C-N    | 5.04  | 127.03      | 120.28   |
| 14  | 9     | 693 | ILE  | C-N-CA    | 5.04  | 127.03      | 120.28   |
| 14  | 9     | 360 | SER  | CA-C-O    | 5.04  | 125.76      | 120.42   |
| 14  | 9     | 157 | ASN  | CA-C-N    | 5.03  | 131.37      | 122.67   |
| 14  | 9     | 157 | ASN  | C-N-CA    | 5.03  | 131.37      | 122.67   |
| 6   | 17    | 949 | HIS  | N-CA-C    | 5.03  | 121.51      | 110.80   |
| 14  | 9     | 729 | PHE  | CA-C-N    | 5.03  | 126.98      | 120.44   |
| 14  | 9     | 729 | PHE  | C-N-CA    | 5.03  | 126.98      | 120.44   |
| 14  | 9     | 81  | GLU  | CA-C-N    | 5.03  | 127.85      | 120.71   |
| 14  | 9     | 81  | GLU  | C-N-CA    | 5.03  | 127.85      | 120.71   |
| 14  | 9     | 494 | ILE  | N-CA-C    | -5.03 | 98.80       | 107.24   |
| 3   | 10    | 40  | VAL  | N-CA-CB   | 5.02  | 117.37      | 110.54   |
| 5   | 12    | 25  | HIS  | O-C-N     | -5.02 | 116.09      | 122.27   |
| 6   | 17    | 949 | HIS  | CA-C-N    | 5.02  | 131.13      | 121.54   |
| 6   | 17    | 949 | HIS  | C-N-CA    | 5.02  | 131.13      | 121.54   |
| 3   | 10    | 243 | ALA  | CA-C-N    | 5.02  | 126.96      | 120.44   |
| 3   | 10    | 243 | ALA  | C-N-CA    | 5.02  | 126.96      | 120.44   |
| 14  | 9     | 280 | PHE  | CA-C-N    | 5.01  | 128.32      | 120.75   |
| 14  | 9     | 280 | PHE  | C-N-CA    | 5.01  | 128.32      | 120.75   |
| 67  | 16    | 242 | ALA  | N-CA-C    | -5.01 | 100.13      | 110.80   |
| 5   | 12    | 121 | VAL  | N-CA-C    | -5.01 | 105.70      | 113.16   |
| 5   | 12    | 50  | ASP  | CA-CB-CG  | -5.00 | 107.59      | 112.60   |
| 14  | 9     | 775 | LEU  | N-CA-CB   | 5.00  | 117.90      | 110.29   |
| 4   | 11    | 61  | LEU  | CA-C-O    | -5.00 | 115.25      | 120.55   |
| 14  | 9     | 271 | GLU  | CA-C-O    | -5.00 | 115.55      | 120.90   |
| 14  | 9     | 741 | GLU  | CA-C-N    | 5.00  | 131.10      | 121.54   |
| 14  | 9     | 741 | GLU  | C-N-CA    | 5.00  | 131.10      | 121.54   |
| 14  | 9     | 782 | ASP  | CA-C-O    | -5.00 | 114.91      | 120.66   |

There are no chirality outliers.

All (61) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 3   | 10    | 129  | ARG  | Sidechain |
| 3   | 10    | 166  | PHE  | Sidechain |
| 3   | 10    | 217  | TYR  | Sidechain |
| 3   | 10    | 26   | ARG  | Sidechain |
| 3   | 10    | 279  | TYR  | Sidechain |
| 3   | 10    | 342  | PHE  | Sidechain |
| 3   | 10    | 344  | TYR  | Sidechain |
| 3   | 10    | 43   | ARG  | Sidechain |
| 3   | 10    | 448  | ARG  | Sidechain |
| 3   | 10    | 467  | ARG  | Sidechain |
| 5   | 12    | 69   | PHE  | Sidechain |
| 64  | 13    | 458  | LYS  | Peptide   |
| 64  | 13    | 987  | GLN  | Peptide   |
| 64  | 13    | 994  | LEU  | Peptide   |
| 64  | 13    | 997  | LYS  | Peptide   |
| 64  | 13    | 998  | GLN  | Peptide   |
| 64  | 13    | 999  | GLN  | Peptide   |
| 65  | 14    | 369  | ASP  | Peptide   |
| 66  | 15    | 1225 | SER  | Peptide   |
| 66  | 15    | 1226 | SER  | Peptide   |
| 66  | 15    | 275  | GLN  | Peptide   |
| 66  | 15    | 432  | ARG  | Sidechain |
| 66  | 15    | 449  | SER  | Peptide   |
| 66  | 15    | 453  | ASN  | Peptide   |
| 66  | 15    | 455  | GLY  | Peptide   |
| 66  | 15    | 457  | SER  | Peptide   |
| 66  | 15    | 458  | SER  | Peptide   |
| 66  | 15    | 460  | GLY  | Peptide   |
| 66  | 15    | 461  | ASN  | Peptide   |
| 66  | 15    | 467  | LEU  | Peptide   |
| 66  | 15    | 594  | ALA  | Peptide   |
| 66  | 15    | 597  | SER  | Peptide   |
| 66  | 15    | 598  | VAL  | Peptide   |
| 66  | 15    | 599  | GLN  | Peptide   |
| 67  | 16    | 244  | LYS  | Peptide   |
| 6   | 17    | 362  | TYR  | Sidechain |
| 6   | 17    | 399  | ARG  | Peptide   |
| 6   | 17    | 419  | ARG  | Sidechain |
| 6   | 17    | 450  | HIS  | Peptide   |
| 6   | 17    | 702  | GLU  | Peptide   |
| 6   | 17    | 703  | ASN  | Peptide   |
| 6   | 17    | 706  | ILE  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 6   | 17    | 948 | ARG  | Peptide   |
| 6   | 17    | 949 | HIS  | Peptide   |
| 6   | 17    | 950 | LYS  | Peptide   |
| 14  | 9     | 13  | ARG  | Sidechain |
| 14  | 9     | 201 | ARG  | Sidechain |
| 14  | 9     | 220 | ARG  | Sidechain |
| 14  | 9     | 280 | PHE  | Sidechain |
| 14  | 9     | 330 | TYR  | Sidechain |
| 14  | 9     | 386 | TYR  | Sidechain |
| 14  | 9     | 449 | TYR  | Sidechain |
| 14  | 9     | 507 | TYR  | Sidechain |
| 14  | 9     | 526 | ARG  | Sidechain |
| 14  | 9     | 529 | ARG  | Sidechain |
| 14  | 9     | 557 | ARG  | Sidechain |
| 14  | 9     | 710 | ARG  | Sidechain |
| 14  | 9     | 738 | ARG  | Sidechain |
| 14  | 9     | 798 | ARG  | Sidechain |
| 14  | 9     | 85  | ARG  | Sidechain |
| 14  | 9     | 92  | TYR  | 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   | 0     | 380   | 0        | 429      | 7       | 0            |
| 2   | 1     | 477   | 0        | 530      | 11      | 0            |
| 3   | 10    | 3487  | 0        | 3650     | 95      | 0            |
| 4   | 11    | 585   | 0        | 646      | 0       | 0            |
| 5   | 12    | 848   | 0        | 924      | 113     | 0            |
| 6   | 17    | 7613  | 0        | 7589     | 1236    | 0            |
| 7   | 2     | 304   | 0        | 348      | 4       | 0            |
| 8   | 3     | 61992 | 0        | 31109    | 993     | 0            |
| 9   | 4     | 2305  | 0        | 1164     | 35      | 0            |
| 10  | 5     | 32256 | 0        | 16213    | 423     | 0            |
| 11  | 6     | 42    | 0        | 23       | 0       | 0            |
| 12  | 7     | 1638  | 0        | 841      | 57      | 0            |
| 13  | 8     | 1635  | 0        | 833      | 61      | 0            |
| 14  | 9     | 6467  | 0        | 6514     | 897     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15  | A     | 2138  | 0        | 2204     | 78      | 0            |
| 16  | AA    | 1191  | 0        | 1284     | 37      | 0            |
| 17  | AB    | 440   | 0        | 220      | 111     | 0            |
| 18  | AC    | 342   | 0        | 354      | 12      | 0            |
| 18  | x     | 366   | 0        | 356      | 18      | 0            |
| 19  | C     | 1669  | 0        | 1729     | 65      | 0            |
| 20  | E     | 1509  | 0        | 1520     | 52      | 0            |
| 21  | F     | 1254  | 0        | 1320     | 32      | 0            |
| 22  | G     | 1110  | 0        | 1226     | 32      | 0            |
| 23  | H     | 1041  | 0        | 1101     | 48      | 0            |
| 24  | I     | 832   | 0        | 918      | 29      | 0            |
| 25  | J     | 829   | 0        | 855      | 18      | 0            |
| 26  | K     | 1071  | 0        | 1165     | 53      | 0            |
| 27  | L     | 975   | 0        | 1041     | 52      | 0            |
| 28  | M     | 474   | 0        | 505      | 11      | 0            |
| 29  | N     | 689   | 0        | 746      | 11      | 0            |
| 30  | O     | 705   | 0        | 755      | 29      | 0            |
| 31  | P     | 693   | 0        | 753      | 16      | 0            |
| 32  | Q     | 590   | 0        | 625      | 30      | 0            |
| 33  | R     | 700   | 0        | 708      | 23      | 0            |
| 34  | S     | 643   | 0        | 694      | 18      | 0            |
| 35  | T     | 519   | 0        | 578      | 13      | 0            |
| 36  | W     | 1764  | 0        | 1833     | 55      | 0            |
| 37  | Y     | 126   | 0        | 56       | 146     | 0            |
| 38  | Z     | 187   | 0        | 65       | 14      | 0            |
| 39  | a     | 2225  | 0        | 2301     | 58      | 0            |
| 40  | b     | 1778  | 0        | 1821     | 51      | 0            |
| 41  | c     | 1654  | 0        | 1744     | 55      | 0            |
| 42  | d     | 1416  | 0        | 1500     | 92      | 0            |
| 43  | e     | 1396  | 0        | 1481     | 38      | 0            |
| 44  | f     | 1208  | 0        | 1254     | 56      | 0            |
| 45  | g     | 951   | 0        | 1001     | 41      | 0            |
| 46  | h     | 959   | 0        | 1039     | 56      | 0            |
| 47  | i     | 1164  | 0        | 1192     | 29      | 0            |
| 48  | j     | 944   | 0        | 1019     | 25      | 0            |
| 49  | k     | 1170  | 0        | 1274     | 34      | 0            |
| 50  | l     | 1079  | 0        | 1134     | 34      | 0            |
| 51  | m     | 958   | 0        | 1011     | 20      | 0            |
| 52  | n     | 918   | 0        | 979      | 28      | 0            |
| 53  | o     | 966   | 0        | 1041     | 38      | 0            |
| 54  | p     | 981   | 0        | 1062     | 47      | 0            |
| 55  | q     | 811   | 0        | 858      | 19      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56  | r     | 1091   | 0        | 1178     | 27      | 0            |
| 57  | s     | 740    | 0        | 819      | 41      | 0            |
| 58  | t     | 871    | 0        | 964      | 103     | 0            |
| 59  | u     | 670    | 0        | 704      | 15      | 0            |
| 60  | v     | 520    | 0        | 565      | 16      | 0            |
| 61  | w     | 906    | 0        | 976      | 164     | 0            |
| 62  | y     | 452    | 0        | 467      | 27      | 0            |
| 63  | z     | 408    | 0        | 436      | 12      | 0            |
| 64  | 13    | 9604   | 0        | 9522     | 377     | 0            |
| 65  | 14    | 10101  | 0        | 9885     | 511     | 0            |
| 66  | 15    | 9894   | 0        | 9743     | 814     | 0            |
| 67  | 16    | 2141   | 0        | 2059     | 113     | 0            |
| 67  | 18    | 2141   | 0        | 2060     | 182     | 0            |
| 68  | 2     | 1      | 0        | 0        | 0       | 0            |
| 68  | M     | 1      | 0        | 0        | 0       | 0            |
| 68  | Q     | 1      | 0        | 0        | 0       | 0            |
| 68  | x     | 2      | 0        | 0        | 0       | 0            |
| 68  | y     | 1      | 0        | 0        | 0       | 0            |
| 68  | z     | 1      | 0        | 0        | 0       | 0            |
| 69  | 3     | 213    | 0        | 0        | 0       | 0            |
| 69  | 4     | 1      | 0        | 0        | 0       | 0            |
| 69  | 5     | 88     | 0        | 0        | 0       | 0            |
| 69  | 6     | 1      | 0        | 0        | 0       | 0            |
| 69  | 7     | 3      | 0        | 0        | 0       | 0            |
| 69  | 8     | 1      | 0        | 0        | 0       | 0            |
| 69  | AB    | 2      | 0        | 0        | 0       | 0            |
| 69  | K     | 1      | 0        | 0        | 0       | 0            |
| 69  | P     | 1      | 0        | 0        | 0       | 0            |
| 69  | Y     | 1      | 0        | 0        | 0       | 0            |
| 69  | b     | 2      | 0        | 0        | 0       | 0            |
| 69  | i     | 1      | 0        | 0        | 0       | 0            |
| 69  | y     | 2      | 0        | 0        | 0       | 0            |
| 70  | 3     | 36     | 0        | 72       | 2       | 0            |
| 70  | 5     | 30     | 0        | 60       | 0       | 0            |
| 70  | b     | 6      | 0        | 12       | 0       | 0            |
| 71  | 3     | 1      | 0        | 0        | 0       | 0            |
| 72  | 3     | 16     | 0        | 0        | 0       | 0            |
| 72  | 5     | 1      | 0        | 0        | 0       | 0            |
| 72  | A     | 1      | 0        | 0        | 0       | 0            |
| 72  | i     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 202419 | 0        | 154657   | 5578    | 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 16.

All (5578) 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) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:10:253:PHE:CE2    | 6:17:15:ILE:HD13    | 1.28                     | 1.65              |
| 64:13:1192:LEU:CD2  | 67:18:88:GLN:HG2    | 1.19                     | 1.63              |
| 14:9:795:GLN:CG     | 61:w:18:LEU:HD21    | 1.18                     | 1.62              |
| 14:9:165:LEU:CD2    | 58:t:62:LYS:CE      | 1.75                     | 1.62              |
| 14:9:165:LEU:HD23   | 58:t:62:LYS:CE      | 1.28                     | 1.61              |
| 14:9:165:LEU:CB     | 58:t:62:LYS:HE3     | 1.31                     | 1.59              |
| 3:10:253:PHE:CD2    | 6:17:15:ILE:HD13    | 1.36                     | 1.58              |
| 64:13:1020:MET:CB   | 67:18:256:HIS:HA    | 1.14                     | 1.58              |
| 6:17:275:ASN:CB     | 65:14:1125:THR:HB   | 1.13                     | 1.58              |
| 6:17:390:ALA:HB3    | 66:15:71:ARG:CZ     | 1.13                     | 1.58              |
| 6:17:426:LYS:CB     | 66:15:184:GLN:HB2   | 1.12                     | 1.58              |
| 14:9:808:GLN:HA     | 61:w:79:THR:CG2     | 1.20                     | 1.57              |
| 6:17:711:PHE:CZ     | 14:9:642:ASN:HB2    | 1.35                     | 1.57              |
| 65:14:610:ILE:CG1   | 66:15:248:THR:HG21  | 1.35                     | 1.57              |
| 14:9:798:ARG:CZ     | 61:w:18:LEU:CA      | 1.75                     | 1.56              |
| 65:14:610:ILE:CB    | 66:15:248:THR:HG21  | 1.11                     | 1.56              |
| 3:10:253:PHE:CE2    | 6:17:15:ILE:HG21    | 1.09                     | 1.56              |
| 6:17:388:ALA:CA     | 66:15:132:LEU:HD22  | 1.24                     | 1.56              |
| 6:17:362:TYR:CZ     | 65:14:1098:THR:HG22 | 1.39                     | 1.55              |
| 64:13:1192:LEU:HD21 | 67:18:88:GLN:CD     | 1.32                     | 1.55              |
| 6:17:388:ALA:HB1    | 66:15:132:LEU:CB    | 1.31                     | 1.55              |
| 6:17:955:LYS:HZ3    | 14:9:799:GLU:CA     | 1.18                     | 1.55              |
| 65:14:610:ILE:HB    | 66:15:248:THR:CG2   | 1.14                     | 1.54              |
| 6:17:388:ALA:HB3    | 66:15:132:LEU:CD1   | 1.34                     | 1.54              |
| 6:17:376:LYS:NZ     | 66:15:178:GLU:CG    | 1.68                     | 1.54              |
| 26:K:57:LYS:HD2     | 37:Y:45:A:C5'       | 1.15                     | 1.54              |
| 6:17:704:ASN:CA     | 14:9:665:HIS:CG     | 1.79                     | 1.53              |
| 14:9:165:LEU:CG     | 58:t:62:LYS:CE      | 1.77                     | 1.53              |
| 14:9:165:LEU:CG     | 58:t:62:LYS:HE2     | 1.29                     | 1.53              |
| 64:13:1192:LEU:CD2  | 67:18:88:GLN:CG     | 1.77                     | 1.53              |
| 6:17:272:ASP:HB3    | 65:14:1127:THR:CG2  | 1.31                     | 1.52              |
| 14:9:188:ARG:NE     | 58:t:59:SER:HB3     | 1.23                     | 1.52              |
| 14:9:275:LYS:HD2    | 57:s:22:GLY:CA      | 1.40                     | 1.52              |
| 6:17:388:ALA:CB     | 66:15:132:LEU:HD22  | 1.37                     | 1.52              |
| 6:17:388:ALA:C      | 66:15:132:LEU:HD22  | 1.31                     | 1.51              |
| 6:17:695:SER:C      | 14:9:633:VAL:CG2    | 1.83                     | 1.50              |
| 5:12:97:LEU:HD11    | 6:17:667:TRP:CE3    | 1.45                     | 1.50              |
| 14:9:376:PHE:CE2    | 14:9:376:PHE:CZ     | 1.98                     | 1.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 64:13:1018:SER:CB  | 67:18:258:VAL:HG13  | 1.34                     | 1.50              |
| 3:10:253:PHE:CE2   | 6:17:15:ILE:CG2     | 1.91                     | 1.50              |
| 6:17:376:LYS:HE2   | 66:15:178:GLU:CD    | 1.24                     | 1.50              |
| 64:13:984:GLN:NE2  | 64:13:1133:THR:CG2  | 1.70                     | 1.50              |
| 8:3:1558:A:H2      | 14:9:247:LYS:NZ     | 1.06                     | 1.50              |
| 6:17:280:ASN:CB    | 66:15:139:ALA:CB    | 1.83                     | 1.49              |
| 6:17:426:LYS:HB2   | 66:15:184:GLN:CB    | 1.07                     | 1.49              |
| 6:17:955:LYS:CE    | 14:9:799:GLU:CB     | 1.87                     | 1.48              |
| 64:13:1020:MET:HB3 | 67:18:256:HIS:CA    | 1.40                     | 1.48              |
| 6:17:845:TRP:CZ2   | 14:9:644:LYS:HG3    | 1.46                     | 1.48              |
| 3:10:275:SER:CB    | 6:17:970:SER:CB     | 1.88                     | 1.48              |
| 6:17:258:ASN:CG    | 65:14:1126:LEU:HD13 | 1.33                     | 1.48              |
| 6:17:388:ALA:HB1   | 66:15:132:LEU:CG    | 1.42                     | 1.48              |
| 17:AB:41:U:H2'     | 37:Y:42:C:C6        | 1.49                     | 1.48              |
| 6:17:259:GLY:C     | 65:14:1098:THR:HA   | 1.09                     | 1.48              |
| 6:17:704:ASN:CA    | 14:9:665:HIS:CD2    | 1.97                     | 1.48              |
| 64:13:10:GLN:HG2   | 67:18:197:ASN:ND2   | 1.17                     | 1.48              |
| 14:9:376:PHE:CZ    | 14:9:376:PHE:CE1    | 2.01                     | 1.47              |
| 14:9:376:PHE:CD1   | 14:9:376:PHE:CG     | 2.02                     | 1.47              |
| 14:9:376:PHE:CD1   | 14:9:376:PHE:CE1    | 2.02                     | 1.47              |
| 65:14:610:ILE:HB   | 66:15:248:THR:CB    | 1.39                     | 1.47              |
| 3:10:275:SER:CB    | 6:17:970:SER:HB2    | 0.99                     | 1.47              |
| 3:10:238:PHE:CE2   | 6:17:559:PHE:HD1    | 1.27                     | 1.47              |
| 6:17:376:LYS:CE    | 66:15:178:GLU:CD    | 1.88                     | 1.47              |
| 14:9:795:GLN:HG2   | 61:w:18:LEU:CD2     | 1.04                     | 1.46              |
| 6:17:388:ALA:C     | 66:15:132:LEU:CD2   | 1.84                     | 1.46              |
| 5:12:92:ILE:CG2    | 6:17:660:GLY:CA     | 1.90                     | 1.46              |
| 14:9:165:LEU:CD2   | 58:t:62:LYS:HE2     | 1.32                     | 1.46              |
| 26:K:57:LYS:CD     | 37:Y:45:A:H5'       | 0.99                     | 1.46              |
| 8:3:1560:U:H5''    | 14:9:249:ASP:N      | 1.24                     | 1.45              |
| 14:9:376:PHE:CG    | 14:9:376:PHE:CD2    | 2.04                     | 1.45              |
| 6:17:701:THR:CA    | 14:9:662:LEU:HA     | 1.41                     | 1.45              |
| 6:17:388:ALA:CB    | 66:15:132:LEU:CD2   | 1.92                     | 1.45              |
| 6:17:704:ASN:HA    | 14:9:665:HIS:CD2    | 1.52                     | 1.44              |
| 65:14:1209:LYS:HE3 | 66:15:250:PHE:CZ    | 1.49                     | 1.44              |
| 3:10:238:PHE:HE2   | 6:17:559:PHE:CD1    | 1.35                     | 1.44              |
| 6:17:388:ALA:CB    | 66:15:132:LEU:CG    | 1.93                     | 1.44              |
| 14:9:798:ARG:NH2   | 61:w:18:LEU:HA      | 1.29                     | 1.44              |
| 6:17:845:TRP:CZ2   | 14:9:644:LYS:CG     | 1.97                     | 1.44              |
| 5:12:92:ILE:CG2    | 6:17:660:GLY:HA2    | 1.41                     | 1.44              |
| 6:17:701:THR:C     | 14:9:662:LEU:HA     | 1.39                     | 1.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:13:1217:LYS:NZ   | 67:18:274:PRO:HG2   | 1.18                     | 1.43              |
| 3:10:275:SER:HB3    | 6:17:970:SER:CB     | 1.48                     | 1.43              |
| 10:5:1473:U:P       | 37:Y:40:U:H4'       | 1.57                     | 1.43              |
| 10:5:1473:U:C4      | 37:Y:41:U:H5'       | 1.51                     | 1.43              |
| 26:K:57:LYS:CG      | 37:Y:45:A:H5''      | 1.48                     | 1.42              |
| 64:13:984:GLN:CG    | 64:13:1133:THR:H    | 1.15                     | 1.42              |
| 6:17:426:LYS:HZ2    | 66:15:183:LEU:CB    | 1.31                     | 1.42              |
| 6:17:704:ASN:HA     | 14:9:665:HIS:CG     | 0.91                     | 1.42              |
| 14:9:165:LEU:CA     | 58:t:62:LYS:HE3     | 1.28                     | 1.42              |
| 14:9:376:PHE:CE2    | 14:9:376:PHE:CD2    | 2.07                     | 1.41              |
| 5:12:97:LEU:HD13    | 6:17:667:TRP:CZ3    | 1.55                     | 1.41              |
| 6:17:693:THR:CB     | 14:9:682:VAL:HG22   | 1.17                     | 1.41              |
| 5:12:88:SER:HB2     | 6:17:615:PHE:CE2    | 1.53                     | 1.41              |
| 6:17:261:LYS:HB2    | 65:14:1126:LEU:CD1  | 1.50                     | 1.41              |
| 6:17:955:LYS:NZ     | 14:9:799:GLU:CA     | 1.75                     | 1.41              |
| 3:10:238:PHE:CE2    | 6:17:559:PHE:CD1    | 2.04                     | 1.41              |
| 6:17:706:ILE:HG13   | 14:9:659:ASN:CG     | 1.44                     | 1.41              |
| 6:17:258:ASN:CG     | 65:14:1126:LEU:CD1  | 1.92                     | 1.41              |
| 6:17:387:VAL:HA     | 66:15:68:ILE:CD1    | 1.51                     | 1.41              |
| 6:17:261:LYS:CB     | 65:14:1126:LEU:HD11 | 1.51                     | 1.40              |
| 6:17:711:PHE:HE1    | 14:9:642:ASN:CG     | 1.27                     | 1.40              |
| 6:17:711:PHE:CD2    | 14:9:650:ASN:HA     | 1.54                     | 1.40              |
| 6:17:385:ASP:N      | 66:15:64:LYS:HB2    | 1.17                     | 1.40              |
| 6:17:362:TYR:OH     | 65:14:1098:THR:CG2  | 1.70                     | 1.40              |
| 6:17:706:ILE:CD1    | 14:9:658:LEU:HB2    | 1.50                     | 1.40              |
| 3:10:253:PHE:CE2    | 6:17:15:ILE:CD1     | 2.03                     | 1.40              |
| 6:17:262:SER:N      | 65:14:1098:THR:H    | 1.15                     | 1.39              |
| 64:13:1213:LEU:CB   | 67:18:276:ASN:HB3   | 1.51                     | 1.39              |
| 64:13:1020:MET:CB   | 67:18:256:HIS:CA    | 1.94                     | 1.39              |
| 6:17:691:THR:C      | 14:9:682:VAL:HG12   | 1.46                     | 1.38              |
| 6:17:711:PHE:CE2    | 14:9:650:ASN:CA     | 2.05                     | 1.38              |
| 6:17:258:ASN:CB     | 65:14:1126:LEU:HD13 | 1.52                     | 1.38              |
| 6:17:262:SER:H      | 65:14:1098:THR:N    | 1.22                     | 1.38              |
| 6:17:428:GLY:O      | 66:15:549:LEU:CD2   | 1.67                     | 1.38              |
| 6:17:711:PHE:CE1    | 14:9:642:ASN:CG     | 2.01                     | 1.38              |
| 6:17:711:PHE:CE2    | 14:9:650:ASN:HA     | 1.59                     | 1.38              |
| 5:12:97:LEU:CD2     | 6:17:664:ILE:HG23   | 1.54                     | 1.37              |
| 6:17:280:ASN:CB     | 66:15:139:ALA:HB1   | 1.33                     | 1.37              |
| 14:9:808:GLN:CA     | 61:w:79:THR:HG21    | 1.50                     | 1.37              |
| 64:13:1192:LEU:HD21 | 67:18:88:GLN:NE2    | 1.33                     | 1.37              |
| 6:17:955:LYS:NZ     | 14:9:799:GLU:CG     | 1.86                     | 1.37              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:5:528:G:C2       | 13:8:35:U:H1'       | 1.55                     | 1.37              |
| 5:12:97:LEU:CD1     | 6:17:667:TRP:CE3    | 2.08                     | 1.37              |
| 6:17:695:SER:C      | 14:9:633:VAL:HG21   | 0.95                     | 1.37              |
| 64:13:173:GLU:OE1   | 66:15:1178:SER:CB   | 1.72                     | 1.36              |
| 66:15:1105:VAL:HG23 | 67:16:255:ARG:CB    | 1.54                     | 1.36              |
| 6:17:272:ASP:CB     | 65:14:1127:THR:CG2  | 1.82                     | 1.36              |
| 6:17:698:SER:CB     | 14:9:769:ILE:HG21   | 1.53                     | 1.36              |
| 12:7:29:G:C5'       | 27:L:117:ALA:HA     | 1.52                     | 1.36              |
| 6:17:390:ALA:CB     | 66:15:71:ARG:CZ     | 1.74                     | 1.36              |
| 64:13:1192:LEU:HD21 | 67:18:88:GLN:CG     | 1.43                     | 1.36              |
| 8:3:519:A:C2        | 14:9:165:LEU:HD13   | 1.60                     | 1.35              |
| 6:17:388:ALA:CB     | 66:15:132:LEU:HB3   | 1.52                     | 1.35              |
| 6:17:598:LYS:CG     | 14:9:641:ARG:HH21   | 1.35                     | 1.35              |
| 6:17:429:ASP:OD2    | 66:15:184:GLN:HG2   | 1.23                     | 1.35              |
| 14:9:451:GLN:NE2    | 62:y:57:TYR:OXT     | 1.60                     | 1.34              |
| 14:9:798:ARG:CZ     | 61:w:18:LEU:HA      | 0.88                     | 1.34              |
| 66:15:1071:PHE:HD2  | 66:15:1247:ARG:CZ   | 1.40                     | 1.34              |
| 3:10:253:PHE:CZ     | 6:17:15:ILE:HG21    | 1.62                     | 1.34              |
| 3:10:275:SER:OG     | 6:17:970:SER:CB     | 1.73                     | 1.34              |
| 6:17:275:ASN:CB     | 65:14:1125:THR:CB   | 2.04                     | 1.34              |
| 6:17:705:ASP:N      | 14:9:665:HIS:ND1    | 1.70                     | 1.34              |
| 6:17:698:SER:HB2    | 14:9:769:ILE:CG2    | 1.58                     | 1.33              |
| 10:5:1473:U:C2'     | 37:Y:41:U:OP1       | 1.76                     | 1.33              |
| 6:17:261:LYS:N      | 65:14:1126:LEU:HD21 | 1.03                     | 1.33              |
| 6:17:386:VAL:CG1    | 66:15:177:GLY:N     | 1.78                     | 1.33              |
| 10:5:1468:A:O2'     | 37:Y:43:A:H1'       | 1.16                     | 1.33              |
| 67:18:15:GLN:OE1    | 67:18:90:GLN:HB2    | 1.25                     | 1.33              |
| 3:10:257:GLU:OE1    | 6:17:11:TRP:CZ3     | 1.72                     | 1.33              |
| 6:17:376:LYS:CE     | 66:15:178:GLU:CG    | 2.04                     | 1.33              |
| 5:12:100:LEU:CD2    | 6:17:668:LEU:HD11   | 1.59                     | 1.32              |
| 6:17:280:ASN:HB3    | 66:15:139:ALA:CB    | 1.43                     | 1.32              |
| 66:15:1154:GLU:HG2  | 67:16:71:GLN:C      | 1.53                     | 1.32              |
| 65:14:605:GLU:O     | 66:15:248:THR:HA    | 1.25                     | 1.32              |
| 14:9:165:LEU:HD23   | 58:t:62:LYS:NZ      | 1.01                     | 1.32              |
| 14:9:795:GLN:HE21   | 61:w:18:LEU:CG      | 1.41                     | 1.32              |
| 64:13:10:GLN:CG     | 67:18:197:ASN:ND2   | 1.89                     | 1.32              |
| 6:17:259:GLY:O      | 65:14:1098:THR:CA   | 1.76                     | 1.31              |
| 6:17:261:LYS:H      | 65:14:1126:LEU:CD2  | 1.41                     | 1.31              |
| 5:12:87:THR:HA      | 6:17:14:LYS:CB      | 1.61                     | 1.31              |
| 6:17:261:LYS:N      | 65:14:1126:LEU:CD2  | 1.91                     | 1.31              |
| 66:15:1071:PHE:CD2  | 66:15:1247:ARG:CZ   | 2.14                     | 1.31              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:17:955:LYS:CE   | 14:9:799:GLU:HB2   | 1.48                     | 1.30              |
| 6:17:706:ILE:CG1  | 14:9:659:ASN:OD1   | 1.78                     | 1.30              |
| 8:3:102:A:OP2     | 14:9:779:GLU:CG    | 1.79                     | 1.30              |
| 10:5:528:G:N3     | 13:8:35:U:H1'      | 1.45                     | 1.30              |
| 10:5:1473:U:C4    | 37:Y:41:U:C5'      | 2.14                     | 1.30              |
| 14:9:795:GLN:NE2  | 61:w:18:LEU:HG     | 1.43                     | 1.30              |
| 6:17:591:GLU:OE2  | 14:9:646:GLN:NE2   | 1.63                     | 1.30              |
| 6:17:701:THR:C    | 14:9:662:LEU:CA    | 2.04                     | 1.30              |
| 6:17:386:VAL:CA   | 66:15:174:ASP:OD1  | 1.77                     | 1.30              |
| 6:17:699:ILE:CG2  | 14:9:689:ILE:HA    | 1.34                     | 1.30              |
| 8:3:1560:U:C5'    | 14:9:249:ASP:N     | 1.94                     | 1.29              |
| 14:9:795:GLN:HG2  | 61:w:18:LEU:CG     | 1.61                     | 1.29              |
| 14:9:801:HIS:NE2  | 61:w:24:GLY:O      | 1.62                     | 1.29              |
| 5:12:86:VAL:O     | 6:17:15:ILE:HG13   | 1.25                     | 1.29              |
| 5:12:88:SER:OG    | 6:17:18:ILE:CG1    | 1.66                     | 1.29              |
| 6:17:277:SER:HB2  | 65:14:1124:LYS:CA  | 1.61                     | 1.29              |
| 6:17:711:PHE:CZ   | 14:9:642:ASN:CB    | 2.16                     | 1.29              |
| 64:13:972:ASN:CG  | 67:18:256:HIS:NE2  | 1.91                     | 1.28              |
| 67:16:15:GLN:OE1  | 67:16:90:GLN:HB2   | 1.29                     | 1.28              |
| 6:17:426:LYS:NZ   | 66:15:183:LEU:HB3  | 1.46                     | 1.28              |
| 6:17:706:ILE:HG13 | 14:9:659:ASN:OD1   | 1.33                     | 1.28              |
| 66:15:1104:SER:OG | 67:16:256:HIS:HA   | 1.29                     | 1.28              |
| 6:17:706:ILE:CD1  | 14:9:658:LEU:CB    | 2.10                     | 1.28              |
| 6:17:955:LYS:HZ1  | 14:9:799:GLU:CG    | 1.40                     | 1.28              |
| 8:3:520:C:OP1     | 14:9:160:ASN:HB3   | 1.20                     | 1.28              |
| 39:a:132:PRO:CD   | 39:a:132:PRO:N     | 1.81                     | 1.27              |
| 66:15:1105:VAL:O  | 67:16:254:LYS:O    | 1.52                     | 1.27              |
| 6:17:277:SER:CB   | 65:14:1124:LYS:C   | 2.06                     | 1.27              |
| 64:13:924:LYS:NZ  | 67:18:79:ALA:HB1   | 1.45                     | 1.27              |
| 6:17:376:LYS:NZ   | 66:15:178:GLU:HG3  | 0.95                     | 1.27              |
| 64:13:147:THR:O   | 66:15:1169:ASP:HB3 | 1.23                     | 1.27              |
| 6:17:429:ASP:OD2  | 66:15:184:GLN:CG   | 1.83                     | 1.27              |
| 10:5:1473:U:C5    | 37:Y:41:U:O5'      | 1.86                     | 1.27              |
| 8:3:1561:G:C4'    | 14:9:299:LYS:HD2   | 1.65                     | 1.26              |
| 13:8:35:U:N3      | 17:AB:44:A:C2      | 2.02                     | 1.26              |
| 6:17:259:GLY:C    | 65:14:1098:THR:CA  | 2.05                     | 1.26              |
| 6:17:362:TYR:CZ   | 65:14:1098:THR:CG2 | 2.15                     | 1.26              |
| 6:17:386:VAL:HA   | 66:15:174:ASP:OD1  | 1.17                     | 1.26              |
| 6:17:695:SER:CA   | 14:9:633:VAL:HG21  | 1.64                     | 1.26              |
| 6:17:706:ILE:HD12 | 14:9:658:LEU:CB    | 1.66                     | 1.26              |
| 6:17:426:LYS:NZ   | 66:15:183:LEU:CB   | 1.97                     | 1.26              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:9:798:ARG:CD    | 61:w:18:LEU:O     | 1.82                     | 1.26              |
| 6:17:428:GLY:H     | 66:15:141:VAL:CG2 | 1.49                     | 1.26              |
| 6:17:704:ASN:N     | 14:9:665:HIS:CD2  | 2.01                     | 1.26              |
| 14:9:798:ARG:HD2   | 61:w:18:LEU:O     | 1.12                     | 1.26              |
| 6:17:874:ARG:HH12  | 14:9:647:ASN:ND2  | 1.32                     | 1.25              |
| 6:17:264:GLU:HB2   | 65:14:1096:ILE:O  | 1.19                     | 1.25              |
| 42:d:38:MET:HE3    | 42:d:151:GLY:O    | 1.25                     | 1.25              |
| 6:17:384:ALA:C     | 66:15:64:LYS:CB   | 1.74                     | 1.25              |
| 6:17:711:PHE:HE2   | 14:9:650:ASN:CB   | 1.49                     | 1.25              |
| 14:9:798:ARG:HG3   | 61:w:21:LYS:C     | 1.53                     | 1.25              |
| 64:13:1217:LYS:HZ2 | 67:18:274:PRO:CG  | 1.49                     | 1.25              |
| 64:13:1213:LEU:HB3 | 67:18:276:ASN:CB  | 1.66                     | 1.25              |
| 5:12:92:ILE:HD11   | 6:17:655:TYR:CE1  | 1.70                     | 1.25              |
| 6:17:594:LEU:O     | 14:9:641:ARG:NH2  | 1.69                     | 1.25              |
| 14:9:275:LYS:CD    | 57:s:22:GLY:HA2   | 1.67                     | 1.25              |
| 8:3:102:A:OP2      | 14:9:779:GLU:HG2  | 1.29                     | 1.24              |
| 6:17:251:ASP:OD1   | 65:14:1104:ALA:C  | 1.79                     | 1.24              |
| 6:17:264:GLU:OE2   | 65:14:1130:LYS:CE | 1.84                     | 1.24              |
| 6:17:690:LEU:C     | 14:9:682:VAL:HG11 | 1.63                     | 1.24              |
| 6:17:845:TRP:CH2   | 14:9:644:LYS:HG3  | 1.70                     | 1.24              |
| 6:17:426:LYS:CD    | 66:15:184:GLN:H   | 1.50                     | 1.24              |
| 17:AB:44:A:C2'     | 37:Y:44:A:H2'     | 1.46                     | 1.24              |
| 66:15:1106:SER:O   | 67:16:254:LYS:HB2 | 1.32                     | 1.24              |
| 12:7:34:G:N1       | 17:AB:42:C:N3     | 1.86                     | 1.24              |
| 6:17:689:ALA:O     | 14:9:682:VAL:HB   | 1.11                     | 1.23              |
| 64:13:1217:LYS:NZ  | 67:18:274:PRO:CG  | 2.01                     | 1.23              |
| 6:17:692:LYS:N     | 14:9:682:VAL:HG12 | 1.29                     | 1.23              |
| 6:17:701:THR:OG1   | 14:9:773:ALA:HB1  | 1.36                     | 1.23              |
| 65:14:605:GLU:O    | 66:15:248:THR:CA  | 1.86                     | 1.23              |
| 6:17:386:VAL:HG13  | 66:15:174:ASP:CG  | 1.61                     | 1.23              |
| 26:K:57:LYS:CG     | 37:Y:45:A:C5'     | 2.08                     | 1.23              |
| 6:17:690:LEU:O     | 14:9:682:VAL:HG11 | 1.10                     | 1.23              |
| 8:3:1560:U:C5'     | 14:9:249:ASP:H    | 1.50                     | 1.23              |
| 8:3:1560:U:H5'     | 14:9:249:ASP:CG   | 1.61                     | 1.23              |
| 13:8:35:U:C4       | 17:AB:44:A:N1     | 2.06                     | 1.23              |
| 64:13:972:ASN:ND2  | 67:18:256:HIS:HE2 | 1.37                     | 1.23              |
| 14:9:798:ARG:HG3   | 61:w:22:LEU:N     | 1.51                     | 1.23              |
| 6:17:702:GLU:CG    | 14:9:663:ASN:ND2  | 1.86                     | 1.22              |
| 10:5:528:G:N3      | 13:8:35:U:C1'     | 2.00                     | 1.22              |
| 10:5:1467:A:H1'    | 37:Y:44:A:O2'     | 1.36                     | 1.22              |
| 65:14:1209:LYS:CE  | 66:15:250:PHE:CZ  | 2.19                     | 1.22              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:388:ALA:CB    | 66:15:132:LEU:HD13  | 1.67                     | 1.22              |
| 6:17:695:SER:O     | 14:9:633:VAL:HG21   | 1.34                     | 1.22              |
| 6:17:955:LYS:CE    | 14:9:799:GLU:HB3    | 1.54                     | 1.22              |
| 5:12:97:LEU:CD1    | 6:17:667:TRP:CZ3    | 2.21                     | 1.22              |
| 6:17:700:LEU:HD22  | 14:9:658:LEU:C      | 1.64                     | 1.22              |
| 10:5:528:G:C4      | 13:8:35:U:H1'       | 1.74                     | 1.22              |
| 14:9:188:ARG:NE    | 58:t:59:SER:CB      | 2.01                     | 1.22              |
| 64:13:984:GLN:NE2  | 64:13:1133:THR:HG23 | 0.91                     | 1.22              |
| 66:15:877:ARG:NH1  | 66:15:1270:ILE:HG22 | 1.54                     | 1.22              |
| 14:9:808:GLN:HB3   | 57:s:48:TYR:O       | 1.40                     | 1.22              |
| 17:AB:44:A:O2'     | 37:Y:44:A:C2'       | 1.86                     | 1.21              |
| 66:15:1105:VAL:O   | 67:16:254:LYS:C     | 1.81                     | 1.21              |
| 6:17:376:LYS:HE2   | 66:15:178:GLU:OE2   | 1.05                     | 1.21              |
| 8:3:1561:G:H4'     | 14:9:299:LYS:CD     | 1.70                     | 1.21              |
| 26:K:57:LYS:HG3    | 37:Y:45:A:H5''      | 1.22                     | 1.21              |
| 6:17:275:ASN:HB3   | 65:14:1125:THR:CB   | 1.66                     | 1.21              |
| 6:17:690:LEU:O     | 14:9:682:VAL:CG1    | 1.88                     | 1.21              |
| 3:10:275:SER:OG    | 6:17:970:SER:HB2    | 1.30                     | 1.21              |
| 6:17:422:ASP:OD2   | 66:15:135:SER:CA    | 1.89                     | 1.21              |
| 5:12:97:LEU:HD23   | 6:17:664:ILE:CG2    | 1.71                     | 1.20              |
| 6:17:258:ASN:ND2   | 65:14:1126:LEU:HD12 | 1.53                     | 1.20              |
| 17:AB:44:A:O2'     | 37:Y:44:A:H2'       | 1.02                     | 1.20              |
| 26:K:57:LYS:CD     | 37:Y:45:A:C5'       | 1.78                     | 1.20              |
| 14:9:275:LYS:CD    | 57:s:22:GLY:CA      | 2.17                     | 1.20              |
| 14:9:804:SER:HG    | 57:s:96:GLU:C       | 1.50                     | 1.20              |
| 6:17:709:ASP:CG    | 14:9:670:PRO:HB2    | 1.67                     | 1.20              |
| 66:15:1154:GLU:HG2 | 67:16:71:GLN:CA     | 1.70                     | 1.20              |
| 6:17:386:VAL:HG22  | 66:15:174:ASP:O     | 1.37                     | 1.19              |
| 8:3:102:A:H62      | 14:9:786:MET:CE     | 1.56                     | 1.19              |
| 6:17:264:GLU:CB    | 65:14:1096:ILE:O    | 1.89                     | 1.19              |
| 14:9:188:ARG:HD3   | 58:t:57:LYS:CG      | 1.71                     | 1.19              |
| 14:9:226:SER:O     | 58:t:53:LYS:O       | 1.61                     | 1.19              |
| 6:17:259:GLY:O     | 65:14:1098:THR:HA   | 1.04                     | 1.19              |
| 8:3:1561:G:H8      | 14:9:248:GLU:CG     | 1.56                     | 1.19              |
| 14:9:162:ALA:CB    | 58:t:61:GLY:O       | 1.89                     | 1.19              |
| 6:17:385:ASP:HA    | 66:15:65:ASP:N      | 1.36                     | 1.19              |
| 14:9:798:ARG:NH2   | 61:w:18:LEU:CA      | 1.92                     | 1.19              |
| 6:17:277:SER:HB2   | 65:14:1124:LYS:C    | 1.65                     | 1.18              |
| 6:17:691:THR:C     | 14:9:682:VAL:CG1    | 2.14                     | 1.18              |
| 6:17:699:ILE:CG2   | 14:9:692:LYS:HB3    | 1.72                     | 1.18              |
| 65:14:605:GLU:HG3  | 66:15:248:THR:CG2   | 1.72                     | 1.18              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 64:13:972:ASN:CG    | 67:18:256:HIS:HE2  | 1.48                     | 1.18              |
| 64:13:10:GLN:HG2    | 67:18:197:ASN:CG   | 1.54                     | 1.18              |
| 64:13:1018:SER:CB   | 67:18:258:VAL:CG1  | 2.09                     | 1.18              |
| 64:13:1192:LEU:HD23 | 67:18:88:GLN:CG    | 1.55                     | 1.18              |
| 65:14:947:SER:OG    | 66:15:247:LYS:NZ   | 1.76                     | 1.18              |
| 3:10:235:ILE:HD11   | 6:17:564:GLY:CA    | 1.74                     | 1.17              |
| 8:3:519:A:N3        | 14:9:165:LEU:CD1   | 2.08                     | 1.17              |
| 8:3:1561:G:C3'      | 14:9:299:LYS:HD2   | 1.74                     | 1.17              |
| 10:5:1468:A:H4'     | 37:Y:43:A:O2'      | 1.39                     | 1.17              |
| 10:5:1473:U:C5      | 37:Y:41:U:C5'      | 2.27                     | 1.17              |
| 6:17:426:LYS:NZ     | 66:15:179:PHE:O    | 1.76                     | 1.17              |
| 6:17:711:PHE:HE2    | 14:9:650:ASN:HB2   | 1.02                     | 1.17              |
| 6:17:708:THR:HA     | 14:9:651:HIS:O     | 1.43                     | 1.17              |
| 6:17:693:THR:HG23   | 14:9:682:VAL:N     | 1.59                     | 1.17              |
| 8:3:1558:A:C2       | 14:9:247:LYS:CE    | 2.26                     | 1.17              |
| 10:5:1473:U:H2'     | 37:Y:41:U:OP1      | 1.45                     | 1.17              |
| 6:17:701:THR:N      | 14:9:662:LEU:HA    | 1.37                     | 1.16              |
| 14:9:165:LEU:HG     | 58:t:62:LYS:HE2    | 1.19                     | 1.16              |
| 6:17:428:GLY:O      | 66:15:549:LEU:HD21 | 1.20                     | 1.16              |
| 64:13:984:GLN:CG    | 64:13:1133:THR:N   | 1.81                     | 1.16              |
| 65:14:605:GLU:C     | 66:15:248:THR:HA   | 1.70                     | 1.16              |
| 65:14:1096:ILE:O    | 65:14:1130:LYS:NZ  | 1.78                     | 1.16              |
| 6:17:700:LEU:HD22   | 14:9:658:LEU:O     | 1.40                     | 1.16              |
| 6:17:701:THR:N      | 14:9:662:LEU:CA    | 2.01                     | 1.16              |
| 8:3:1562:A:C5'      | 14:9:298:VAL:O     | 1.93                     | 1.16              |
| 5:12:100:LEU:CD2    | 6:17:668:LEU:CD1   | 2.23                     | 1.16              |
| 6:17:390:ALA:HB2    | 66:15:71:ARG:NH2   | 1.53                     | 1.16              |
| 6:17:701:THR:OG1    | 14:9:773:ALA:CB    | 1.91                     | 1.16              |
| 8:3:1561:G:C8       | 14:9:248:GLU:CG    | 2.29                     | 1.16              |
| 14:9:802:GLU:OE2    | 61:w:20:ILE:HD12   | 1.46                     | 1.16              |
| 6:17:262:SER:N      | 65:14:1098:THR:N   | 1.80                     | 1.16              |
| 6:17:693:THR:HB     | 14:9:637:CYS:HB3   | 1.20                     | 1.16              |
| 10:5:528:G:C2       | 13:8:35:U:C1'      | 2.13                     | 1.16              |
| 17:AB:41:U:C4       | 37:Y:42:C:N4       | 2.13                     | 1.16              |
| 6:17:711:PHE:CE1    | 14:9:642:ASN:OD1   | 1.95                     | 1.15              |
| 8:3:1561:G:C8       | 14:9:248:GLU:HG2   | 1.80                     | 1.15              |
| 14:9:188:ARG:HD2    | 58:t:59:SER:OG     | 1.46                     | 1.15              |
| 14:9:801:HIS:CD2    | 61:w:24:GLY:C      | 2.24                     | 1.15              |
| 6:17:692:LYS:N      | 14:9:683:HIS:HD1   | 1.43                     | 1.15              |
| 6:17:693:THR:CB     | 14:9:682:VAL:CG2   | 1.82                     | 1.15              |
| 6:17:699:ILE:N      | 14:9:689:ILE:HG21  | 1.52                     | 1.15              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:15:1106:SER:C    | 67:16:254:LYS:HB2   | 1.72                     | 1.15              |
| 6:17:261:LYS:HG3    | 65:14:1130:LYS:CE   | 1.76                     | 1.15              |
| 6:17:689:ALA:O      | 14:9:682:VAL:CB     | 1.93                     | 1.15              |
| 64:13:1191:GLN:HE21 | 67:18:92:ARG:NH2    | 1.43                     | 1.15              |
| 14:9:791:LEU:HD21   | 61:w:7:LEU:CD2      | 1.76                     | 1.15              |
| 14:9:798:ARG:NH1    | 61:w:21:LYS:HB3     | 1.61                     | 1.15              |
| 14:9:808:GLN:CA     | 61:w:79:THR:CG2     | 2.15                     | 1.15              |
| 64:13:1020:MET:CA   | 67:18:256:HIS:HA    | 1.76                     | 1.15              |
| 6:17:373:VAL:HB     | 66:15:172:PRO:HG2   | 1.29                     | 1.14              |
| 66:15:1071:PHE:CD2  | 66:15:1247:ARG:NE   | 2.15                     | 1.14              |
| 6:17:80:GLY:HA3     | 65:14:1268:ASN:OD1  | 1.43                     | 1.14              |
| 6:17:706:ILE:HD12   | 14:9:658:LEU:C      | 1.70                     | 1.14              |
| 6:17:711:PHE:CE1    | 14:9:642:ASN:CB     | 2.30                     | 1.14              |
| 64:13:171:PHE:HB3   | 66:15:1183:LEU:HD11 | 1.28                     | 1.14              |
| 66:15:962:LEU:HA    | 66:15:1269:LEU:HD11 | 1.24                     | 1.14              |
| 6:17:388:ALA:HB1    | 66:15:132:LEU:CD2   | 1.58                     | 1.14              |
| 6:17:695:SER:C      | 14:9:686:HIS:HA     | 1.70                     | 1.14              |
| 10:5:1468:A:O2'     | 37:Y:43:A:C1'       | 1.94                     | 1.14              |
| 13:8:34:U8U:S2      | 17:AB:45:A:C2       | 2.40                     | 1.14              |
| 5:12:86:VAL:HB      | 6:17:15:ILE:HD11    | 1.25                     | 1.14              |
| 6:17:264:GLU:H      | 65:14:1096:ILE:C    | 1.55                     | 1.14              |
| 64:13:1062:ARG:HH11 | 67:18:73:VAL:N      | 1.45                     | 1.14              |
| 3:10:238:PHE:HE2    | 6:17:559:PHE:CE1    | 1.65                     | 1.14              |
| 3:10:238:PHE:CE1    | 6:17:563:VAL:HG23   | 1.81                     | 1.14              |
| 6:17:699:ILE:N      | 14:9:689:ILE:CG2    | 1.86                     | 1.14              |
| 14:9:165:LEU:CG     | 58:t:62:LYS:HE3     | 1.57                     | 1.14              |
| 66:15:900:GLN:NE2   | 66:15:934:GLU:HG2   | 1.62                     | 1.14              |
| 6:17:693:THR:HB     | 14:9:637:CYS:CB     | 1.74                     | 1.13              |
| 10:5:1473:U:O4      | 37:Y:41:U:H4'       | 1.48                     | 1.13              |
| 8:3:1561:G:H4'      | 14:9:299:LYS:HD2    | 1.18                     | 1.13              |
| 14:9:165:LEU:HG     | 58:t:62:LYS:CE      | 1.69                     | 1.13              |
| 6:17:699:ILE:HG23   | 14:9:692:LYS:CB     | 1.77                     | 1.13              |
| 6:17:702:GLU:CG     | 14:9:663:ASN:HD22   | 1.40                     | 1.13              |
| 14:9:165:LEU:CA     | 58:t:62:LYS:CE      | 2.04                     | 1.13              |
| 64:13:1018:SER:HB3  | 67:18:258:VAL:CG1   | 1.67                     | 1.13              |
| 6:17:427:ASN:OD1    | 66:15:140:ASN:O     | 1.66                     | 1.13              |
| 6:17:706:ILE:HD12   | 14:9:659:ASN:N      | 1.62                     | 1.12              |
| 12:7:34:G:O6        | 17:AB:42:C:N4       | 1.82                     | 1.13              |
| 14:9:165:LEU:HA     | 58:t:62:LYS:HE3     | 1.25                     | 1.13              |
| 14:9:798:ARG:HD3    | 61:w:22:LEU:HG      | 1.23                     | 1.13              |
| 6:17:275:ASN:HB2    | 65:14:1125:THR:HB   | 1.16                     | 1.12              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:387:VAL:HA    | 66:15:68:ILE:HD11   | 1.28                     | 1.12              |
| 6:17:693:THR:OG1   | 14:9:682:VAL:HG21   | 1.34                     | 1.12              |
| 6:17:710:PHE:CE2   | 14:9:654:LEU:HD23   | 1.84                     | 1.12              |
| 14:9:804:SER:OG    | 57:s:96:GLU:O       | 1.67                     | 1.12              |
| 66:15:1103:GLN:NE2 | 67:16:259:GLN:O     | 1.82                     | 1.12              |
| 3:10:275:SER:HG    | 6:17:970:SER:CB     | 1.56                     | 1.12              |
| 66:15:900:GLN:HE21 | 66:15:934:GLU:CG    | 1.62                     | 1.12              |
| 6:17:426:LYS:HD2   | 66:15:184:GLN:N     | 1.65                     | 1.12              |
| 13:8:35:U:N3       | 17:AB:44:A:N1       | 1.97                     | 1.12              |
| 14:9:795:GLN:HE21  | 61:w:18:LEU:CD1     | 1.63                     | 1.12              |
| 64:13:1062:ARG:HD2 | 67:18:73:VAL:HG23   | 1.30                     | 1.12              |
| 66:15:130:GLN:HE22 | 66:15:560:GLN:HG2   | 1.11                     | 1.12              |
| 5:12:92:ILE:HG21   | 6:17:660:GLY:CA     | 1.76                     | 1.11              |
| 5:12:92:ILE:HG23   | 6:17:660:GLY:HA3    | 1.23                     | 1.11              |
| 6:17:385:ASP:N     | 66:15:175:PRO:HB2   | 1.53                     | 1.11              |
| 6:17:429:ASP:OD2   | 66:15:184:GLN:CB    | 1.98                     | 1.11              |
| 6:17:706:ILE:HD13  | 14:9:658:LEU:HB2    | 1.14                     | 1.11              |
| 6:17:710:PHE:CE1   | 14:9:649:VAL:HG21   | 1.72                     | 1.11              |
| 12:7:34:G:N2       | 17:AB:42:C:O2       | 1.83                     | 1.11              |
| 64:13:986:ILE:HD12 | 64:13:1130:PRO:HB3  | 1.21                     | 1.11              |
| 3:10:238:PHE:HE1   | 6:17:563:VAL:CG2    | 1.60                     | 1.11              |
| 6:17:362:TYR:OH    | 65:14:1098:THR:HG22 | 1.28                     | 1.11              |
| 6:17:390:ALA:CA    | 66:15:71:ARG:NH2    | 2.13                     | 1.11              |
| 6:17:432:LYS:CG    | 66:15:556:GLN:HE22  | 1.62                     | 1.11              |
| 64:13:984:GLN:HG3  | 64:13:1133:THR:H    | 0.97                     | 1.11              |
| 6:17:703:ASN:HB2   | 14:9:663:ASN:HB3    | 1.32                     | 1.11              |
| 17:AB:43:A:OP1     | 37:Y:43:A:OP1       | 1.68                     | 1.11              |
| 66:15:1154:GLU:HG2 | 67:16:71:GLN:HA     | 1.31                     | 1.11              |
| 6:17:264:GLU:N     | 65:14:1096:ILE:C    | 2.09                     | 1.11              |
| 17:AB:41:U:C2'     | 37:Y:42:C:C6        | 2.33                     | 1.11              |
| 66:15:1105:VAL:C   | 67:16:254:LYS:CB    | 2.23                     | 1.11              |
| 6:17:429:ASP:O     | 66:15:137:ILE:HG12  | 1.36                     | 1.10              |
| 6:17:692:LYS:N     | 14:9:682:VAL:CG1    | 2.13                     | 1.10              |
| 14:9:13:ARG:CZ     | 14:9:376:PHE:CD1    | 2.33                     | 1.10              |
| 5:12:87:THR:HA     | 6:17:14:LYS:HB2     | 1.14                     | 1.10              |
| 6:17:388:ALA:O     | 66:15:132:LEU:HD21  | 1.51                     | 1.10              |
| 6:17:390:ALA:HB2   | 66:15:71:ARG:NH1    | 1.65                     | 1.10              |
| 6:17:699:ILE:HG21  | 14:9:689:ILE:HA     | 1.21                     | 1.10              |
| 6:17:874:ARG:NH1   | 14:9:647:ASN:HD21   | 1.48                     | 1.10              |
| 8:3:102:A:N7       | 14:9:786:MET:HE3    | 1.66                     | 1.10              |
| 8:3:519:A:C2       | 14:9:165:LEU:CD1    | 2.34                     | 1.10              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:9:165:LEU:CD2   | 58:t:62:LYS:NZ      | 1.98                     | 1.10              |
| 3:10:238:PHE:CE1   | 6:17:563:VAL:CG2    | 2.33                     | 1.10              |
| 6:17:388:ALA:CB    | 66:15:132:LEU:CD1   | 2.14                     | 1.10              |
| 6:17:693:THR:OG1   | 14:9:682:VAL:CB     | 1.98                     | 1.10              |
| 6:17:706:ILE:CG1   | 14:9:659:ASN:CG     | 2.19                     | 1.10              |
| 10:5:1473:U:C6     | 37:Y:41:U:O5'       | 2.02                     | 1.10              |
| 64:13:984:GLN:CD   | 64:13:1133:THR:N    | 2.07                     | 1.10              |
| 6:17:256:THR:O     | 65:14:1099:GLN:NE2  | 1.84                     | 1.10              |
| 39:a:128:ILE:HG22  | 39:a:129:ASP:H      | 1.11                     | 1.10              |
| 6:17:80:GLY:CA     | 65:14:1268:ASN:OD1  | 1.98                     | 1.09              |
| 6:17:432:LYS:HG2   | 66:15:556:GLN:HE22  | 1.05                     | 1.09              |
| 14:9:791:LEU:HD11  | 61:w:7:LEU:HD21     | 1.30                     | 1.09              |
| 6:17:386:VAL:CG2   | 66:15:177:GLY:N     | 2.01                     | 1.09              |
| 14:9:188:ARG:CD    | 58:t:59:SER:HB3     | 1.81                     | 1.09              |
| 14:9:13:ARG:NH2    | 14:9:376:PHE:CD1    | 2.21                     | 1.09              |
| 5:12:23:LYS:HE2    | 51:m:85:LYS:HD2     | 1.32                     | 1.09              |
| 6:17:385:ASP:CA    | 66:15:65:ASP:N      | 2.14                     | 1.09              |
| 6:17:598:LYS:HG3   | 14:9:641:ARG:NH2    | 1.27                     | 1.09              |
| 10:5:528:G:N1      | 13:8:35:U:O2        | 1.84                     | 1.09              |
| 64:13:171:PHE:CB   | 66:15:1183:LEU:HD11 | 1.83                     | 1.09              |
| 66:15:900:GLN:NE2  | 66:15:934:GLU:CG    | 2.15                     | 1.09              |
| 6:17:275:ASN:HB2   | 65:14:1125:THR:CB   | 1.74                     | 1.09              |
| 6:17:385:ASP:H     | 66:15:175:PRO:HB2   | 0.93                     | 1.09              |
| 6:17:706:ILE:CD1   | 14:9:659:ASN:N      | 2.16                     | 1.09              |
| 13:8:34:U8U:O4     | 17:AB:44:A:N6       | 1.83                     | 1.09              |
| 14:9:13:ARG:CZ     | 14:9:376:PHE:CZ     | 2.35                     | 1.09              |
| 12:7:29:G:H5''     | 27:L:117:ALA:HA     | 1.12                     | 1.08              |
| 14:9:795:GLN:CB    | 61:w:18:LEU:HD21    | 1.83                     | 1.08              |
| 64:13:1192:LEU:CD2 | 67:18:88:GLN:NE2    | 2.14                     | 1.08              |
| 66:15:1103:GLN:HB3 | 67:16:259:GLN:N     | 1.58                     | 1.08              |
| 5:12:89:LYS:HZ3    | 6:17:612:LYS:HA     | 1.06                     | 1.08              |
| 6:17:700:LEU:CD2   | 14:9:658:LEU:HB3    | 1.83                     | 1.08              |
| 14:9:13:ARG:CZ     | 14:9:376:PHE:CG     | 2.36                     | 1.08              |
| 14:9:798:ARG:NE    | 61:w:18:LEU:HA      | 1.68                     | 1.08              |
| 6:17:428:GLY:H     | 66:15:141:VAL:HG22  | 0.97                     | 1.08              |
| 6:17:701:THR:HB    | 14:9:774:ASN:OD1    | 1.52                     | 1.08              |
| 66:15:1105:VAL:CG2 | 67:16:255:ARG:HB2   | 1.84                     | 1.08              |
| 6:17:261:LYS:HG3   | 65:14:1130:LYS:HE2  | 1.22                     | 1.08              |
| 14:9:165:LEU:HA    | 58:t:62:LYS:CE      | 1.68                     | 1.08              |
| 6:17:251:ASP:OD1   | 65:14:1105:LEU:N    | 1.85                     | 1.08              |
| 66:15:1154:GLU:HG2 | 67:16:71:GLN:O      | 1.54                     | 1.08              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:702:GLU:HG2   | 14:9:663:ASN:ND2    | 1.20                     | 1.07              |
| 65:14:610:ILE:HD12 | 66:15:248:THR:CG2   | 1.84                     | 1.07              |
| 6:17:430:PRO:HG2   | 66:15:556:GLN:HG3   | 1.34                     | 1.07              |
| 6:17:80:GLY:HA3    | 65:14:1268:ASN:HA   | 1.32                     | 1.07              |
| 6:17:428:GLY:N     | 66:15:141:VAL:HG22  | 1.68                     | 1.07              |
| 14:9:798:ARG:CG    | 61:w:22:LEU:N       | 2.14                     | 1.07              |
| 6:17:373:VAL:HG11  | 66:15:171:LYS:C     | 1.42                     | 1.07              |
| 6:17:390:ALA:CB    | 66:15:71:ARG:NH1    | 2.14                     | 1.07              |
| 14:9:13:ARG:CZ     | 14:9:13:ARG:NH2     | 2.18                     | 1.07              |
| 5:12:88:SER:CB     | 6:17:615:PHE:CE2    | 2.37                     | 1.07              |
| 14:9:13:ARG:CZ     | 14:9:376:PHE:CE1    | 2.38                     | 1.07              |
| 14:9:13:ARG:NH2    | 14:9:376:PHE:CE1    | 2.22                     | 1.07              |
| 14:9:807:GLY:O     | 61:w:79:THR:HG23    | 1.54                     | 1.07              |
| 46:h:122:LYS:HA    | 46:h:125:LEU:HD13   | 1.32                     | 1.07              |
| 66:15:877:ARG:CZ   | 66:15:1270:ILE:HG22 | 1.85                     | 1.07              |
| 6:17:697:TYR:CE2   | 14:9:636:PHE:C      | 2.33                     | 1.06              |
| 6:17:874:ARG:NH1   | 14:9:647:ASN:ND2    | 2.01                     | 1.06              |
| 14:9:791:LEU:CD2   | 61:w:7:LEU:HD23     | 1.84                     | 1.06              |
| 64:13:1020:MET:HB2 | 67:18:256:HIS:HA    | 1.27                     | 1.06              |
| 66:15:1103:GLN:CB  | 67:16:259:GLN:N     | 2.14                     | 1.06              |
| 12:7:29:G:H5'      | 27:L:117:ALA:HA     | 1.32                     | 1.06              |
| 5:12:97:LEU:HD23   | 6:17:664:ILE:HG23   | 1.14                     | 1.06              |
| 6:17:280:ASN:HB2   | 66:15:139:ALA:HB1   | 1.09                     | 1.06              |
| 6:17:695:SER:CA    | 14:9:633:VAL:CG2    | 2.23                     | 1.06              |
| 6:17:701:THR:CB    | 14:9:774:ASN:OD1    | 2.04                     | 1.06              |
| 66:15:1106:SER:N   | 67:16:254:LYS:HB3   | 1.68                     | 1.06              |
| 14:9:13:ARG:CZ     | 14:9:376:PHE:CD2    | 2.39                     | 1.06              |
| 65:14:610:ILE:CG1  | 66:15:248:THR:CG2   | 2.22                     | 1.06              |
| 3:10:253:PHE:CD2   | 6:17:15:ILE:CD1     | 2.31                     | 1.06              |
| 6:17:387:VAL:HG13  | 66:15:68:ILE:HG13   | 1.32                     | 1.06              |
| 6:17:694:SER:CA    | 14:9:633:VAL:O      | 1.89                     | 1.06              |
| 6:17:701:THR:O     | 14:9:662:LEU:C      | 1.99                     | 1.06              |
| 6:17:711:PHE:CE2   | 14:9:650:ASN:HB2    | 1.90                     | 1.06              |
| 14:9:13:ARG:NH2    | 14:9:376:PHE:CD2    | 2.24                     | 1.06              |
| 66:15:707:ARG:NH2  | 66:15:886:GLU:O     | 1.89                     | 1.06              |
| 66:15:1071:PHE:HB2 | 66:15:1247:ARG:NH2  | 1.69                     | 1.06              |
| 6:17:703:ASN:C     | 14:9:665:HIS:HD2    | 1.61                     | 1.05              |
| 64:13:569:THR:HG23 | 66:15:1122:GLN:OE1  | 1.54                     | 1.05              |
| 64:13:1020:MET:HA  | 67:18:255:ARG:O     | 1.54                     | 1.05              |
| 5:12:92:ILE:CG2    | 6:17:660:GLY:HA3    | 1.67                     | 1.05              |
| 17:AB:40:U:C2      | 37:Y:41:U:C5        | 2.43                     | 1.05              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 10:5:1438:U:P     | 53:o:110:LYS:HE2    | 1.94                     | 1.05              |
| 10:5:1473:U:O2'   | 37:Y:41:U:OP1       | 1.73                     | 1.05              |
| 14:9:188:ARG:CZ   | 58:t:59:SER:HB3     | 1.86                     | 1.05              |
| 64:13:986:ILE:CD1 | 64:13:1130:PRO:HB3  | 1.86                     | 1.05              |
| 6:17:362:TYR:OH   | 65:14:1098:THR:HG21 | 1.55                     | 1.05              |
| 6:17:426:LYS:HB2  | 66:15:184:GLN:CG    | 1.83                     | 1.05              |
| 10:5:1438:U:OP1   | 53:o:110:LYS:HE2    | 1.55                     | 1.05              |
| 14:9:13:ARG:NH2   | 14:9:376:PHE:CE2    | 2.23                     | 1.05              |
| 65:14:610:ILE:CD1 | 66:15:248:THR:HG21  | 1.86                     | 1.05              |
| 6:17:81:ASN:HB2   | 65:14:1293:GLN:CG   | 1.87                     | 1.05              |
| 6:17:701:THR:C    | 14:9:662:LEU:C      | 2.23                     | 1.05              |
| 14:9:13:ARG:CZ    | 14:9:376:PHE:CE2    | 2.39                     | 1.05              |
| 14:9:788:ALA:N    | 61:w:6:GLU:HG3      | 1.71                     | 1.05              |
| 65:14:610:ILE:CB  | 66:15:248:THR:CG2   | 1.90                     | 1.05              |
| 66:15:343:LYS:HE2 | 66:15:439:MET:HB2   | 1.12                     | 1.05              |
| 6:17:385:ASP:N    | 66:15:64:LYS:CB     | 2.01                     | 1.04              |
| 6:17:705:ASP:H    | 14:9:665:HIS:CG     | 1.75                     | 1.04              |
| 8:3:1561:G:H8     | 14:9:248:GLU:HG2    | 0.89                     | 1.04              |
| 14:9:787:LYS:HE3  | 61:w:2:THR:OG1      | 1.53                     | 1.04              |
| 6:17:388:ALA:CB   | 66:15:132:LEU:CB    | 2.04                     | 1.04              |
| 6:17:388:ALA:O    | 66:15:132:LEU:CD2   | 2.04                     | 1.04              |
| 6:17:694:SER:H    | 14:9:682:VAL:HG13   | 1.05                     | 1.04              |
| 6:17:712:ILE:O    | 14:9:674:GLU:C      | 2.00                     | 1.04              |
| 8:3:102:A:C6      | 14:9:781:PHE:HA     | 1.55                     | 1.04              |
| 14:9:801:HIS:HD2  | 61:w:25:GLU:N       | 1.54                     | 1.04              |
| 66:15:997:ASP:HB2 | 66:15:1241:PRO:HB3  | 1.36                     | 1.04              |
| 6:17:706:ILE:HD12 | 14:9:658:LEU:CA     | 1.87                     | 1.04              |
| 3:10:312:THR:HG22 | 65:14:85:GLN:NE2    | 1.72                     | 1.04              |
| 6:17:261:LYS:HA   | 65:14:1130:LYS:CE   | 1.87                     | 1.04              |
| 6:17:386:VAL:CG2  | 66:15:177:GLY:H     | 1.57                     | 1.04              |
| 13:8:35:U:O4      | 17:AB:44:A:C6       | 2.11                     | 1.04              |
| 65:14:605:GLU:HG3 | 66:15:248:THR:HG22  | 1.39                     | 1.04              |
| 6:17:704:ASN:C    | 14:9:665:HIS:CG     | 2.35                     | 1.04              |
| 6:17:705:ASP:N    | 14:9:665:HIS:CE1    | 2.26                     | 1.04              |
| 14:9:188:ARG:CD   | 58:t:59:SER:CB      | 2.35                     | 1.04              |
| 64:13:283:ARG:HD3 | 64:13:290:ASP:OD1   | 1.58                     | 1.04              |
| 6:17:256:THR:C    | 65:14:1099:GLN:HG3  | 1.72                     | 1.03              |
| 6:17:258:ASN:ND2  | 65:14:1126:LEU:CD1  | 2.16                     | 1.03              |
| 14:9:794:LEU:HD13 | 61:w:50:LEU:HD22    | 1.04                     | 1.03              |
| 66:15:343:LYS:CE  | 66:15:439:MET:HB2   | 1.87                     | 1.03              |
| 14:9:798:ARG:HE   | 61:w:18:LEU:CD2     | 1.71                     | 1.03              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:1560:U:H5''    | 14:9:248:GLU:C     | 1.73                     | 1.03              |
| 6:17:428:GLY:O     | 66:15:549:LEU:HD22 | 1.55                     | 1.03              |
| 6:17:696:ASN:H     | 14:9:633:VAL:CG1   | 1.70                     | 1.03              |
| 8:3:102:A:O2'      | 14:9:783:GLU:HA    | 1.59                     | 1.03              |
| 14:9:13:ARG:NH2    | 14:9:376:PHE:CG    | 2.25                     | 1.03              |
| 17:AB:41:U:H2'     | 37:Y:42:C:C5       | 1.92                     | 1.03              |
| 6:17:376:LYS:HE3   | 66:15:178:GLU:HB2  | 1.41                     | 1.03              |
| 6:17:388:ALA:H     | 66:15:68:ILE:HD11  | 1.19                     | 1.03              |
| 14:9:798:ARG:NH2   | 61:w:18:LEU:HD23   | 1.74                     | 1.03              |
| 14:9:798:ARG:NE    | 61:w:18:LEU:HD23   | 1.73                     | 1.03              |
| 26:K:57:LYS:HD3    | 37:Y:45:A:H5'      | 1.41                     | 1.03              |
| 65:14:806:VAL:HG13 | 65:14:818:GLY:HA2  | 1.37                     | 1.03              |
| 66:15:962:LEU:HA   | 66:15:1269:LEU:CD1 | 1.87                     | 1.03              |
| 6:17:710:PHE:O     | 14:9:649:VAL:O     | 1.76                     | 1.02              |
| 6:17:955:LYS:CD    | 14:9:799:GLU:HB3   | 1.88                     | 1.02              |
| 3:10:235:ILE:HA    | 6:17:562:ALA:O     | 1.59                     | 1.02              |
| 6:17:277:SER:HA    | 65:14:1124:LYS:O   | 1.57                     | 1.02              |
| 6:17:694:SER:N     | 14:9:682:VAL:HG13  | 1.59                     | 1.02              |
| 6:17:702:GLU:OE2   | 14:9:781:PHE:CE2   | 2.11                     | 1.02              |
| 14:9:801:HIS:CD2   | 61:w:25:GLU:HA     | 1.94                     | 1.02              |
| 65:14:610:ILE:CD1  | 66:15:248:THR:CG2  | 2.37                     | 1.02              |
| 66:15:1154:GLU:CG  | 67:16:71:GLN:C     | 2.32                     | 1.02              |
| 13:8:34:U8U:S2     | 17:AB:45:A:H2      | 1.72                     | 1.02              |
| 17:AB:41:U:N3      | 37:Y:42:C:N4       | 2.07                     | 1.02              |
| 64:13:785:LEU:HD21 | 64:13:793:LEU:HD12 | 1.36                     | 1.02              |
| 64:13:1099:PHE:HE1 | 64:13:1103:ARG:NH2 | 1.58                     | 1.02              |
| 3:10:238:PHE:CZ    | 6:17:559:PHE:HD1   | 1.76                     | 1.02              |
| 5:12:100:LEU:HD23  | 6:17:668:LEU:HD11  | 1.41                     | 1.02              |
| 6:17:261:LYS:HE3   | 65:14:1130:LYS:HG2 | 1.40                     | 1.02              |
| 6:17:594:LEU:O     | 14:9:641:ARG:CZ    | 2.06                     | 1.02              |
| 6:17:699:ILE:CG2   | 14:9:692:LYS:CB    | 2.35                     | 1.02              |
| 14:9:13:ARG:NH2    | 14:9:376:PHE:CZ    | 2.28                     | 1.02              |
| 14:9:795:GLN:NE2   | 61:w:18:LEU:CD1    | 2.22                     | 1.02              |
| 64:13:10:GLN:CG    | 67:18:197:ASN:HD22 | 1.56                     | 1.02              |
| 64:13:283:ARG:CD   | 64:13:290:ASP:OD1  | 2.06                     | 1.02              |
| 64:13:1062:ARG:NH1 | 67:18:73:VAL:CG2   | 2.21                     | 1.02              |
| 66:15:866:PHE:CE1  | 66:15:1262:LYS:HG2 | 1.93                     | 1.02              |
| 6:17:279:GLN:HG3   | 65:14:1122:LYS:HB3 | 1.40                     | 1.02              |
| 6:17:390:ALA:CB    | 66:15:71:ARG:NH2   | 0.87                     | 1.02              |
| 6:17:426:LYS:HB3   | 66:15:184:GLN:HB2  | 1.41                     | 1.02              |
| 6:17:598:LYS:O     | 14:9:678:PHE:CE2   | 2.13                     | 1.02              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:706:ILE:HD11  | 14:9:668:ILE:HD12   | 1.36                     | 1.02              |
| 17:AB:43:A:H5''    | 37:Y:43:A:OP1       | 0.95                     | 1.02              |
| 5:12:92:ILE:HG22   | 6:17:660:GLY:HA2    | 1.01                     | 1.01              |
| 6:17:384:ALA:C     | 66:15:64:LYS:HB2    | 0.94                     | 1.01              |
| 6:17:388:ALA:N     | 66:15:68:ILE:HD11   | 1.74                     | 1.01              |
| 64:13:1020:MET:HB2 | 67:18:256:HIS:CG    | 1.95                     | 1.01              |
| 64:13:1192:LEU:CD2 | 67:18:88:GLN:CD     | 2.13                     | 1.01              |
| 6:17:709:ASP:OD1   | 14:9:670:PRO:HB2    | 1.57                     | 1.01              |
| 8:3:1558:A:C2      | 14:9:247:LYS:NZ     | 1.93                     | 1.01              |
| 64:13:756:ARG:NH2  | 64:13:1205:GLY:O    | 1.93                     | 1.01              |
| 66:15:1106:SER:N   | 67:16:254:LYS:CB    | 2.23                     | 1.01              |
| 6:17:81:ASN:CB     | 65:14:1293:GLN:HG2  | 1.89                     | 1.01              |
| 6:17:712:ILE:C     | 14:9:674:GLU:C      | 2.28                     | 1.01              |
| 27:L:117:ALA:O     | 33:R:86:ASN:ND2     | 1.93                     | 1.01              |
| 66:15:961:THR:HB   | 66:15:1269:LEU:CD2  | 1.88                     | 1.01              |
| 3:10:235:ILE:HD11  | 6:17:564:GLY:HA3    | 1.42                     | 1.01              |
| 6:17:277:SER:HB2   | 65:14:1124:LYS:HA   | 1.40                     | 1.01              |
| 6:17:386:VAL:HG21  | 66:15:177:GLY:N     | 1.54                     | 1.01              |
| 6:17:706:ILE:HG12  | 14:9:659:ASN:OD1    | 1.55                     | 1.01              |
| 14:9:188:ARG:HD3   | 58:t:57:LYS:HG3     | 1.03                     | 1.01              |
| 14:9:808:GLN:HA    | 61:w:79:THR:HG23    | 1.41                     | 1.01              |
| 65:14:605:GLU:HG3  | 66:15:248:THR:HG23  | 1.43                     | 1.01              |
| 6:17:845:TRP:CZ2   | 14:9:644:LYS:HG2    | 1.95                     | 1.00              |
| 6:17:697:TYR:CD2   | 14:9:636:PHE:C      | 2.39                     | 1.00              |
| 6:17:387:VAL:CA    | 66:15:68:ILE:HD11   | 1.91                     | 1.00              |
| 6:17:432:LYS:HG2   | 66:15:556:GLN:NE2   | 1.76                     | 1.00              |
| 8:3:1562:A:H5'     | 14:9:298:VAL:O      | 1.62                     | 1.00              |
| 14:9:275:LYS:HD2   | 57:s:22:GLY:HA2     | 1.28                     | 1.00              |
| 10:5:1473:U:OP1    | 37:Y:40:U:H4'       | 1.60                     | 1.00              |
| 45:g:96:VAL:O      | 45:g:100:VAL:HG22   | 1.61                     | 1.00              |
| 66:15:1105:VAL:C   | 67:16:254:LYS:HB3   | 1.82                     | 1.00              |
| 6:17:272:ASP:HB3   | 65:14:1127:THR:HG22 | 1.01                     | 1.00              |
| 10:5:1473:U:P      | 37:Y:40:U:C4'       | 2.49                     | 1.00              |
| 10:5:1473:U:N3     | 37:Y:41:U:H5'       | 1.77                     | 1.00              |
| 6:17:426:LYS:NZ    | 66:15:183:LEU:H     | 1.59                     | 1.00              |
| 6:17:430:PRO:CG    | 66:15:556:GLN:HG3   | 1.91                     | 1.00              |
| 10:5:1467:A:C1'    | 37:Y:44:A:O2'       | 2.09                     | 1.00              |
| 15:A:214:ILE:HG22  | 15:A:216:PRO:HD3    | 1.44                     | 1.00              |
| 6:17:388:ALA:HB2   | 66:15:132:LEU:HB3   | 1.39                     | 1.00              |
| 6:17:696:ASN:H     | 14:9:633:VAL:HG11   | 1.25                     | 1.00              |
| 5:12:100:LEU:HD22  | 6:17:668:LEU:HD11   | 1.44                     | 0.99              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:17:387:VAL:HA    | 66:15:68:ILE:CG1   | 1.92                     | 0.99              |
| 6:17:397:LYS:NZ    | 66:15:65:ASP:OD1   | 1.93                     | 0.99              |
| 64:13:1062:ARG:CD  | 67:18:73:VAL:HG23  | 1.92                     | 0.99              |
| 6:17:426:LYS:HZ2   | 66:15:183:LEU:HB3  | 0.89                     | 0.99              |
| 14:9:275:LYS:CB    | 57:s:22:GLY:HA2    | 1.91                     | 0.99              |
| 65:14:610:ILE:HD12 | 66:15:248:THR:HG23 | 1.38                     | 0.99              |
| 66:15:807:LYS:HE3  | 66:15:811:ASN:OD1  | 1.62                     | 0.99              |
| 6:17:690:LEU:HA    | 14:9:682:VAL:HG21  | 1.42                     | 0.99              |
| 43:e:118:GLU:OE1   | 43:e:150:GLU:HG3   | 1.62                     | 0.99              |
| 62:y:53:VAL:HG12   | 62:y:54:LYS:HG3    | 1.44                     | 0.99              |
| 6:17:426:LYS:HB3   | 66:15:181:ALA:O    | 1.61                     | 0.99              |
| 6:17:81:ASN:HB2    | 65:14:1293:GLN:HG2 | 1.00                     | 0.99              |
| 64:13:1020:MET:CB  | 67:18:256:HIS:CB   | 2.40                     | 0.99              |
| 66:15:22:PHE:CE1   | 66:15:827:ILE:HD11 | 1.97                     | 0.99              |
| 3:10:253:PHE:HE2   | 6:17:15:ILE:CB     | 1.74                     | 0.99              |
| 14:9:791:LEU:CD1   | 61:w:7:LEU:HD21    | 1.92                     | 0.99              |
| 66:15:396:GLN:NE2  | 66:15:412:GLY:HA2  | 1.77                     | 0.99              |
| 6:17:690:LEU:N     | 14:9:679:ASP:OD2   | 1.95                     | 0.99              |
| 6:17:709:ASP:CG    | 14:9:670:PRO:CB    | 2.28                     | 0.99              |
| 45:g:100:VAL:HG12  | 45:g:106:MET:HG3   | 1.45                     | 0.99              |
| 5:12:89:LYS:NZ     | 6:17:612:LYS:HA    | 1.76                     | 0.99              |
| 6:17:156:ALA:HB2   | 6:17:165:ILE:HD12  | 1.43                     | 0.99              |
| 6:17:700:LEU:O     | 14:9:661:GLU:C     | 2.05                     | 0.99              |
| 6:17:711:PHE:CE2   | 14:9:650:ASN:CB    | 2.36                     | 0.99              |
| 3:10:253:PHE:HE2   | 6:17:15:ILE:CG2    | 1.48                     | 0.99              |
| 10:5:1473:U:C4     | 37:Y:41:U:H4'      | 1.98                     | 0.99              |
| 14:9:795:GLN:HE21  | 61:w:18:LEU:HG     | 0.97                     | 0.99              |
| 64:13:972:ASN:OD1  | 67:18:256:HIS:CD2  | 2.16                     | 0.99              |
| 6:17:386:VAL:CG1   | 66:15:174:ASP:CG   | 2.36                     | 0.98              |
| 6:17:845:TRP:HZ2   | 14:9:644:LYS:CB    | 1.76                     | 0.98              |
| 14:9:165:LEU:HD23  | 58:t:62:LYS:HZ3    | 1.24                     | 0.98              |
| 6:17:390:ALA:HB1   | 66:15:71:ARG:NH2   | 1.33                     | 0.98              |
| 14:9:798:ARG:HH11  | 61:w:21:LYS:HB3    | 1.16                     | 0.98              |
| 6:17:696:ASN:N     | 14:9:633:VAL:CG1   | 2.25                     | 0.98              |
| 64:13:10:GLN:CG    | 67:18:197:ASN:CG   | 2.17                     | 0.98              |
| 65:14:605:GLU:CA   | 66:15:248:THR:HA   | 1.92                     | 0.98              |
| 6:17:279:GLN:CG    | 65:14:1122:LYS:HB3 | 1.60                     | 0.98              |
| 14:9:801:HIS:CD2   | 61:w:25:GLU:N      | 2.30                     | 0.98              |
| 65:14:948:VAL:CG2  | 66:15:247:LYS:HD2  | 1.93                     | 0.98              |
| 6:17:701:THR:CG2   | 14:9:774:ASN:OD1   | 2.10                     | 0.98              |
| 8:3:1562:A:H5''    | 14:9:298:VAL:O     | 1.61                     | 0.98              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:9:795:GLN:NE2   | 61:w:18:LEU:CG      | 2.11                     | 0.98              |
| 65:14:1036:GLN:HG3 | 66:15:539:GLU:HA    | 1.44                     | 0.98              |
| 67:18:15:GLN:OE1   | 67:18:90:GLN:CB     | 2.11                     | 0.98              |
| 5:12:88:SER:OG     | 6:17:18:ILE:HG13    | 1.09                     | 0.98              |
| 6:17:376:LYS:CE    | 66:15:178:GLU:CB    | 2.40                     | 0.98              |
| 6:17:597:ILE:O     | 14:9:641:ARG:HD2    | 1.60                     | 0.98              |
| 8:3:102:A:C5       | 14:9:786:MET:HE3    | 1.99                     | 0.98              |
| 14:9:798:ARG:HH21  | 61:w:18:LEU:HD23    | 1.25                     | 0.98              |
| 6:17:376:LYS:CE    | 66:15:178:GLU:OE2   | 1.96                     | 0.98              |
| 6:17:430:PRO:CD    | 66:15:555:PHE:HD1   | 1.76                     | 0.98              |
| 14:9:795:GLN:CG    | 61:w:18:LEU:CD2     | 1.97                     | 0.98              |
| 8:3:102:A:N6       | 14:9:786:MET:CE     | 2.27                     | 0.97              |
| 6:17:429:ASP:CA    | 66:15:549:LEU:HD22  | 1.93                     | 0.97              |
| 17:AB:44:A:C5      | 37:Y:45:A:N6        | 2.32                     | 0.97              |
| 64:13:1126:ARG:NH1 | 65:14:505:ASP:OD2   | 1.96                     | 0.97              |
| 6:17:376:LYS:NZ    | 66:15:178:GLU:CD    | 2.12                     | 0.97              |
| 8:3:1561:G:O2'     | 14:9:299:LYS:CD     | 2.12                     | 0.97              |
| 6:17:386:VAL:HG22  | 66:15:174:ASP:C     | 1.82                     | 0.97              |
| 64:13:984:GLN:CD   | 64:13:1133:THR:HG23 | 1.89                     | 0.97              |
| 6:17:697:TYR:N     | 14:9:633:VAL:HG22   | 1.79                     | 0.97              |
| 14:9:225:ILE:HD12  | 58:t:57:LYS:HG2     | 1.45                     | 0.97              |
| 14:9:791:LEU:HD21  | 61:w:7:LEU:HD23     | 0.97                     | 0.97              |
| 66:15:1106:SER:O   | 67:16:254:LYS:CB    | 2.12                     | 0.97              |
| 3:10:311:GLN:O     | 65:14:89:ASN:OD1    | 1.83                     | 0.97              |
| 6:17:261:LYS:CG    | 65:14:1130:LYS:HE2  | 1.94                     | 0.97              |
| 17:AB:45:A:O5'     | 37:Y:45:A:C8        | 2.18                     | 0.97              |
| 6:17:711:PHE:CE2   | 14:9:650:ASN:N      | 2.31                     | 0.97              |
| 6:17:426:LYS:HD2   | 66:15:184:GLN:H     | 0.84                     | 0.97              |
| 6:17:955:LYS:HD3   | 14:9:803:LYS:CE     | 1.95                     | 0.97              |
| 41:c:5:LYS:HD2     | 41:c:13:PHE:CD2     | 1.99                     | 0.97              |
| 10:5:1467:A:C2     | 37:Y:44:A:C2        | 2.53                     | 0.96              |
| 17:AB:41:U:C2      | 37:Y:42:C:C4        | 2.52                     | 0.96              |
| 64:13:283:ARG:HH22 | 64:13:492:LYS:HB2   | 1.30                     | 0.96              |
| 64:13:1099:PHE:CE1 | 64:13:1103:ARG:NH2  | 2.32                     | 0.96              |
| 66:15:877:ARG:NH1  | 66:15:1270:ILE:CG2  | 2.28                     | 0.96              |
| 67:16:255:ARG:HH11 | 67:16:259:GLN:HE21  | 1.05                     | 0.96              |
| 6:17:261:LYS:CA    | 65:14:1126:LEU:HD21 | 1.93                     | 0.96              |
| 66:15:900:GLN:HE21 | 66:15:934:GLU:HG2   | 1.19                     | 0.96              |
| 6:17:376:LYS:CE    | 66:15:178:GLU:HB2   | 1.95                     | 0.96              |
| 64:13:147:THR:O    | 66:15:1169:ASP:CB   | 2.13                     | 0.96              |
| 6:17:429:ASP:N     | 66:15:167:PHE:HE1   | 1.43                     | 0.96              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 64:13:1062:ARG:NH1 | 67:18:72:ALA:C      | 2.23                     | 0.96              |
| 5:12:92:ILE:CD1    | 6:17:655:TYR:CE1    | 2.49                     | 0.96              |
| 6:17:258:ASN:HB3   | 65:14:1126:LEU:HD13 | 1.41                     | 0.96              |
| 14:9:227:GLY:HA2   | 58:t:53:LYS:C       | 1.74                     | 0.96              |
| 6:17:711:PHE:HZ    | 14:9:642:ASN:CB     | 1.68                     | 0.96              |
| 14:9:794:LEU:HD13  | 61:w:50:LEU:CD2     | 1.94                     | 0.96              |
| 6:17:388:ALA:HB3   | 66:15:132:LEU:CG    | 1.74                     | 0.96              |
| 6:17:423:PRO:O     | 66:15:170:SER:OG    | 1.82                     | 0.96              |
| 6:17:705:ASP:N     | 14:9:665:HIS:CG     | 2.26                     | 0.96              |
| 17:AB:44:A:C6      | 37:Y:45:A:N6        | 2.34                     | 0.96              |
| 6:17:79:SER:OG     | 65:14:1270:LEU:N    | 1.89                     | 0.96              |
| 6:17:700:LEU:O     | 14:9:661:GLU:CB     | 2.13                     | 0.96              |
| 14:9:802:GLU:OE2   | 61:w:20:ILE:CD1     | 2.14                     | 0.96              |
| 6:17:373:VAL:CG1   | 66:15:171:LYS:C     | 2.28                     | 0.96              |
| 6:17:376:LYS:HE2   | 66:15:178:GLU:CG    | 1.81                     | 0.96              |
| 10:5:1473:U:H2'    | 37:Y:41:U:P         | 2.05                     | 0.96              |
| 6:17:387:VAL:CA    | 66:15:68:ILE:CD1    | 2.43                     | 0.95              |
| 6:17:698:SER:C     | 14:9:689:ILE:HG21   | 1.90                     | 0.95              |
| 26:K:57:LYS:HG3    | 37:Y:45:A:C5'       | 1.85                     | 0.95              |
| 65:14:745:GLN:O    | 65:14:751:LYS:HE3   | 1.66                     | 0.95              |
| 6:17:697:TYR:CD2   | 14:9:637:CYS:N      | 2.35                     | 0.95              |
| 14:9:275:LYS:HD2   | 57:s:22:GLY:HA3     | 0.98                     | 0.95              |
| 66:15:1237:PRO:HG2 | 66:15:1239:HIS:NE2  | 1.81                     | 0.95              |
| 64:13:318:GLU:OE2  | 64:13:498:ASN:HB2   | 1.65                     | 0.95              |
| 6:17:710:PHE:CE2   | 14:9:654:LEU:CD2    | 2.49                     | 0.95              |
| 14:9:798:ARG:NE    | 61:w:18:LEU:CD2     | 2.29                     | 0.95              |
| 3:10:431:MET:HE2   | 6:17:667:TRP:CH2    | 2.02                     | 0.95              |
| 5:12:87:THR:CA     | 6:17:14:LYS:CB      | 2.42                     | 0.95              |
| 64:13:1020:MET:HB2 | 67:18:256:HIS:CA    | 1.84                     | 0.95              |
| 65:14:610:ILE:CB   | 66:15:248:THR:CB    | 2.32                     | 0.95              |
| 66:15:130:GLN:NE2  | 66:15:560:GLN:HG2   | 1.80                     | 0.95              |
| 66:15:1105:VAL:CG2 | 67:16:255:ARG:CB    | 2.39                     | 0.95              |
| 6:17:264:GLU:H     | 65:14:1097:GLN:N    | 1.64                     | 0.95              |
| 5:12:87:THR:HA     | 6:17:14:LYS:HB3     | 1.46                     | 0.95              |
| 6:17:426:LYS:HZ2   | 66:15:183:LEU:CA    | 1.79                     | 0.95              |
| 8:3:1560:U:C5'     | 14:9:249:ASP:CG     | 2.40                     | 0.95              |
| 8:3:1560:U:H4'     | 14:9:249:ASP:H      | 1.23                     | 0.95              |
| 14:9:804:SER:OG    | 57:s:96:GLU:C       | 2.06                     | 0.95              |
| 6:17:264:GLU:OE2   | 65:14:1130:LYS:CD   | 2.15                     | 0.94              |
| 6:17:388:ALA:HB1   | 66:15:132:LEU:HB3   | 1.11                     | 0.94              |
| 14:9:163:PRO:HG2   | 58:t:63:VAL:HG23    | 1.49                     | 0.94              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:9:794:LEU:CD1   | 61:w:50:LEU:HD22    | 1.97                     | 0.94              |
| 17:AB:40:U:H2'     | 37:Y:41:U:C6        | 2.02                     | 0.94              |
| 6:17:707:GLN:OE1   | 14:9:669:SER:HA     | 1.66                     | 0.94              |
| 6:17:709:ASP:O     | 14:9:674:GLU:CA     | 2.16                     | 0.94              |
| 14:9:798:ARG:HE    | 61:w:18:LEU:HD23    | 1.24                     | 0.94              |
| 66:15:1071:PHE:HB2 | 66:15:1247:ARG:HH22 | 1.32                     | 0.94              |
| 5:12:86:VAL:O      | 6:17:15:ILE:CG1     | 2.15                     | 0.94              |
| 6:17:262:SER:CA    | 65:14:1098:THR:H    | 1.78                     | 0.94              |
| 45:g:29:TYR:HA     | 45:g:32:MET:HE1     | 1.45                     | 0.94              |
| 64:13:173:GLU:OE1  | 66:15:1178:SER:HB3  | 0.76                     | 0.94              |
| 64:13:1213:LEU:CB  | 67:18:276:ASN:CB    | 2.35                     | 0.94              |
| 66:15:877:ARG:HD2  | 66:15:1270:ILE:HG21 | 1.47                     | 0.94              |
| 3:10:431:MET:CE    | 6:17:667:TRP:HH2    | 1.79                     | 0.94              |
| 6:17:262:SER:OG    | 65:14:1098:THR:OG1  | 1.86                     | 0.94              |
| 6:17:692:LYS:N     | 14:9:683:HIS:ND1    | 2.15                     | 0.94              |
| 8:3:1558:A:C2      | 14:9:247:LYS:HE2    | 2.00                     | 0.94              |
| 3:10:257:GLU:OE1   | 6:17:11:TRP:HZ3     | 0.79                     | 0.94              |
| 6:17:694:SER:HA    | 14:9:633:VAL:O      | 0.97                     | 0.94              |
| 6:17:700:LEU:CD2   | 14:9:658:LEU:O      | 2.15                     | 0.94              |
| 6:17:710:PHE:HE1   | 14:9:649:VAL:HG21   | 1.24                     | 0.94              |
| 10:5:787:A:H1'     | 12:7:38:A:H4'       | 1.48                     | 0.94              |
| 43:e:92:LEU:HD21   | 43:e:97:TYR:HB3     | 1.50                     | 0.94              |
| 64:13:149:PRO:HB3  | 66:15:1168:VAL:HA   | 1.50                     | 0.94              |
| 39:a:128:ILE:HG22  | 39:a:129:ASP:N      | 1.79                     | 0.94              |
| 5:12:85:TRP:HB3    | 6:17:12:LEU:N       | 1.61                     | 0.94              |
| 6:17:264:GLU:H     | 65:14:1097:GLN:CA   | 1.80                     | 0.94              |
| 6:17:387:VAL:HG11  | 66:15:67:ASN:HB2    | 1.50                     | 0.94              |
| 8:3:519:A:N3       | 14:9:165:LEU:HD13   | 1.75                     | 0.94              |
| 14:9:798:ARG:CZ    | 61:w:18:LEU:HD23    | 1.97                     | 0.94              |
| 5:12:100:LEU:HD22  | 6:17:668:LEU:CD1    | 1.95                     | 0.93              |
| 6:17:277:SER:CB    | 65:14:1124:LYS:CA   | 2.41                     | 0.93              |
| 6:17:385:ASP:C     | 66:15:65:ASP:HB2    | 1.93                     | 0.93              |
| 6:17:397:LYS:HE2   | 66:15:67:ASN:CG     | 1.64                     | 0.93              |
| 64:13:1099:PHE:HE1 | 64:13:1103:ARG:HH21 | 0.99                     | 0.93              |
| 14:9:188:ARG:HD2   | 58:t:59:SER:CB      | 1.96                     | 0.93              |
| 6:17:387:VAL:CG1   | 66:15:68:ILE:HG13   | 1.98                     | 0.93              |
| 14:9:164:HIS:HB3   | 58:t:62:LYS:O       | 1.41                     | 0.93              |
| 14:9:795:GLN:CG    | 61:w:18:LEU:CG      | 2.37                     | 0.93              |
| 64:13:1020:MET:HB3 | 67:18:256:HIS:CB    | 1.98                     | 0.93              |
| 6:17:698:SER:HB2   | 14:9:769:ILE:HG21   | 0.93                     | 0.93              |
| 64:13:569:THR:CG2  | 66:15:1122:GLN:OE1  | 2.16                     | 0.93              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 66:15:343:LYS:HE2   | 66:15:439:MET:CB   | 1.99                     | 0.93              |
| 6:17:386:VAL:HG11   | 66:15:177:GLY:CA   | 1.98                     | 0.93              |
| 6:17:694:SER:H      | 14:9:682:VAL:CG1   | 1.81                     | 0.93              |
| 14:9:313:LYS:HE3    | 38:Z:2:UNK:C       | 1.99                     | 0.93              |
| 65:14:948:VAL:HG23  | 66:15:247:LYS:HD2  | 1.49                     | 0.93              |
| 5:12:92:ILE:HD11    | 6:17:655:TYR:HE1   | 1.33                     | 0.93              |
| 6:17:277:SER:CA     | 65:14:1124:LYS:O   | 2.17                     | 0.93              |
| 6:17:698:SER:HB3    | 14:9:632:PHE:HB3   | 1.48                     | 0.93              |
| 14:9:451:GLN:HA     | 62:y:56:ALA:HB3    | 1.48                     | 0.93              |
| 64:13:1020:MET:HB3  | 67:18:256:HIS:C    | 1.93                     | 0.93              |
| 64:13:1191:GLN:HE21 | 67:18:92:ARG:HH22  | 1.03                     | 0.93              |
| 6:17:426:LYS:N      | 66:15:140:ASN:HD22 | 1.53                     | 0.93              |
| 6:17:699:ILE:HG23   | 14:9:692:LYS:HB3   | 0.95                     | 0.93              |
| 14:9:313:LYS:HD2    | 38:Z:2:UNK:CB      | 1.99                     | 0.93              |
| 66:15:1103:GLN:CD   | 67:16:259:GLN:O    | 2.12                     | 0.93              |
| 10:5:1468:A:H1'     | 37:Y:43:A:N3       | 1.82                     | 0.93              |
| 64:13:173:GLU:CD    | 66:15:1178:SER:HB3 | 1.92                     | 0.93              |
| 6:17:387:VAL:HG13   | 66:15:68:ILE:CG1   | 1.99                     | 0.93              |
| 10:5:1468:A:N3      | 37:Y:43:A:H2       | 1.64                     | 0.93              |
| 64:13:734:LEU:CD1   | 64:13:885:LYS:O    | 2.16                     | 0.93              |
| 66:15:1154:GLU:CG   | 67:16:71:GLN:O     | 2.16                     | 0.93              |
| 67:16:15:GLN:OE1    | 67:16:90:GLN:CB    | 2.16                     | 0.93              |
| 6:17:430:PRO:CD     | 66:15:555:PHE:CD1  | 2.52                     | 0.92              |
| 64:13:1062:ARG:NH1  | 67:18:73:VAL:N     | 2.17                     | 0.92              |
| 14:9:798:ARG:HD2    | 61:w:22:LEU:H      | 1.33                     | 0.92              |
| 64:13:662:ASN:O     | 64:13:966:GLN:NE2  | 2.03                     | 0.92              |
| 66:15:1104:SER:OG   | 67:16:256:HIS:CA   | 2.18                     | 0.92              |
| 8:3:925:C:P         | 27:L:92:ARG:NH1    | 2.43                     | 0.92              |
| 14:9:165:LEU:HD23   | 58:t:62:LYS:HZ1    | 1.13                     | 0.92              |
| 65:14:316:LYS:CE    | 65:14:454:GLN:NE2  | 2.32                     | 0.92              |
| 12:7:29:G:OP1       | 33:R:87:ARG:NH2    | 1.75                     | 0.92              |
| 14:9:162:ALA:HB1    | 58:t:61:GLY:O      | 1.11                     | 0.92              |
| 6:17:702:GLU:OE2    | 14:9:781:PHE:CZ    | 2.23                     | 0.92              |
| 66:15:1154:GLU:CG   | 67:16:71:GLN:HA    | 1.98                     | 0.92              |
| 5:12:85:TRP:CB      | 6:17:12:LEU:N      | 2.32                     | 0.92              |
| 6:17:430:PRO:HD3    | 66:15:555:PHE:CD1  | 2.04                     | 0.92              |
| 6:17:699:ILE:HG21   | 14:9:689:ILE:CA    | 1.91                     | 0.92              |
| 8:3:520:C:OP1       | 14:9:160:ASN:CB    | 2.15                     | 0.92              |
| 14:9:801:HIS:CD2    | 61:w:25:GLU:CA     | 2.52                     | 0.92              |
| 64:13:924:LYS:HZ2   | 67:18:79:ALA:HB1   | 1.32                     | 0.92              |
| 5:12:85:TRP:CG      | 6:17:12:LEU:H      | 1.88                     | 0.92              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:12:88:SER:HB2     | 6:17:615:PHE:CZ    | 2.05                     | 0.92              |
| 65:14:1183:ARG:NH1  | 65:14:1243:ASN:HB2 | 1.84                     | 0.92              |
| 10:5:715:A:N7       | 32:Q:69:LYS:NZ     | 2.17                     | 0.91              |
| 14:9:451:GLN:CA     | 62:y:56:ALA:HB3    | 1.99                     | 0.91              |
| 14:9:795:GLN:CG     | 61:w:18:LEU:HD11   | 1.99                     | 0.91              |
| 6:17:261:LYS:HG2    | 65:14:1096:ILE:HB  | 1.49                     | 0.91              |
| 14:9:188:ARG:CD     | 58:t:59:SER:OG     | 2.18                     | 0.91              |
| 14:9:798:ARG:CG     | 61:w:21:LYS:C      | 2.12                     | 0.91              |
| 17:AB:45:A:N6       | 37:Y:45:A:H61      | 1.59                     | 0.91              |
| 5:12:97:LEU:CD2     | 6:17:664:ILE:CG2   | 2.38                     | 0.91              |
| 6:17:427:ASN:HD21   | 66:15:168:VAL:HG23 | 1.35                     | 0.91              |
| 6:17:388:ALA:C      | 66:15:132:LEU:HD21 | 1.90                     | 0.91              |
| 6:17:845:TRP:HZ2    | 14:9:644:LYS:CG    | 1.70                     | 0.91              |
| 10:5:787:A:O4'      | 12:7:38:A:O2'      | 1.89                     | 0.91              |
| 10:5:1473:U:C4      | 37:Y:41:U:C4'      | 2.53                     | 0.91              |
| 14:9:275:LYS:CD     | 57:s:22:GLY:HA3    | 1.92                     | 0.91              |
| 3:10:235:ILE:HD11   | 6:17:564:GLY:HA2   | 1.50                     | 0.91              |
| 6:17:264:GLU:OE2    | 65:14:1130:LYS:HE3 | 1.70                     | 0.91              |
| 6:17:711:PHE:CE1    | 14:9:642:ASN:HB2   | 1.97                     | 0.91              |
| 65:14:605:GLU:O     | 66:15:248:THR:C    | 2.13                     | 0.91              |
| 64:13:1192:LEU:HD21 | 67:18:88:GLN:HE21  | 1.19                     | 0.91              |
| 6:17:706:ILE:O      | 14:9:656:GLU:CG    | 2.19                     | 0.91              |
| 8:3:1560:U:O2       | 14:9:246:LEU:O     | 1.87                     | 0.91              |
| 64:13:972:ASN:OD1   | 67:18:256:HIS:NE2  | 2.01                     | 0.91              |
| 6:17:697:TYR:HB2    | 14:9:633:VAL:HA    | 1.49                     | 0.91              |
| 6:17:955:LYS:HZ3    | 14:9:799:GLU:C     | 1.77                     | 0.91              |
| 64:13:1062:ARG:NH1  | 67:18:73:VAL:CA    | 2.33                     | 0.91              |
| 66:15:1271:ARG:HH22 | 67:16:256:HIS:HD2  | 1.18                     | 0.91              |
| 6:17:277:SER:CB     | 65:14:1124:LYS:HA  | 2.00                     | 0.90              |
| 6:17:599:ASN:ND2    | 14:9:641:ARG:O     | 1.84                     | 0.90              |
| 14:9:791:LEU:CD2    | 61:w:7:LEU:CD2     | 2.45                     | 0.90              |
| 6:17:373:VAL:HG13   | 66:15:174:ASP:H    | 1.36                     | 0.90              |
| 66:15:71:ARG:NH1    | 66:15:132:LEU:HD21 | 1.86                     | 0.90              |
| 5:12:88:SER:HB2     | 6:17:615:PHE:HE2   | 1.08                     | 0.90              |
| 6:17:79:SER:HB3     | 65:14:1269:ALA:C   | 1.94                     | 0.90              |
| 6:17:422:ASP:O      | 66:15:136:ASN:HA   | 1.72                     | 0.90              |
| 64:13:290:ASP:HB2   | 64:13:511:SER:OG   | 1.70                     | 0.90              |
| 64:13:924:LYS:NZ    | 67:18:79:ALA:CB    | 2.33                     | 0.90              |
| 66:15:1071:PHE:CD2  | 66:15:1247:ARG:NH2 | 2.39                     | 0.90              |
| 6:17:697:TYR:HE2    | 14:9:637:CYS:HA    | 1.34                     | 0.90              |
| 5:12:88:SER:CB      | 6:17:615:PHE:HE2   | 1.80                     | 0.90              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:12:92:ILE:HG21   | 6:17:660:GLY:HA2    | 1.41                     | 0.90              |
| 6:17:272:ASP:CB    | 65:14:1127:THR:HG21 | 1.54                     | 0.90              |
| 6:17:280:ASN:HB3   | 66:15:139:ALA:HB2   | 0.90                     | 0.90              |
| 13:8:35:U:O4       | 17:AB:44:A:N1       | 2.01                     | 0.90              |
| 64:13:10:GLN:CB    | 67:18:197:ASN:ND2   | 2.35                     | 0.90              |
| 6:17:426:LYS:CE    | 66:15:179:PHE:O     | 2.20                     | 0.90              |
| 10:5:1468:A:C4'    | 37:Y:43:A:O2'       | 2.19                     | 0.90              |
| 12:7:29:G:H5''     | 27:L:117:ALA:CA     | 2.02                     | 0.90              |
| 64:13:216:ILE:HG21 | 64:13:406:LEU:HD23  | 1.54                     | 0.90              |
| 6:17:275:ASN:HB3   | 65:14:1125:THR:HB   | 0.91                     | 0.90              |
| 6:17:712:ILE:O     | 14:9:674:GLU:O      | 1.89                     | 0.89              |
| 66:15:1103:GLN:O   | 67:16:255:ARG:HB3   | 1.72                     | 0.89              |
| 6:17:710:PHE:CD2   | 14:9:673:PHE:HB3    | 2.07                     | 0.89              |
| 64:13:1191:GLN:NE2 | 67:18:92:ARG:HH22   | 1.70                     | 0.89              |
| 5:12:87:THR:CA     | 6:17:14:LYS:HB3     | 2.03                     | 0.89              |
| 5:12:97:LEU:CG     | 6:17:664:ILE:HG23   | 2.03                     | 0.89              |
| 6:17:386:VAL:HG11  | 66:15:177:GLY:N     | 1.22                     | 0.89              |
| 6:17:700:LEU:HD22  | 14:9:658:LEU:CA     | 2.01                     | 0.89              |
| 8:3:1559:A:O3'     | 14:9:249:ASP:OD1    | 1.90                     | 0.89              |
| 64:13:924:LYS:HZ1  | 67:18:79:ALA:HB1    | 1.06                     | 0.89              |
| 3:10:431:MET:CE    | 6:17:667:TRP:CH2    | 2.56                     | 0.89              |
| 6:17:261:LYS:HG2   | 65:14:1096:ILE:CG2  | 2.02                     | 0.89              |
| 8:3:102:A:H62      | 14:9:786:MET:HE3    | 1.35                     | 0.89              |
| 6:17:710:PHE:CD2   | 14:9:673:PHE:CB     | 2.56                     | 0.89              |
| 10:5:1473:U:C6     | 37:Y:41:U:P         | 2.66                     | 0.89              |
| 14:9:351:VAL:O     | 58:t:53:LYS:HE3     | 1.70                     | 0.89              |
| 66:15:958:PHE:CE2  | 66:15:1270:ILE:HG13 | 2.07                     | 0.89              |
| 66:15:995:TYR:O    | 66:15:1241:PRO:O    | 1.90                     | 0.89              |
| 6:17:280:ASN:CB    | 66:15:139:ALA:HB2   | 1.68                     | 0.89              |
| 6:17:706:ILE:HG13  | 14:9:659:ASN:CB     | 2.02                     | 0.89              |
| 13:8:35:U:O4       | 17:AB:44:A:N6       | 2.05                     | 0.89              |
| 64:13:1126:ARG:NH1 | 65:14:152:LYS:HZ1   | 1.71                     | 0.89              |
| 66:15:958:PHE:HE2  | 66:15:1270:ILE:HG13 | 1.36                     | 0.89              |
| 66:15:1071:PHE:CE2 | 66:15:1247:ARG:NE   | 2.40                     | 0.89              |
| 6:17:260:GLN:HB3   | 65:14:1126:LEU:HD23 | 1.54                     | 0.89              |
| 6:17:275:ASN:CA    | 65:14:1125:THR:HB   | 1.99                     | 0.89              |
| 64:13:1191:GLN:NE2 | 67:18:92:ARG:NH2    | 2.21                     | 0.89              |
| 3:10:253:PHE:HD2   | 6:17:15:ILE:HD13    | 1.38                     | 0.88              |
| 66:15:807:LYS:HE3  | 66:15:811:ASN:CG    | 1.97                     | 0.88              |
| 6:17:432:LYS:CG    | 66:15:556:GLN:NE2   | 2.34                     | 0.88              |
| 8:3:1560:U:H5'     | 14:9:249:ASP:OD2    | 1.73                     | 0.88              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:15:986:ARG:NH2   | 66:15:1131:GLY:O    | 2.06                     | 0.88              |
| 6:17:272:ASP:CB     | 65:14:1127:THR:HG23 | 1.80                     | 0.88              |
| 6:17:700:LEU:C      | 14:9:662:LEU:N      | 2.25                     | 0.88              |
| 12:7:29:G:C5'       | 27:L:117:ALA:CA     | 2.46                     | 0.88              |
| 14:9:188:ARG:CD     | 58:t:57:LYS:HG3     | 1.98                     | 0.88              |
| 14:9:787:LYS:C      | 61:w:6:GLU:HG3      | 1.98                     | 0.88              |
| 44:f:41:LYS:HB3     | 44:f:46:ASP:HB3     | 1.53                     | 0.88              |
| 66:15:343:LYS:CE    | 66:15:439:MET:CB    | 2.52                     | 0.88              |
| 66:15:1105:VAL:HG23 | 67:16:255:ARG:HB2   | 0.90                     | 0.88              |
| 6:17:262:SER:CB     | 65:14:1098:THR:OG1  | 2.20                     | 0.88              |
| 6:17:693:THR:OG1    | 14:9:682:VAL:CG2    | 0.58                     | 0.88              |
| 6:17:709:ASP:O      | 14:9:674:GLU:HA     | 1.74                     | 0.88              |
| 6:17:386:VAL:CG1    | 66:15:174:ASP:OD1   | 2.21                     | 0.88              |
| 6:17:955:LYS:CD     | 14:9:803:LYS:CE     | 2.48                     | 0.88              |
| 64:13:1062:ARG:CZ   | 67:18:73:VAL:HG22   | 2.03                     | 0.88              |
| 66:15:54:GLU:HG2    | 66:15:814:GLN:NE2   | 1.87                     | 0.88              |
| 66:15:1139:LYS:HE3  | 66:15:1197:VAL:O    | 1.74                     | 0.88              |
| 14:9:801:HIS:NE2    | 61:w:24:GLY:C       | 2.27                     | 0.88              |
| 64:13:1217:LYS:HZ3  | 67:18:274:PRO:CG    | 1.85                     | 0.88              |
| 6:17:697:TYR:H      | 14:9:633:VAL:HG22   | 1.36                     | 0.88              |
| 6:17:706:ILE:CD1    | 14:9:668:ILE:HD12   | 2.03                     | 0.88              |
| 14:9:798:ARG:NH2    | 61:w:18:LEU:N       | 2.22                     | 0.88              |
| 66:15:958:PHE:N     | 66:15:1273:VAL:HG11 | 1.89                     | 0.88              |
| 6:17:82:ASN:OD1     | 65:14:1268:ASN:ND2  | 2.06                     | 0.88              |
| 52:n:29:VAL:HG21    | 52:n:46:PHE:CE1     | 2.08                     | 0.88              |
| 6:17:397:LYS:CE     | 66:15:65:ASP:OD1    | 2.22                     | 0.88              |
| 14:9:451:GLN:HB3    | 62:y:56:ALA:O       | 1.73                     | 0.88              |
| 64:13:699:LYS:NZ    | 64:13:714:GLU:OE1   | 2.06                     | 0.87              |
| 66:15:1105:VAL:O    | 67:16:256:HIS:CD2   | 2.27                     | 0.87              |
| 6:17:261:LYS:HA     | 65:14:1130:LYS:HE3  | 1.57                     | 0.87              |
| 14:9:798:ARG:CD     | 61:w:22:LEU:N       | 2.36                     | 0.87              |
| 64:13:1062:ARG:NH1  | 67:18:73:VAL:HG22   | 1.86                     | 0.87              |
| 5:12:97:LEU:HD13    | 6:17:667:TRP:HZ3    | 1.37                     | 0.87              |
| 6:17:422:ASP:CG     | 66:15:135:SER:HB2   | 1.99                     | 0.87              |
| 6:17:264:GLU:OE2    | 65:14:1130:LYS:HD2  | 1.74                     | 0.87              |
| 6:17:693:THR:HB     | 14:9:682:VAL:HG22   | 1.56                     | 0.87              |
| 6:17:261:LYS:HG2    | 65:14:1096:ILE:CB   | 2.03                     | 0.87              |
| 6:17:697:TYR:CZ     | 14:9:636:PHE:O      | 2.28                     | 0.87              |
| 6:17:703:ASN:HB2    | 14:9:663:ASN:CB     | 2.05                     | 0.87              |
| 64:13:290:ASP:CB    | 64:13:511:SER:OG    | 2.23                     | 0.87              |
| 6:17:80:GLY:CA      | 65:14:1268:ASN:HA   | 1.95                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:17:258:ASN:CB    | 65:14:1126:LEU:CD1 | 2.43                     | 0.87              |
| 6:17:422:ASP:CG    | 66:15:135:SER:CB   | 2.48                     | 0.87              |
| 64:13:1020:MET:HB2 | 67:18:256:HIS:CB   | 2.05                     | 0.87              |
| 6:17:422:ASP:OD2   | 66:15:135:SER:HA   | 1.06                     | 0.87              |
| 6:17:700:LEU:HD21  | 14:9:658:LEU:HB3   | 1.54                     | 0.87              |
| 6:17:706:ILE:CG1   | 14:9:659:ASN:N     | 2.38                     | 0.87              |
| 8:3:1485:A:H2      | 8:3:2710:G:H1      | 1.15                     | 0.87              |
| 5:12:88:SER:CB     | 6:17:615:PHE:CZ    | 2.58                     | 0.86              |
| 6:17:598:LYS:HA    | 14:9:678:PHE:CD1   | 2.10                     | 0.86              |
| 6:17:701:THR:HG1   | 14:9:773:ALA:HB1   | 1.41                     | 0.86              |
| 65:14:638:LYS:HE3  | 65:14:668:GLU:OE2  | 1.75                     | 0.86              |
| 6:17:385:ASP:HB2   | 66:15:64:LYS:HB3   | 1.56                     | 0.86              |
| 6:17:699:ILE:O     | 14:9:662:LEU:HB3   | 1.73                     | 0.86              |
| 8:3:519:A:H2       | 14:9:165:LEU:HD13  | 1.32                     | 0.86              |
| 64:13:283:ARG:CG   | 64:13:290:ASP:OD1  | 2.23                     | 0.86              |
| 3:10:275:SER:HB3   | 6:17:970:SER:CA    | 2.04                     | 0.86              |
| 6:17:429:ASP:C     | 66:15:549:LEU:HD22 | 1.99                     | 0.86              |
| 14:9:798:ARG:HH21  | 61:w:18:LEU:CD2    | 1.87                     | 0.86              |
| 41:c:162:ASN:HB3   | 41:c:202:GLU:OE2   | 1.74                     | 0.86              |
| 8:3:102:A:H62      | 14:9:786:MET:HE1   | 1.39                     | 0.86              |
| 6:17:80:GLY:HA3    | 65:14:1268:ASN:CA  | 2.05                     | 0.86              |
| 6:17:385:ASP:H     | 66:15:175:PRO:CB   | 1.84                     | 0.86              |
| 15:A:199:VAL:HG12  | 15:A:213:PHE:HB2   | 1.55                     | 0.86              |
| 6:17:703:ASN:O     | 14:9:785:LEU:HD21  | 1.76                     | 0.86              |
| 8:3:1619:A:H2'     | 8:3:1620:A:C8      | 2.09                     | 0.86              |
| 6:17:430:PRO:HG2   | 66:15:556:GLN:CG   | 2.06                     | 0.85              |
| 6:17:697:TYR:CE2   | 14:9:637:CYS:HA    | 2.11                     | 0.85              |
| 14:9:798:ARG:HD3   | 61:w:22:LEU:CG     | 2.04                     | 0.85              |
| 64:13:1217:LYS:HZ3 | 67:18:274:PRO:HG2  | 1.40                     | 0.85              |
| 14:9:798:ARG:NH1   | 61:w:18:LEU:CA     | 2.36                     | 0.85              |
| 6:17:385:ASP:N     | 66:15:175:PRO:CB   | 2.33                     | 0.85              |
| 6:17:390:ALA:HB2   | 66:15:71:ARG:CZ    | 1.73                     | 0.85              |
| 6:17:690:LEU:C     | 14:9:682:VAL:CG1   | 2.43                     | 0.85              |
| 6:17:695:SER:HA    | 14:9:633:VAL:CG2   | 2.03                     | 0.85              |
| 8:3:1560:U:C4'     | 14:9:249:ASP:H     | 1.66                     | 0.85              |
| 64:13:1062:ARG:CZ  | 67:18:73:VAL:CG2   | 2.53                     | 0.85              |
| 66:15:900:GLN:NE2  | 66:15:934:GLU:HG3  | 1.91                     | 0.85              |
| 66:15:1071:PHE:CB  | 66:15:1247:ARG:NH2 | 2.39                     | 0.85              |
| 5:12:89:LYS:HB3    | 6:17:659:TYR:OH    | 1.76                     | 0.85              |
| 6:17:711:PHE:HB2   | 14:9:651:HIS:CE1   | 2.11                     | 0.85              |
| 12:7:29:G:H5'      | 27:L:117:ALA:CA    | 2.06                     | 0.85              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 65:14:745:GLN:O    | 65:14:751:LYS:CE    | 2.25                     | 0.85              |
| 6:17:706:ILE:HG13  | 14:9:659:ASN:CA     | 2.06                     | 0.85              |
| 6:17:256:THR:H     | 65:14:1100:THR:HA   | 1.42                     | 0.85              |
| 6:17:426:LYS:NZ    | 66:15:183:LEU:HB2   | 1.91                     | 0.85              |
| 6:17:699:ILE:HB    | 14:9:689:ILE:CG1    | 1.74                     | 0.85              |
| 6:17:711:PHE:CZ    | 14:9:642:ASN:CG     | 2.53                     | 0.85              |
| 26:K:57:LYS:HG2    | 37:Y:45:A:H5''      | 1.55                     | 0.85              |
| 18:x:6:HIS:ND1     | 18:x:7:PHE:CE1      | 2.44                     | 0.85              |
| 66:15:877:ARG:CD   | 66:15:1270:ILE:HG21 | 2.07                     | 0.85              |
| 6:17:277:SER:CA    | 65:14:1124:LYS:C    | 2.50                     | 0.85              |
| 8:3:1561:G:OP1     | 14:9:251:TYR:CE2    | 2.29                     | 0.85              |
| 6:17:390:ALA:HB2   | 66:15:71:ARG:HH12   | 1.36                     | 0.85              |
| 6:17:704:ASN:O     | 14:9:659:ASN:C      | 1.99                     | 0.85              |
| 14:9:798:ARG:CZ    | 61:w:18:LEU:C       | 2.50                     | 0.85              |
| 64:13:171:PHE:HB3  | 66:15:1183:LEU:CD1  | 2.07                     | 0.85              |
| 64:13:734:LEU:HD13 | 64:13:885:LYS:O     | 1.76                     | 0.85              |
| 65:14:605:GLU:HA   | 66:15:248:THR:HA    | 1.56                     | 0.85              |
| 5:12:93:THR:O      | 6:17:664:ILE:HG12   | 1.76                     | 0.84              |
| 6:17:264:GLU:OE2   | 65:14:1130:LYS:NZ   | 1.88                     | 0.84              |
| 6:17:845:TRP:CZ2   | 14:9:644:LYS:CB     | 2.56                     | 0.84              |
| 6:17:264:GLU:CA    | 65:14:1096:ILE:O    | 2.24                     | 0.84              |
| 14:9:228:PRO:HG3   | 58:t:52:THR:HG22    | 1.56                     | 0.84              |
| 5:12:97:LEU:HD11   | 6:17:667:TRP:HE3    | 1.38                     | 0.84              |
| 14:9:805:ASN:OD1   | 57:s:96:GLU:OE1     | 1.94                     | 0.84              |
| 6:17:599:ASN:HA    | 14:9:641:ARG:H      | 1.40                     | 0.84              |
| 10:5:1473:U:OP2    | 37:Y:40:U:C4'       | 2.24                     | 0.84              |
| 14:9:275:LYS:CG    | 57:s:22:GLY:HA2     | 2.06                     | 0.84              |
| 66:15:1209:GLU:OE1 | 66:15:1249:TRP:NE1  | 2.10                     | 0.84              |
| 3:10:312:THR:CG2   | 65:14:85:GLN:HE21   | 1.90                     | 0.84              |
| 6:17:277:SER:HB3   | 65:14:1124:LYS:C    | 2.00                     | 0.84              |
| 6:17:703:ASN:C     | 14:9:665:HIS:CD2    | 2.46                     | 0.84              |
| 66:15:1143:LYS:HE3 | 66:15:1194:VAL:HG13 | 1.58                     | 0.84              |
| 65:14:1209:LYS:HE3 | 66:15:250:PHE:HZ    | 0.86                     | 0.84              |
| 6:17:386:VAL:N     | 66:15:175:PRO:C     | 2.34                     | 0.84              |
| 6:17:699:ILE:HB    | 14:9:689:ILE:HG12   | 1.58                     | 0.84              |
| 6:17:706:ILE:HD13  | 14:9:658:LEU:CB     | 1.91                     | 0.84              |
| 6:17:259:GLY:CA    | 65:14:1098:THR:HA   | 2.07                     | 0.84              |
| 6:17:388:ALA:HB3   | 66:15:132:LEU:HD13  | 0.84                     | 0.84              |
| 6:17:431:VAL:O     | 66:15:550:GLU:HA    | 1.76                     | 0.84              |
| 6:17:697:TYR:CE2   | 14:9:636:PHE:O      | 2.29                     | 0.84              |
| 6:17:704:ASN:N     | 14:9:665:HIS:HD2    | 1.56                     | 0.84              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:9:795:GLN:CG     | 61:w:18:LEU:CD1     | 2.55                     | 0.84              |
| 42:d:38:MET:CE      | 42:d:151:GLY:O      | 2.18                     | 0.84              |
| 64:13:1192:LEU:HD11 | 67:18:88:GLN:NE2    | 1.92                     | 0.84              |
| 6:17:598:LYS:HA     | 14:9:678:PHE:CE1    | 2.13                     | 0.84              |
| 6:17:712:ILE:C      | 14:9:675:ASN:N      | 2.31                     | 0.84              |
| 66:15:961:THR:CB    | 66:15:1269:LEU:CD2  | 2.55                     | 0.84              |
| 66:15:1154:GLU:CG   | 67:16:71:GLN:CA     | 2.54                     | 0.84              |
| 6:17:385:ASP:HA     | 66:15:65:ASP:H      | 1.03                     | 0.83              |
| 6:17:701:THR:O      | 14:9:662:LEU:O      | 1.95                     | 0.83              |
| 65:14:605:GLU:CG    | 66:15:248:THR:HG22  | 2.07                     | 0.83              |
| 6:17:706:ILE:O      | 14:9:656:GLU:HG3    | 1.77                     | 0.83              |
| 66:15:1091:PHE:CZ   | 66:15:1247:ARG:HD2  | 2.13                     | 0.83              |
| 6:17:386:VAL:HG22   | 66:15:177:GLY:H     | 1.44                     | 0.83              |
| 6:17:700:LEU:O      | 14:9:661:GLU:HB2    | 1.75                     | 0.83              |
| 66:15:961:THR:C     | 66:15:1269:LEU:HD21 | 2.03                     | 0.83              |
| 5:12:96:LEU:HD22    | 6:17:661:LEU:CB     | 2.08                     | 0.83              |
| 6:17:697:TYR:CE2    | 14:9:637:CYS:N      | 2.47                     | 0.83              |
| 66:15:1105:VAL:CA   | 67:16:254:LYS:HB3   | 2.07                     | 0.83              |
| 8:3:102:A:N6        | 14:9:786:MET:HE3    | 1.91                     | 0.83              |
| 44:f:96:GLN:HE21    | 44:f:121:PHE:HB3    | 1.43                     | 0.83              |
| 64:13:1192:LEU:CD2  | 67:18:88:GLN:HG3    | 2.08                     | 0.83              |
| 6:17:275:ASN:HB3    | 65:14:1125:THR:CA   | 2.08                     | 0.83              |
| 6:17:386:VAL:C      | 66:15:174:ASP:OD1   | 2.20                     | 0.83              |
| 6:17:700:LEU:CD2    | 14:9:658:LEU:CB     | 2.56                     | 0.83              |
| 6:17:710:PHE:CE1    | 14:9:649:VAL:CG2    | 2.50                     | 0.83              |
| 8:3:1558:A:N1       | 14:9:247:LYS:CE     | 2.40                     | 0.83              |
| 56:r:15:GLN:OE1     | 62:y:17:ARG:NH1     | 2.12                     | 0.83              |
| 66:15:396:GLN:HE21  | 66:15:412:GLY:HA2   | 1.42                     | 0.83              |
| 3:10:313:GLU:OE2    | 65:14:88:ARG:NH1    | 2.12                     | 0.83              |
| 6:17:424:VAL:O      | 66:15:184:GLN:NE2   | 2.10                     | 0.83              |
| 6:17:599:ASN:C      | 14:9:638:ASP:OD1    | 2.11                     | 0.83              |
| 8:3:102:A:OP2       | 14:9:779:GLU:HG3    | 1.77                     | 0.83              |
| 8:3:925:C:P         | 27:L:92:ARG:HH11    | 1.99                     | 0.83              |
| 3:10:253:PHE:HE2    | 6:17:15:ILE:CG1     | 1.90                     | 0.83              |
| 17:AB:43:A:C2       | 37:Y:44:A:N6        | 2.46                     | 0.83              |
| 65:14:948:VAL:HG23  | 66:15:247:LYS:HZ2   | 1.44                     | 0.83              |
| 66:15:178:GLU:OE2   | 66:15:632:LYS:NZ    | 2.10                     | 0.83              |
| 3:10:312:THR:CG2    | 65:14:85:GLN:NE2    | 2.41                     | 0.83              |
| 6:17:80:GLY:C       | 65:14:1268:ASN:OD1  | 2.21                     | 0.83              |
| 6:17:261:LYS:HB3    | 65:14:1102:PHE:HB2  | 1.60                     | 0.83              |
| 6:17:696:ASN:N      | 14:9:633:VAL:CG2    | 2.41                     | 0.83              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 64:13:1192:LEU:CD2 | 67:18:88:GLN:HE21   | 1.82                     | 0.83              |
| 6:17:258:ASN:OD1   | 65:14:1126:LEU:HB2  | 1.80                     | 0.82              |
| 6:17:699:ILE:CG2   | 14:9:689:ILE:CA     | 2.26                     | 0.82              |
| 64:13:972:ASN:ND2  | 67:18:256:HIS:NE2   | 2.19                     | 0.82              |
| 64:13:984:GLN:NE2  | 64:13:1133:THR:HG22 | 1.90                     | 0.82              |
| 67:16:105:TRP:HZ3  | 67:16:152:TYR:HD2   | 1.27                     | 0.82              |
| 65:14:608:ASN:HD22 | 66:15:251:ASP:N     | 1.71                     | 0.82              |
| 6:17:428:GLY:C     | 66:15:549:LEU:CD2   | 2.52                     | 0.82              |
| 8:3:2465:U:H3      | 8:3:2502:G:H1       | 0.86                     | 0.82              |
| 10:5:1473:U:OP2    | 37:Y:40:U:H4'       | 1.79                     | 0.82              |
| 14:9:188:ARG:HD2   | 58:t:59:SER:HG      | 1.44                     | 0.82              |
| 54:p:68:LEU:HD12   | 54:p:73:MET:HG2     | 1.61                     | 0.82              |
| 6:17:264:GLU:H     | 65:14:1097:GLN:HA   | 1.41                     | 0.82              |
| 6:17:430:PRO:HD3   | 66:15:555:PHE:HD1   | 1.39                     | 0.82              |
| 14:9:451:GLN:O     | 62:y:56:ALA:N       | 2.10                     | 0.82              |
| 64:13:358:LYS:NZ   | 64:13:374:ASN:O     | 2.12                     | 0.82              |
| 6:17:264:GLU:N     | 65:14:1097:GLN:N    | 2.22                     | 0.82              |
| 6:17:428:GLY:C     | 66:15:549:LEU:HD22  | 2.04                     | 0.82              |
| 6:17:711:PHE:CZ    | 14:9:642:ASN:OD1    | 2.32                     | 0.82              |
| 17:AB:44:A:C4      | 37:Y:45:A:C5        | 2.67                     | 0.82              |
| 66:15:1209:GLU:HG2 | 66:15:1249:TRP:CD1  | 2.15                     | 0.82              |
| 6:17:690:LEU:CA    | 14:9:682:VAL:HG21   | 2.10                     | 0.82              |
| 6:17:706:ILE:CG1   | 14:9:659:ASN:H      | 1.92                     | 0.82              |
| 42:d:40:VAL:HG22   | 42:d:42:ASP:H       | 1.42                     | 0.82              |
| 18:x:6:HIS:CE1     | 18:x:7:PHE:CE1      | 2.66                     | 0.82              |
| 6:17:710:PHE:CD2   | 14:9:654:LEU:HD23   | 2.13                     | 0.82              |
| 14:9:163:PRO:CG    | 58:t:63:VAL:HG23    | 2.09                     | 0.82              |
| 6:17:712:ILE:HG13  | 14:9:651:HIS:NE2    | 1.95                     | 0.82              |
| 6:17:845:TRP:HZ2   | 14:9:644:LYS:HB3    | 1.45                     | 0.82              |
| 6:17:264:GLU:N     | 65:14:1096:ILE:O    | 2.12                     | 0.82              |
| 6:17:710:PHE:CE2   | 14:9:673:PHE:HB3    | 2.15                     | 0.82              |
| 66:15:1219:MET:HE2 | 66:15:1247:ARG:HH21 | 1.45                     | 0.82              |
| 17:AB:40:U:O2      | 37:Y:41:U:C5        | 2.33                     | 0.81              |
| 6:17:261:LYS:CB    | 65:14:1102:PHE:HB2  | 2.10                     | 0.81              |
| 10:5:528:G:N3      | 13:8:35:U:C2'       | 2.23                     | 0.81              |
| 14:9:13:ARG:NE     | 14:9:376:PHE:CD2    | 2.48                     | 0.81              |
| 17:AB:41:U:C2'     | 37:Y:42:C:C5        | 2.60                     | 0.81              |
| 66:15:838:GLU:HG2  | 66:15:956:LEU:HD12  | 1.62                     | 0.81              |
| 66:15:877:ARG:CD   | 66:15:1270:ILE:CG2  | 2.58                     | 0.81              |
| 6:17:252:SER:N     | 65:14:1104:ALA:HB2  | 1.79                     | 0.81              |
| 6:17:262:SER:HB2   | 65:14:1098:THR:OG1  | 1.80                     | 0.81              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:17:277:SER:HB3    | 65:14:1125:THR:N    | 1.94                     | 0.81              |
| 6:17:698:SER:C      | 14:9:689:ILE:CG2    | 2.50                     | 0.81              |
| 6:17:703:ASN:HB3    | 14:9:785:LEU:HG     | 1.62                     | 0.81              |
| 17:AB:45:A:O3'      | 37:Y:45:A:O3'       | 1.74                     | 0.81              |
| 64:13:7:SER:N       | 67:18:198:LEU:HD11  | 1.95                     | 0.81              |
| 66:15:82:GLU:OE2    | 66:15:120:LYS:HE2   | 1.80                     | 0.81              |
| 10:5:1467:A:C2      | 37:Y:44:A:H2        | 1.95                     | 0.81              |
| 17:AB:45:A:C5'      | 37:Y:45:A:C8        | 2.63                     | 0.81              |
| 8:3:881:A:H1'       | 8:3:882:C:H5''      | 1.61                     | 0.81              |
| 10:5:1467:A:H2      | 37:Y:44:A:C2        | 1.98                     | 0.81              |
| 6:17:706:ILE:CD1    | 14:9:658:LEU:HB3    | 2.10                     | 0.81              |
| 57:s:25:LYS:HE3     | 57:s:90:ALA:HB2     | 1.61                     | 0.81              |
| 64:13:1062:ARG:HH11 | 67:18:72:ALA:C      | 1.84                     | 0.81              |
| 6:17:701:THR:HG21   | 14:9:774:ASN:OD1    | 1.79                     | 0.81              |
| 6:17:706:ILE:CD1    | 14:9:658:LEU:C      | 2.49                     | 0.81              |
| 6:17:711:PHE:CD2    | 14:9:650:ASN:CA     | 2.45                     | 0.81              |
| 8:3:925:C:OP2       | 27:L:92:ARG:NH1     | 2.12                     | 0.81              |
| 64:13:924:LYS:HZ2   | 67:18:79:ALA:CB     | 1.92                     | 0.81              |
| 65:14:209:VAL:HG23  | 65:14:467:HIS:ND1   | 1.95                     | 0.81              |
| 65:14:68:ARG:NH1    | 65:14:126:ASP:OD1   | 2.13                     | 0.81              |
| 66:15:965:LEU:HB3   | 66:15:1265:LEU:CD2  | 2.11                     | 0.81              |
| 6:17:428:GLY:N      | 66:15:141:VAL:CG2   | 2.34                     | 0.81              |
| 65:14:1122:LYS:N    | 66:15:150:PHE:CE1   | 2.49                     | 0.81              |
| 6:17:426:LYS:NZ     | 66:15:183:LEU:N     | 2.27                     | 0.81              |
| 6:17:691:THR:OG1    | 14:9:683:HIS:CE1    | 2.33                     | 0.81              |
| 6:17:693:THR:O      | 14:9:633:VAL:HG13   | 1.81                     | 0.81              |
| 14:9:808:GLN:CB     | 57:s:48:TYR:O       | 2.27                     | 0.80              |
| 6:17:425:ALA:HB3    | 66:15:140:ASN:H     | 1.45                     | 0.80              |
| 6:17:376:LYS:HZ2    | 66:15:178:GLU:CG    | 1.54                     | 0.80              |
| 64:13:1194:LEU:HD23 | 64:13:1197:ILE:HD11 | 1.62                     | 0.80              |
| 64:13:1217:LYS:HE2  | 67:18:275:LEU:O     | 1.80                     | 0.80              |
| 66:15:434:THR:HG22  | 66:15:489:THR:HG21  | 1.62                     | 0.80              |
| 66:15:877:ARG:CZ    | 66:15:1270:ILE:CG2  | 2.58                     | 0.80              |
| 64:13:811:ALA:HB1   | 64:13:901:ILE:HG22  | 1.62                     | 0.80              |
| 65:14:1122:LYS:H    | 66:15:150:PHE:HE1   | 1.27                     | 0.80              |
| 66:15:847:PHE:CD2   | 66:15:963:MET:HE1   | 2.17                     | 0.80              |
| 6:17:373:VAL:HB     | 66:15:172:PRO:CG    | 2.11                     | 0.80              |
| 52:n:29:VAL:HG21    | 52:n:46:PHE:CD1     | 2.15                     | 0.80              |
| 64:13:1062:ARG:HH11 | 67:18:73:VAL:CA     | 1.93                     | 0.80              |
| 6:17:692:LYS:HE3    | 14:9:683:HIS:CD2    | 2.15                     | 0.80              |
| 8:3:102:A:N7        | 14:9:786:MET:HG2    | 1.97                     | 0.80              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:9:451:GLN:O     | 62:y:56:ALA:CB      | 2.30                     | 0.80              |
| 3:10:227:ILE:CD1   | 6:17:112:VAL:H      | 1.93                     | 0.80              |
| 6:17:387:VAL:HA    | 66:15:68:ILE:HG13   | 1.64                     | 0.80              |
| 42:d:165:GLU:OE1   | 42:d:165:GLU:HA     | 1.80                     | 0.80              |
| 18:x:6:HIS:ND1     | 18:x:7:PHE:CD1      | 2.50                     | 0.80              |
| 65:14:610:ILE:HB   | 66:15:248:THR:HB    | 1.57                     | 0.80              |
| 66:15:962:LEU:CA   | 66:15:1269:LEU:CD1  | 2.60                     | 0.80              |
| 6:17:595:ARG:NH2   | 14:9:644:LYS:NZ     | 2.19                     | 0.79              |
| 17:AB:41:U:C2      | 37:Y:42:C:C5        | 2.70                     | 0.79              |
| 66:15:839:TRP:NE1  | 66:15:843:ASN:ND2   | 2.30                     | 0.79              |
| 6:17:261:LYS:HB2   | 65:14:1126:LEU:CG   | 2.11                     | 0.79              |
| 6:17:388:ALA:H     | 66:15:68:ILE:CD1    | 1.95                     | 0.79              |
| 6:17:693:THR:HG23  | 14:9:681:THR:C      | 2.07                     | 0.79              |
| 10:5:1467:A:C2     | 37:Y:44:A:N3        | 2.49                     | 0.79              |
| 17:AB:40:U:H2'     | 37:Y:41:U:C5        | 2.16                     | 0.79              |
| 50:l:32:TYR:HD2    | 50:l:114:MET:HE3    | 1.47                     | 0.79              |
| 3:10:238:PHE:CZ    | 6:17:559:PHE:CD1    | 2.58                     | 0.79              |
| 6:17:689:ALA:C     | 14:9:682:VAL:HB     | 2.07                     | 0.79              |
| 14:9:13:ARG:NE     | 14:9:376:PHE:CE2    | 2.50                     | 0.79              |
| 10:5:1438:U:OP1    | 53:o:110:LYS:CE     | 2.31                     | 0.79              |
| 66:15:343:LYS:HE3  | 66:15:439:MET:SD    | 2.23                     | 0.79              |
| 6:17:426:LYS:HB2   | 66:15:184:GLN:HB3   | 1.57                     | 0.79              |
| 6:17:701:THR:O     | 14:9:662:LEU:CA     | 2.28                     | 0.79              |
| 8:3:102:A:C6       | 14:9:786:MET:HE3    | 2.17                     | 0.79              |
| 6:17:387:VAL:HA    | 66:15:68:ILE:HD12   | 1.60                     | 0.79              |
| 6:17:706:ILE:HG13  | 14:9:659:ASN:N      | 1.98                     | 0.79              |
| 6:17:707:GLN:OE1   | 14:9:669:SER:CA     | 2.30                     | 0.79              |
| 21:F:69:MET:HG2    | 21:F:95:LYS:HG2     | 1.63                     | 0.79              |
| 26:K:42:LEU:HD13   | 26:K:94:LEU:HD21    | 1.62                     | 0.79              |
| 54:p:66:ALA:O      | 54:p:70:GLU:OE1     | 2.00                     | 0.79              |
| 65:14:948:VAL:HG23 | 66:15:247:LYS:CD    | 2.13                     | 0.79              |
| 14:9:188:ARG:CD    | 58:t:57:LYS:CG      | 2.58                     | 0.79              |
| 8:3:1561:G:O2'     | 14:9:299:LYS:HD3    | 1.82                     | 0.79              |
| 14:9:704:ILE:HD13  | 58:t:6:LYS:HE2      | 1.63                     | 0.79              |
| 42:d:146:ILE:HG22  | 42:d:148:ARG:H      | 1.48                     | 0.79              |
| 5:12:96:LEU:HD22   | 6:17:661:LEU:HB2    | 1.64                     | 0.79              |
| 6:17:258:ASN:HB2   | 65:14:1099:GLN:NE2  | 1.71                     | 0.79              |
| 46:h:105:ALA:HA    | 46:h:123:MET:CE     | 2.13                     | 0.79              |
| 65:14:316:LYS:HE3  | 65:14:454:GLN:HE21  | 1.47                     | 0.79              |
| 66:15:954:LYS:HB3  | 66:15:1274:LEU:HD23 | 1.65                     | 0.79              |
| 67:18:105:TRP:HZ3  | 67:18:152:TYR:HD2   | 1.26                     | 0.79              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:17:385:ASP:O      | 66:15:65:ASP:HB2    | 1.82                     | 0.79              |
| 8:3:1561:G:O3'      | 14:9:299:LYS:HA     | 1.83                     | 0.79              |
| 12:7:43:C:H2'       | 12:7:44:G:C8        | 2.18                     | 0.79              |
| 31:P:61:VAL:HG12    | 31:P:80:ILE:HG12    | 1.65                     | 0.79              |
| 66:15:1154:GLU:OE1  | 67:16:72:ALA:CA     | 2.31                     | 0.79              |
| 5:12:100:LEU:HD21   | 6:17:668:LEU:CD1    | 2.12                     | 0.78              |
| 5:12:100:LEU:HD21   | 6:17:668:LEU:HD13   | 1.66                     | 0.78              |
| 6:17:258:ASN:OD1    | 65:14:1126:LEU:CB   | 2.30                     | 0.78              |
| 6:17:275:ASN:HB3    | 65:14:1126:LEU:N    | 1.98                     | 0.78              |
| 14:9:798:ARG:CZ     | 61:w:21:LYS:HB3     | 2.12                     | 0.78              |
| 17:AB:44:A:C5       | 37:Y:45:A:C6        | 2.71                     | 0.78              |
| 8:3:102:A:N7        | 14:9:786:MET:CE     | 2.45                     | 0.78              |
| 8:3:1560:U:H4'      | 14:9:249:ASP:N      | 1.89                     | 0.78              |
| 10:5:1473:U:O4      | 37:Y:41:U:C4'       | 2.28                     | 0.78              |
| 14:9:795:GLN:CD     | 61:w:18:LEU:HG      | 2.08                     | 0.78              |
| 66:15:1251:MET:SD   | 66:15:1256:PRO:HD3  | 2.23                     | 0.78              |
| 5:12:96:LEU:CD2     | 6:17:661:LEU:CA     | 2.61                     | 0.78              |
| 6:17:251:ASP:OD1    | 65:14:1105:LEU:CA   | 2.31                     | 0.78              |
| 10:5:528:G:C4       | 13:8:35:U:C1'       | 2.53                     | 0.78              |
| 64:13:7:SER:H       | 67:18:198:LEU:HD11  | 1.49                     | 0.78              |
| 64:13:1126:ARG:HH11 | 65:14:152:LYS:HZ1   | 1.28                     | 0.78              |
| 66:15:961:THR:HB    | 66:15:1269:LEU:HD22 | 1.66                     | 0.78              |
| 3:10:253:PHE:HE2    | 6:17:15:ILE:CD1     | 1.66                     | 0.78              |
| 5:12:86:VAL:HB      | 6:17:15:ILE:CD1     | 2.09                     | 0.78              |
| 14:9:798:ARG:CD     | 61:w:22:LEU:HG      | 2.10                     | 0.78              |
| 20:E:84:ARG:NH1     | 32:Q:95:TYR:O       | 2.16                     | 0.78              |
| 17:AB:40:U:H2'      | 37:Y:41:U:H6        | 1.46                     | 0.78              |
| 65:14:46:ALA:HB2    | 65:14:527:ILE:HD13  | 1.65                     | 0.78              |
| 66:15:33:VAL:HA     | 66:15:832:ILE:CD1   | 2.13                     | 0.78              |
| 8:3:47:G:H5''       | 8:3:48:G:H5'        | 1.63                     | 0.78              |
| 8:3:2312:G:H22      | 8:3:2320:U:H3       | 1.29                     | 0.78              |
| 41:c:130:GLN:NE2    | 41:c:200:GLU:OE2    | 2.17                     | 0.78              |
| 65:14:1122:LYS:HB2  | 66:15:150:PHE:CZ    | 2.18                     | 0.78              |
| 65:14:1209:LYS:CE   | 66:15:250:PHE:CE2   | 2.66                     | 0.78              |
| 66:15:900:GLN:HE21  | 66:15:934:GLU:HG3   | 1.46                     | 0.78              |
| 6:17:710:PHE:C      | 14:9:649:VAL:O      | 2.26                     | 0.78              |
| 8:3:1095:U:H5''     | 46:h:68:LYS:HE2     | 1.66                     | 0.78              |
| 8:3:1561:G:H1'      | 14:9:299:LYS:NZ     | 1.98                     | 0.78              |
| 33:R:11:VAL:HG12    | 33:R:38:SER:HB3     | 1.64                     | 0.78              |
| 65:14:1032:GLN:NE2  | 66:15:540:ASN:CG    | 2.41                     | 0.78              |
| 3:10:312:THR:HG22   | 65:14:85:GLN:HE21   | 1.46                     | 0.78              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 17:AB:41:U:N3       | 37:Y:42:C:C4        | 2.52                     | 0.78              |
| 8:3:1559:A:C2'      | 14:9:247:LYS:HD3    | 2.13                     | 0.78              |
| 8:3:1561:G:H1'      | 14:9:299:LYS:HZ2    | 1.49                     | 0.78              |
| 61:w:20:ILE:HD12    | 61:w:21:LYS:N       | 1.98                     | 0.78              |
| 14:9:228:PRO:CG     | 58:t:53:LYS:H       | 1.93                     | 0.78              |
| 17:AB:44:A:C2       | 37:Y:45:A:N1        | 2.52                     | 0.78              |
| 6:17:362:TYR:CE2    | 65:14:1098:THR:CG2  | 2.67                     | 0.77              |
| 66:15:707:ARG:HE    | 66:15:711:GLY:HA2   | 1.48                     | 0.77              |
| 6:17:258:ASN:HB3    | 65:14:1126:LEU:CD1  | 2.11                     | 0.77              |
| 6:17:704:ASN:C      | 14:9:665:HIS:CD2    | 2.56                     | 0.77              |
| 45:g:29:TYR:HA      | 45:g:32:MET:CE      | 2.15                     | 0.77              |
| 64:13:1020:MET:HB3  | 67:18:256:HIS:HA    | 0.98                     | 0.77              |
| 6:17:426:LYS:HZ3    | 66:15:183:LEU:H     | 1.30                     | 0.77              |
| 17:AB:40:U:O4'      | 37:Y:40:U:O4'       | 1.69                     | 0.77              |
| 6:17:955:LYS:HZ2    | 14:9:799:GLU:CG     | 1.67                     | 0.77              |
| 14:9:164:HIS:CB     | 58:t:62:LYS:O       | 2.18                     | 0.77              |
| 14:9:788:ALA:N      | 61:w:6:GLU:CG       | 2.47                     | 0.77              |
| 5:12:84:VAL:HA      | 6:17:8:SER:N        | 2.00                     | 0.77              |
| 6:17:387:VAL:C      | 66:15:68:ILE:HD11   | 2.08                     | 0.77              |
| 64:13:1192:LEU:HD11 | 67:18:88:GLN:HE21   | 1.49                     | 0.77              |
| 6:17:260:GLN:C      | 65:14:1126:LEU:HD21 | 2.06                     | 0.77              |
| 40:b:227:GLU:HG3    | 53:o:19:LYS:HD2     | 1.67                     | 0.77              |
| 47:i:136:GLU:OE2    | 47:i:136:GLU:N      | 2.13                     | 0.77              |
| 14:9:808:GLN:CB     | 61:w:79:THR:HG21    | 2.15                     | 0.77              |
| 6:17:693:THR:C      | 14:9:633:VAL:CG1    | 2.56                     | 0.77              |
| 6:17:698:SER:HB2    | 14:9:769:ILE:HG23   | 1.65                     | 0.77              |
| 39:a:179:TYR:HB3    | 39:a:191:LYS:HB3    | 1.66                     | 0.77              |
| 42:d:104:ILE:HA     | 42:d:108:LEU:HD12   | 1.65                     | 0.77              |
| 65:14:316:LYS:HE2   | 65:14:454:GLN:NE2   | 2.00                     | 0.77              |
| 6:17:427:ASN:OD1    | 66:15:168:VAL:N     | 2.10                     | 0.77              |
| 6:17:595:ARG:NH2    | 14:9:644:LYS:HZ3    | 1.81                     | 0.77              |
| 17:AB:45:A:N6       | 37:Y:45:A:N6        | 2.26                     | 0.77              |
| 17:AB:44:A:C4       | 37:Y:45:A:C6        | 2.72                     | 0.77              |
| 6:17:256:THR:HG23   | 65:14:1100:THR:O    | 1.84                     | 0.76              |
| 64:13:986:ILE:HG13  | 64:13:1130:PRO:HB2  | 1.66                     | 0.76              |
| 65:14:52:VAL:CG2    | 65:14:563:ILE:HD12  | 2.14                     | 0.76              |
| 29:N:26:VAL:HG11    | 29:N:78:LEU:HD21    | 1.64                     | 0.76              |
| 18:x:6:HIS:CE1      | 18:x:7:PHE:HE1      | 2.03                     | 0.76              |
| 65:14:605:GLU:HA    | 66:15:248:THR:CA    | 2.14                     | 0.76              |
| 6:17:277:SER:CB     | 65:14:1125:THR:N    | 2.48                     | 0.76              |
| 10:5:1468:A:HO2'    | 37:Y:43:A:H1'       | 1.50                     | 0.76              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:9:795:GLN:HG2   | 61:w:18:LEU:CD1     | 2.15                     | 0.76              |
| 66:15:1208:PHE:CD2 | 66:15:1216:LYS:HE3  | 2.19                     | 0.76              |
| 66:15:1271:ARG:NH2 | 67:16:256:HIS:HD2   | 1.83                     | 0.76              |
| 8:3:530:G:N3       | 56:r:61:ASN:ND2     | 2.33                     | 0.76              |
| 17:AB:44:A:C6      | 37:Y:45:A:C6        | 2.73                     | 0.76              |
| 27:L:119:LYS:HA    | 33:R:86:ASN:OD1     | 1.86                     | 0.76              |
| 65:14:610:ILE:N    | 66:15:248:THR:HB    | 2.00                     | 0.76              |
| 66:15:847:PHE:CD2  | 66:15:963:MET:CE    | 2.69                     | 0.76              |
| 8:3:1561:G:C2'     | 14:9:299:LYS:HD2    | 2.13                     | 0.76              |
| 14:9:807:GLY:O     | 61:w:78:LYS:HB3     | 1.85                     | 0.76              |
| 42:d:49:PHE:HZ     | 42:d:147:LYS:HB2    | 1.51                     | 0.76              |
| 14:9:798:ARG:HH11  | 61:w:21:LYS:H       | 1.33                     | 0.76              |
| 14:9:801:HIS:CD2   | 61:w:24:GLY:O       | 2.33                     | 0.76              |
| 6:17:696:ASN:N     | 14:9:686:HIS:HA     | 2.01                     | 0.76              |
| 10:5:169:G:N2      | 10:5:219:A:O2'      | 2.19                     | 0.76              |
| 10:5:369:A:O2'     | 10:5:448:A:N7       | 2.17                     | 0.76              |
| 66:15:68:ILE:HD12  | 66:15:176:ASN:ND2   | 2.01                     | 0.76              |
| 6:17:80:GLY:HA3    | 65:14:1268:ASN:CG   | 2.09                     | 0.76              |
| 6:17:259:GLY:O     | 65:14:1098:THR:CB   | 2.33                     | 0.76              |
| 66:15:326:GLN:OE1  | 66:15:432:ARG:NH1   | 2.17                     | 0.76              |
| 66:15:962:LEU:CA   | 66:15:1269:LEU:HD11 | 2.12                     | 0.76              |
| 14:9:275:LYS:HB2   | 57:s:22:GLY:HA2     | 1.68                     | 0.76              |
| 6:17:386:VAL:HG13  | 66:15:174:ASP:OD1   | 1.82                     | 0.76              |
| 65:14:609:GLN:N    | 66:15:248:THR:O     | 2.15                     | 0.76              |
| 3:10:275:SER:HB3   | 6:17:970:SER:HB2    | 0.76                     | 0.75              |
| 6:17:373:VAL:C     | 66:15:172:PRO:C     | 2.52                     | 0.75              |
| 8:3:1561:G:C8      | 14:9:248:GLU:HG3    | 2.21                     | 0.75              |
| 34:S:60:ILE:HD11   | 34:S:64:ARG:HD3     | 1.68                     | 0.75              |
| 47:i:3:LYS:HG3     | 47:i:4:THR:H        | 1.49                     | 0.75              |
| 66:15:961:THR:HG22 | 66:15:1269:LEU:HD21 | 1.67                     | 0.75              |
| 66:15:965:LEU:HD12 | 66:15:1269:LEU:HG   | 1.67                     | 0.75              |
| 66:15:1106:SER:N   | 67:16:254:LYS:HB2   | 1.99                     | 0.75              |
| 3:10:227:ILE:HD11  | 6:17:112:VAL:O      | 1.86                     | 0.75              |
| 6:17:700:LEU:HD22  | 14:9:658:LEU:CB     | 2.17                     | 0.75              |
| 8:3:1485:A:C2      | 8:3:2710:G:N1       | 2.54                     | 0.75              |
| 36:W:61:THR:HG22   | 36:W:62:GLN:H       | 1.51                     | 0.75              |
| 58:t:1:MET:HG2     | 58:t:2:GLN:H        | 1.51                     | 0.75              |
| 64:13:195:ASP:OD2  | 64:13:329:LYS:NZ    | 2.19                     | 0.75              |
| 65:14:677:LYS:NZ   | 65:14:834:GLU:O     | 2.19                     | 0.75              |
| 66:15:958:PHE:CA   | 66:15:1273:VAL:HG11 | 2.17                     | 0.75              |
| 6:17:599:ASN:HA    | 14:9:641:ARG:N      | 2.00                     | 0.75              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:709:ASP:N     | 14:9:670:PRO:HB3    | 2.00                     | 0.75              |
| 8:3:427:A:H1'      | 8:3:447:G:O4'       | 1.86                     | 0.75              |
| 64:13:1018:SER:HB2 | 67:18:258:VAL:CG1   | 2.16                     | 0.75              |
| 6:17:264:GLU:N     | 65:14:1097:GLN:CA   | 2.42                     | 0.75              |
| 10:5:1468:A:N3     | 37:Y:43:A:C2        | 2.53                     | 0.75              |
| 43:e:16:VAL:HA     | 43:e:28:LYS:O       | 1.85                     | 0.75              |
| 6:17:387:VAL:CB    | 66:15:68:ILE:HG13   | 2.16                     | 0.75              |
| 66:15:930:GLN:OE1  | 66:15:935:LEU:HD21  | 1.86                     | 0.75              |
| 6:17:690:LEU:O     | 14:9:682:VAL:HG21   | 1.85                     | 0.75              |
| 17:AB:44:A:C2      | 37:Y:45:A:C2        | 2.74                     | 0.75              |
| 53:o:15:GLN:HA     | 53:o:18:LEU:HD12    | 1.68                     | 0.75              |
| 58:t:90:LYS:HG3    | 58:t:105:LYS:HG2    | 1.66                     | 0.75              |
| 66:15:839:TRP:CE2  | 66:15:843:ASN:ND2   | 2.54                     | 0.75              |
| 66:15:1103:GLN:CD  | 67:16:259:GLN:C     | 2.39                     | 0.75              |
| 6:17:700:LEU:C     | 14:9:661:GLU:C      | 2.55                     | 0.75              |
| 8:3:788:G:N2       | 51:m:3:TYR:OH       | 2.20                     | 0.75              |
| 8:3:1561:G:O3'     | 14:9:299:LYS:HD2    | 1.87                     | 0.75              |
| 64:13:1213:LEU:HB2 | 67:18:276:ASN:CG    | 2.12                     | 0.75              |
| 6:17:800:LEU:CD1   | 6:17:839:ILE:HD11   | 2.17                     | 0.75              |
| 12:7:52:G:N2       | 12:7:62:C:O2        | 2.13                     | 0.75              |
| 64:13:1213:LEU:HB3 | 67:18:276:ASN:HB3   | 0.78                     | 0.75              |
| 3:10:431:MET:HE2   | 6:17:667:TRP:HH2    | 1.45                     | 0.74              |
| 6:17:386:VAL:CB    | 66:15:174:ASP:OD1   | 2.36                     | 0.74              |
| 13:8:34:U8U:C4     | 17:AB:44:A:H61      | 2.00                     | 0.74              |
| 66:15:1103:GLN:HA  | 67:16:259:GLN:HG3   | 1.69                     | 0.74              |
| 8:3:2308:U:H2'     | 8:3:2309:A:H8       | 1.52                     | 0.74              |
| 14:9:13:ARG:NH1    | 14:9:376:PHE:CD1    | 2.55                     | 0.74              |
| 3:10:235:ILE:CD1   | 6:17:564:GLY:HA3    | 2.16                     | 0.74              |
| 6:17:702:GLU:HG2   | 14:9:663:ASN:HD21   | 1.43                     | 0.74              |
| 6:17:710:PHE:CE2   | 14:9:673:PHE:CG     | 2.75                     | 0.74              |
| 6:17:387:VAL:HG11  | 66:15:67:ASN:CB     | 2.18                     | 0.74              |
| 6:17:691:THR:OG1   | 14:9:683:HIS:HE1    | 1.70                     | 0.74              |
| 6:17:700:LEU:HD23  | 14:9:662:LEU:HB2    | 1.69                     | 0.74              |
| 8:3:1560:U:C5'     | 14:9:248:GLU:C      | 2.44                     | 0.74              |
| 41:c:5:LYS:HD2     | 41:c:13:PHE:HD2     | 1.49                     | 0.74              |
| 8:3:1619:A:H2'     | 8:3:1620:A:H8       | 1.53                     | 0.74              |
| 17:AB:43:A:C2'     | 37:Y:43:A:C4        | 2.48                     | 0.74              |
| 64:13:868:ASN:HD22 | 64:13:1002:GLN:HE21 | 1.33                     | 0.74              |
| 64:13:1062:ARG:NH1 | 67:18:73:VAL:HG23   | 2.02                     | 0.74              |
| 14:9:313:LYS:CE    | 38:Z:1:UNK:O        | 2.36                     | 0.74              |
| 14:9:795:GLN:CD    | 61:w:18:LEU:HD11    | 2.12                     | 0.74              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:A:182:VAL:HG23   | 15:A:206:THR:HG22   | 1.70                     | 0.74              |
| 6:17:703:ASN:C      | 14:9:663:ASN:HA     | 1.88                     | 0.74              |
| 14:9:808:GLN:HA     | 61:w:79:THR:CB      | 2.17                     | 0.74              |
| 64:13:1217:LYS:NZ   | 67:18:274:PRO:CB    | 2.51                     | 0.74              |
| 6:17:595:ARG:HH22   | 14:9:644:LYS:HZ3    | 1.35                     | 0.74              |
| 8:3:436:G:O6        | 60:v:56:ARG:NH2     | 2.21                     | 0.74              |
| 13:8:35:U:C2        | 17:AB:44:A:C2       | 2.75                     | 0.74              |
| 14:9:452:GLU:HA     | 62:y:55:LYS:HB2     | 1.69                     | 0.74              |
| 66:15:1103:GLN:OE1  | 67:16:259:GLN:O     | 2.05                     | 0.74              |
| 3:10:227:ILE:HD12   | 6:17:112:VAL:N      | 2.03                     | 0.73              |
| 3:10:235:ILE:CD1    | 6:17:564:GLY:CA     | 2.62                     | 0.73              |
| 8:3:316:C:H2'       | 8:3:392:A:H61       | 1.53                     | 0.73              |
| 8:3:1029:A:OP1      | 54:p:49:ARG:NH1     | 2.21                     | 0.73              |
| 8:3:1031:U:O2'      | 54:p:92:LYS:NZ      | 2.21                     | 0.73              |
| 8:3:1485:A:N1       | 8:3:2710:G:O6       | 2.20                     | 0.73              |
| 64:13:171:PHE:HB2   | 66:15:1183:LEU:HD11 | 1.69                     | 0.73              |
| 64:13:1192:LEU:CG   | 67:18:88:GLN:NE2    | 2.50                     | 0.73              |
| 66:15:1207:LYS:HE2  | 66:15:1252:SER:CB   | 2.18                     | 0.73              |
| 6:17:598:LYS:CG     | 14:9:641:ARG:NH2    | 2.09                     | 0.73              |
| 6:17:700:LEU:O      | 14:9:662:LEU:N      | 2.19                     | 0.73              |
| 14:9:13:ARG:NH1     | 14:9:376:PHE:CE1    | 2.55                     | 0.73              |
| 14:9:164:HIS:O      | 58:t:62:LYS:HD2     | 1.59                     | 0.73              |
| 64:13:20:PHE:HB3    | 64:13:1209:ILE:HD11 | 1.71                     | 0.73              |
| 65:14:934:GLN:OE1   | 65:14:1004:LYS:HD3  | 1.88                     | 0.73              |
| 5:12:92:ILE:HG22    | 6:17:660:GLY:CA     | 1.80                     | 0.73              |
| 6:17:251:ASP:OD1    | 65:14:1104:ALA:O    | 2.06                     | 0.73              |
| 14:9:313:LYS:HE3    | 38:Z:1:UNK:O        | 1.89                     | 0.73              |
| 27:L:71:ARG:NH2     | 42:d:112:ARG:HE     | 1.86                     | 0.73              |
| 64:13:1062:ARG:NH1  | 67:18:73:VAL:HA     | 2.01                     | 0.73              |
| 65:14:209:VAL:CG2   | 65:14:467:HIS:CE1   | 2.70                     | 0.73              |
| 65:14:605:GLU:HA    | 66:15:248:THR:CB    | 2.19                     | 0.73              |
| 66:15:1103:GLN:NE2  | 67:16:259:GLN:C     | 2.46                     | 0.73              |
| 8:3:1561:G:C1'      | 14:9:299:LYS:HZ2    | 2.01                     | 0.73              |
| 10:5:1473:U:C1'     | 37:Y:41:U:OP1       | 2.36                     | 0.73              |
| 14:9:795:GLN:CD     | 61:w:18:LEU:CG      | 2.61                     | 0.73              |
| 64:13:1018:SER:HB2  | 67:18:258:VAL:HG13  | 1.60                     | 0.73              |
| 66:15:1271:ARG:HH22 | 67:16:256:HIS:CD2   | 2.05                     | 0.73              |
| 6:17:429:ASP:N      | 66:15:167:PHE:CE1   | 2.19                     | 0.73              |
| 17:AB:44:A:C2       | 37:Y:45:A:C6        | 2.76                     | 0.73              |
| 64:13:702:TRP:HE1   | 64:13:736:ASN:HD22  | 1.36                     | 0.73              |
| 65:14:1209:LYS:HE3  | 66:15:250:PHE:CE2   | 2.22                     | 0.73              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:10:275:SER:CB     | 6:17:970:SER:HB3    | 2.12                     | 0.73              |
| 14:9:798:ARG:HA     | 61:w:25:GLU:HG3     | 1.71                     | 0.73              |
| 48:j:90:ASP:O       | 48:j:91:LYS:HB2     | 1.88                     | 0.73              |
| 65:14:316:LYS:CG    | 65:14:454:GLN:NE2   | 2.51                     | 0.73              |
| 55:q:40:MET:HG3     | 55:q:45:ILE:HB      | 1.70                     | 0.73              |
| 66:15:1105:VAL:HG11 | 67:16:253:VAL:O     | 1.86                     | 0.73              |
| 6:17:941:VAL:HG13   | 6:17:945:ILE:HD12   | 1.70                     | 0.73              |
| 64:13:1204:ILE:CD1  | 64:13:1213:LEU:HD11 | 2.19                     | 0.73              |
| 65:14:1124:LYS:HB3  | 65:14:1128:GLU:OE2  | 1.87                     | 0.73              |
| 6:17:383:ALA:CA     | 66:15:64:LYS:HZ3    | 2.02                     | 0.73              |
| 6:17:695:SER:C      | 14:9:686:HIS:CA     | 2.58                     | 0.73              |
| 8:3:2736:U:HO2'     | 8:3:2737:G:H8       | 1.37                     | 0.73              |
| 10:5:681:U:H1'      | 25:J:33:ASN:HA      | 1.70                     | 0.73              |
| 15:A:82:ILE:HG22    | 15:A:175:LEU:HB3    | 1.69                     | 0.73              |
| 12:7:35:A:N6        | 17:AB:41:U:H3       | 1.86                     | 0.73              |
| 14:9:188:ARG:HE     | 58:t:59:SER:CB      | 2.02                     | 0.73              |
| 64:13:984:GLN:CD    | 64:13:1133:THR:CA   | 2.62                     | 0.73              |
| 6:17:426:LYS:CD     | 66:15:184:GLN:N     | 2.35                     | 0.72              |
| 44:f:100:GLN:OE1    | 44:f:110:LYS:NZ     | 2.22                     | 0.72              |
| 3:10:253:PHE:CE2    | 6:17:15:ILE:HG23    | 2.21                     | 0.72              |
| 6:17:260:GLN:C      | 65:14:1126:LEU:CD2  | 2.60                     | 0.72              |
| 6:17:277:SER:HA     | 65:14:1124:LYS:C    | 2.13                     | 0.72              |
| 6:17:429:ASP:O      | 66:15:549:LEU:HD13  | 1.88                     | 0.72              |
| 6:17:429:ASP:H      | 66:15:167:PHE:HE1   | 0.77                     | 0.72              |
| 6:17:711:PHE:CD1    | 14:9:648:LEU:HB3    | 2.22                     | 0.72              |
| 15:A:65:LEU:HD21    | 15:A:231:LEU:HD13   | 1.70                     | 0.72              |
| 66:15:1208:PHE:CE2  | 66:15:1216:LYS:HE2  | 2.24                     | 0.72              |
| 67:18:195:LYS:HE2   | 67:18:199:ASP:HA    | 1.71                     | 0.72              |
| 6:17:699:ILE:CG2    | 14:9:692:LYS:HB2    | 2.18                     | 0.72              |
| 10:5:1467:A:N3      | 37:Y:44:A:N3        | 2.37                     | 0.72              |
| 15:A:286:ARG:O      | 15:A:287:ASN:ND2    | 2.22                     | 0.72              |
| 6:17:256:THR:O      | 65:14:1099:GLN:HG3  | 1.89                     | 0.72              |
| 6:17:371:SER:O      | 66:15:173:ASN:ND2   | 2.23                     | 0.72              |
| 10:5:1269:U:O2'     | 27:L:14:ARG:NH1     | 2.22                     | 0.72              |
| 64:13:1217:LYS:HZ3  | 67:18:274:PRO:C     | 1.96                     | 0.72              |
| 67:16:18:VAL:HG12   | 67:16:87:LYS:HE3    | 1.70                     | 0.72              |
| 6:17:706:ILE:HD12   | 14:9:658:LEU:HB2    | 1.32                     | 0.72              |
| 15:A:32:MET:SD      | 15:A:281:ARG:NH1    | 2.63                     | 0.72              |
| 15:A:46:GLU:OE1     | 15:A:46:GLU:N       | 2.22                     | 0.72              |
| 36:W:46:VAL:HG23    | 36:W:47:ASN:H       | 1.54                     | 0.72              |
| 65:14:563:ILE:HG23  | 65:14:567:LEU:HD12  | 1.71                     | 0.72              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:15:1071:PHE:CG  | 66:15:1247:ARG:NH2  | 2.58                     | 0.72              |
| 3:10:431:MET:HE2   | 6:17:667:TRP:CZ3    | 2.25                     | 0.72              |
| 6:17:426:LYS:HE2   | 66:15:179:PHE:O     | 1.87                     | 0.72              |
| 6:17:430:PRO:HD2   | 66:15:555:PHE:CD1   | 2.24                     | 0.72              |
| 6:17:709:ASP:O     | 14:9:674:GLU:N      | 2.22                     | 0.72              |
| 6:17:711:PHE:HD2   | 14:9:650:ASN:HA     | 1.47                     | 0.72              |
| 15:A:49:ARG:HG3    | 15:A:50:LYS:H       | 1.54                     | 0.72              |
| 64:13:984:GLN:HE22 | 64:13:1133:THR:CG2  | 1.99                     | 0.72              |
| 64:13:1217:LYS:HZ3 | 67:18:274:PRO:CB    | 2.03                     | 0.72              |
| 8:3:102:A:C6       | 14:9:781:PHE:CA     | 2.43                     | 0.72              |
| 64:13:171:PHE:CZ   | 66:15:1184:ILE:HG12 | 2.24                     | 0.72              |
| 65:14:948:VAL:HG21 | 66:15:247:LYS:HD2   | 1.71                     | 0.72              |
| 6:17:277:SER:HB2   | 65:14:1124:LYS:N    | 2.03                     | 0.72              |
| 6:17:691:THR:C     | 14:9:682:VAL:HG11   | 2.12                     | 0.72              |
| 6:17:700:LEU:HD22  | 14:9:658:LEU:HB3    | 1.67                     | 0.72              |
| 10:5:787:A:C8      | 12:7:37:MIA:C11     | 2.73                     | 0.72              |
| 10:5:1354:G:O6     | 21:F:2:ARG:NH2      | 2.23                     | 0.72              |
| 66:15:958:PHE:HZ   | 66:15:1266:VAL:HG13 | 1.54                     | 0.72              |
| 6:17:800:LEU:CD2   | 6:17:920:VAL:HG22   | 2.20                     | 0.72              |
| 8:3:102:A:O2'      | 14:9:783:GLU:CA     | 2.37                     | 0.72              |
| 8:3:1559:A:N9      | 14:9:247:LYS:HE2    | 1.67                     | 0.72              |
| 23:H:20:TYR:HB2    | 23:H:66:ASN:HB3     | 1.70                     | 0.72              |
| 3:10:235:ILE:HD13  | 6:17:37:LEU:HD21    | 1.72                     | 0.71              |
| 14:9:163:PRO:CB    | 58:t:63:VAL:HG23    | 2.19                     | 0.71              |
| 65:14:1280:LYS:HE3 | 65:14:1296:ARG:NH2  | 2.05                     | 0.71              |
| 66:15:962:LEU:HB2  | 66:15:1269:LEU:HD13 | 1.70                     | 0.71              |
| 66:15:1154:GLU:OE1 | 67:16:72:ALA:N      | 2.23                     | 0.71              |
| 6:17:382:ASP:CB    | 66:15:64:LYS:HZ1    | 2.02                     | 0.71              |
| 6:17:955:LYS:HD3   | 14:9:803:LYS:HE3    | 1.72                     | 0.71              |
| 17:AB:41:U:C2'     | 37:Y:42:C:H6        | 2.03                     | 0.71              |
| 42:d:148:ARG:HE    | 42:d:149:ILE:H      | 1.37                     | 0.71              |
| 50:l:116:LYS:O     | 50:l:120:ARG:HG2    | 1.90                     | 0.71              |
| 6:17:43:GLY:HA3    | 6:17:46:PHE:CE2     | 2.25                     | 0.71              |
| 6:17:429:ASP:OD2   | 66:15:184:GLN:CA    | 2.36                     | 0.71              |
| 6:17:708:THR:O     | 14:9:651:HIS:CD2    | 2.42                     | 0.71              |
| 8:3:101:C:O2'      | 14:9:699:VAL:CG1    | 2.37                     | 0.71              |
| 8:3:1559:A:H2'     | 14:9:247:LYS:HB3    | 1.72                     | 0.71              |
| 10:5:1468:A:N1     | 13:8:36:U:C2'       | 2.54                     | 0.71              |
| 66:15:1207:LYS:HE2 | 66:15:1252:SER:HB3  | 1.73                     | 0.71              |
| 5:12:100:LEU:CD2   | 6:17:668:LEU:HD13   | 2.17                     | 0.71              |
| 6:17:275:ASN:HB3   | 65:14:1125:THR:C    | 2.16                     | 0.71              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:3:1559:A:C1'      | 14:9:247:LYS:HE2    | 2.19                     | 0.71              |
| 10:5:196:G:O2'      | 10:5:197:A:OP1      | 2.08                     | 0.71              |
| 12:7:29:G:OP1       | 27:L:117:ALA:HB1    | 1.90                     | 0.71              |
| 66:15:1166:VAL:HG23 | 66:15:1168:VAL:HG23 | 1.70                     | 0.71              |
| 66:15:1219:MET:HE2  | 66:15:1247:ARG:NH2  | 2.04                     | 0.71              |
| 6:17:262:SER:H      | 65:14:1098:THR:CA   | 2.02                     | 0.71              |
| 6:17:264:GLU:N      | 65:14:1097:GLN:HA   | 2.05                     | 0.71              |
| 6:17:429:ASP:HA     | 66:15:549:LEU:HD22  | 1.72                     | 0.71              |
| 39:a:125:GLU:N      | 39:a:125:GLU:OE2    | 2.24                     | 0.71              |
| 64:13:1018:SER:HB3  | 67:18:258:VAL:HG13  | 0.72                     | 0.71              |
| 65:14:806:VAL:HG13  | 65:14:818:GLY:CA    | 2.19                     | 0.71              |
| 66:15:1105:VAL:HG23 | 67:16:255:ARG:CG    | 2.20                     | 0.71              |
| 6:17:696:ASN:N      | 14:9:633:VAL:HG11   | 1.78                     | 0.71              |
| 8:3:1561:G:H4'      | 14:9:299:LYS:CE     | 2.21                     | 0.71              |
| 10:5:93:A:H5'       | 10:5:94:A:H5''      | 1.73                     | 0.71              |
| 14:9:227:GLY:N      | 58:t:53:LYS:HG3     | 1.55                     | 0.71              |
| 49:k:126:PHE:HB2    | 49:k:146:VAL:HG22   | 1.71                     | 0.71              |
| 66:15:20:ILE:HG23   | 66:15:24:GLU:HA     | 1.72                     | 0.71              |
| 6:17:695:SER:HA     | 14:9:633:VAL:HG21   | 1.67                     | 0.71              |
| 8:3:2465:U:O4       | 8:3:2502:G:O6       | 2.08                     | 0.71              |
| 10:5:949:G:H4'      | 27:L:119:LYS:HD3    | 1.73                     | 0.71              |
| 15:A:93:LYS:HG3     | 15:A:109:THR:HB     | 1.71                     | 0.71              |
| 66:15:958:PHE:HA    | 66:15:1273:VAL:HG21 | 1.73                     | 0.71              |
| 6:17:260:GLN:CB     | 65:14:1126:LEU:HD23 | 2.20                     | 0.71              |
| 6:17:688:GLN:O      | 14:9:679:ASP:O      | 2.09                     | 0.71              |
| 8:3:102:A:N7        | 14:9:786:MET:CG     | 2.54                     | 0.71              |
| 14:9:798:ARG:HD2    | 61:w:22:LEU:N       | 2.01                     | 0.71              |
| 67:16:255:ARG:HH11  | 67:16:259:GLN:NE2   | 1.86                     | 0.71              |
| 6:17:261:LYS:CG     | 65:14:1130:LYS:CE   | 2.60                     | 0.71              |
| 6:17:373:VAL:HG13   | 66:15:174:ASP:N     | 1.91                     | 0.71              |
| 6:17:700:LEU:HB3    | 14:9:658:LEU:HA     | 1.73                     | 0.71              |
| 8:3:656:G:H4'       | 8:3:657:A:H5'       | 1.73                     | 0.71              |
| 10:5:206:G:N2       | 10:5:209:A:OP2      | 2.23                     | 0.71              |
| 12:7:34:G:C6        | 17:AB:42:C:N3       | 2.58                     | 0.71              |
| 3:10:238:PHE:CE2    | 6:17:559:PHE:CE1    | 2.57                     | 0.71              |
| 3:10:238:PHE:CE1    | 6:17:563:VAL:HG22   | 2.23                     | 0.71              |
| 6:17:691:THR:CA     | 14:9:682:VAL:HG11   | 2.20                     | 0.71              |
| 6:17:693:THR:HG23   | 14:9:682:VAL:CA     | 2.21                     | 0.71              |
| 6:17:706:ILE:CD1    | 14:9:668:ILE:CD1    | 2.69                     | 0.71              |
| 64:13:1020:MET:HB2  | 67:18:256:HIS:ND1   | 2.05                     | 0.71              |
| 65:14:316:LYS:CE    | 65:14:454:GLN:HE21  | 2.03                     | 0.71              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 65:14:610:ILE:HB   | 66:15:248:THR:OG1   | 1.89                     | 0.71              |
| 6:17:252:SER:H     | 65:14:1104:ALA:HB2  | 1.54                     | 0.70              |
| 6:17:845:TRP:CE2   | 14:9:644:LYS:HG2    | 2.26                     | 0.70              |
| 14:9:165:LEU:HD21  | 58:t:62:LYS:HE2     | 1.63                     | 0.70              |
| 20:E:9:VAL:HG23    | 20:E:56:HIS:HB2     | 1.73                     | 0.70              |
| 64:13:1062:ARG:NH2 | 67:18:69:ASN:O      | 2.24                     | 0.70              |
| 66:15:129:PHE:CE1  | 66:15:133:ILE:HD11  | 2.26                     | 0.70              |
| 6:17:259:GLY:O     | 65:14:1098:THR:CG2  | 2.38                     | 0.70              |
| 14:9:798:ARG:HG3   | 61:w:22:LEU:CA      | 2.19                     | 0.70              |
| 41:c:24:LEU:O      | 41:c:113:HIS:HE1    | 1.74                     | 0.70              |
| 64:13:195:ASP:HA   | 64:13:545:ARG:NH1   | 2.06                     | 0.70              |
| 65:14:531:PHE:HZ   | 65:14:563:ILE:HG21  | 1.54                     | 0.70              |
| 66:15:33:VAL:HA    | 66:15:832:ILE:HD12  | 1.73                     | 0.70              |
| 6:17:711:PHE:CG    | 14:9:649:VAL:O      | 2.44                     | 0.70              |
| 54:p:64:LEU:HD11   | 54:p:94:LEU:HB3     | 1.73                     | 0.70              |
| 58:t:95:PRO:HG2    | 58:t:96:LYS:N       | 2.06                     | 0.70              |
| 65:14:166:LEU:HD21 | 65:14:515:PHE:CZ    | 2.26                     | 0.70              |
| 66:15:1173:LEU:O   | 66:15:1189:LYS:HE2  | 1.90                     | 0.70              |
| 10:5:1241:G:N2     | 10:5:1244:A:OP2     | 2.22                     | 0.70              |
| 18:x:32:LYS:HE3    | 18:x:34:ILE:HD13    | 1.71                     | 0.70              |
| 3:10:312:THR:HG22  | 65:14:85:GLN:HE22   | 1.54                     | 0.70              |
| 6:17:697:TYR:CE2   | 14:9:637:CYS:CA     | 2.75                     | 0.70              |
| 8:3:1561:G:OP1     | 14:9:248:GLU:O      | 2.08                     | 0.70              |
| 20:E:163:MET:SD    | 22:G:50:LYS:NZ      | 2.65                     | 0.70              |
| 61:w:40:LYS:HD3    | 61:w:42:HIS:NE2     | 2.07                     | 0.70              |
| 64:13:10:GLN:CB    | 67:18:197:ASN:HD22  | 2.00                     | 0.70              |
| 65:14:605:GLU:CB   | 66:15:248:THR:HG22  | 2.22                     | 0.70              |
| 65:14:1209:LYS:HE2 | 66:15:250:PHE:CE2   | 2.26                     | 0.70              |
| 66:15:996:ASP:HB2  | 66:15:1057:LEU:CD1  | 2.20                     | 0.70              |
| 6:17:388:ALA:C     | 66:15:132:LEU:HD23  | 2.12                     | 0.70              |
| 6:17:955:LYS:HZ1   | 14:9:799:GLU:CD     | 1.99                     | 0.70              |
| 8:3:1446:G:O2'     | 8:3:1613:A:N6       | 2.24                     | 0.70              |
| 26:K:84:GLY:O      | 26:K:112:ARG:NH2    | 2.25                     | 0.70              |
| 39:a:137:PRO:HA    | 39:a:197:ARG:HA     | 1.74                     | 0.70              |
| 64:13:1192:LEU:CD1 | 67:18:88:GLN:HE21   | 2.03                     | 0.70              |
| 65:14:608:ASN:ND2  | 66:15:251:ASP:N     | 2.38                     | 0.70              |
| 66:15:989:VAL:HG11 | 66:15:1260:LEU:HD21 | 1.71                     | 0.70              |
| 6:17:275:ASN:HB2   | 65:14:1125:THR:OG1  | 1.91                     | 0.70              |
| 64:13:209:PRO:HD3  | 64:13:234:PHE:CD1   | 2.27                     | 0.70              |
| 67:16:195:LYS:HE2  | 67:16:199:ASP:HA    | 1.73                     | 0.70              |
| 6:17:259:GLY:O     | 65:14:1098:THR:HG22 | 1.91                     | 0.70              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:691:THR:N     | 14:9:682:VAL:HG11   | 2.07                     | 0.70              |
| 8:3:1561:G:O2'     | 14:9:299:LYS:HD2    | 1.89                     | 0.70              |
| 10:5:528:G:C5      | 13:8:35:U:H1'       | 2.27                     | 0.70              |
| 17:AB:43:A:H2'     | 37:Y:44:A:C8        | 2.27                     | 0.70              |
| 65:14:313:ALA:HB1  | 65:14:455:PRO:HG2   | 1.73                     | 0.70              |
| 65:14:610:ILE:H    | 66:15:248:THR:HB    | 1.57                     | 0.70              |
| 3:10:253:PHE:CE2   | 6:17:15:ILE:CG1     | 2.68                     | 0.70              |
| 5:12:96:LEU:CD2    | 6:17:661:LEU:HB2    | 2.20                     | 0.70              |
| 8:3:1103:G:N2      | 8:3:1130:A:O2'      | 2.25                     | 0.70              |
| 12:7:28:G:O3'      | 27:L:117:ALA:CB     | 2.40                     | 0.70              |
| 46:h:122:LYS:CA    | 46:h:125:LEU:HD13   | 2.18                     | 0.70              |
| 66:15:961:THR:CB   | 66:15:1269:LEU:HD21 | 2.21                     | 0.70              |
| 3:10:238:PHE:HB2   | 6:17:562:ALA:HB1    | 1.73                     | 0.69              |
| 6:17:78:GLY:O      | 65:14:1268:ASN:O    | 2.10                     | 0.69              |
| 6:17:690:LEU:O     | 14:9:682:VAL:CG2    | 2.40                     | 0.69              |
| 8:3:2688:C:OP2     | 40:b:117:ARG:NH2    | 2.23                     | 0.69              |
| 44:f:5:LEU:HA      | 44:f:36:ALA:HA      | 1.74                     | 0.69              |
| 64:13:984:GLN:HG3  | 64:13:1133:THR:OG1  | 1.92                     | 0.69              |
| 65:14:316:LYS:HE3  | 65:14:454:GLN:NE2   | 2.03                     | 0.69              |
| 65:14:1032:GLN:NE2 | 66:15:540:ASN:OD1   | 2.26                     | 0.69              |
| 66:15:284:ARG:NH1  | 66:15:527:TYR:CD2   | 2.59                     | 0.69              |
| 3:10:251:THR:HG22  | 3:10:424:VAL:HG11   | 1.74                     | 0.69              |
| 6:17:384:ALA:O     | 66:15:63:ASN:OD1    | 2.10                     | 0.69              |
| 8:3:892:G:H2'      | 8:3:893:A:H8        | 1.57                     | 0.69              |
| 10:5:528:G:N1      | 13:8:35:U:H1'       | 2.05                     | 0.69              |
| 12:7:35:A:N1       | 17:AB:41:U:O2       | 2.25                     | 0.69              |
| 39:a:137:PRO:HG2   | 39:a:140:PHE:CE1    | 2.26                     | 0.69              |
| 42:d:108:LEU:HB3   | 42:d:114:PHE:CE2    | 2.28                     | 0.69              |
| 66:15:961:THR:CG2  | 66:15:1269:LEU:CD2  | 2.70                     | 0.69              |
| 5:12:97:LEU:HD11   | 6:17:667:TRP:CD2    | 2.24                     | 0.69              |
| 6:17:429:ASP:OD1   | 66:15:555:PHE:CE1   | 2.44                     | 0.69              |
| 6:17:711:PHE:HZ    | 14:9:642:ASN:HB2    | 0.92                     | 0.69              |
| 8:3:1558:A:N1      | 14:9:247:LYS:HE3    | 2.07                     | 0.69              |
| 8:3:1561:G:C1'     | 14:9:299:LYS:NZ     | 2.55                     | 0.69              |
| 13:8:34:U8U:C4     | 17:AB:44:A:N6       | 2.55                     | 0.69              |
| 14:9:165:LEU:HG    | 58:t:62:LYS:CG      | 2.21                     | 0.69              |
| 64:13:53:ALA:O     | 64:13:612:LEU:HD12  | 1.93                     | 0.69              |
| 64:13:1020:MET:HA  | 67:18:256:HIS:HA    | 1.73                     | 0.69              |
| 67:18:195:LYS:HE2  | 67:18:199:ASP:OD1   | 1.92                     | 0.69              |
| 10:5:1468:A:H61    | 13:8:36:U:HO2'      | 1.38                     | 0.69              |
| 15:A:95:LEU:HD11   | 15:A:226:CYS:HA     | 1.74                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:J:43:MET:HA     | 25:J:43:MET:HE3    | 1.73                     | 0.69              |
| 36:W:84:ASN:O      | 36:W:88:ILE:HG23   | 1.93                     | 0.69              |
| 65:14:242:LYS:NZ   | 65:14:396:GLU:OE1  | 2.24                     | 0.69              |
| 65:14:971:TYR:HE2  | 65:14:973:LYS:HE3  | 1.56                     | 0.69              |
| 5:12:85:TRP:CB     | 6:17:12:LEU:H      | 2.01                     | 0.69              |
| 6:17:706:ILE:HD12  | 14:9:659:ASN:H     | 1.55                     | 0.69              |
| 8:3:1129:U:N3      | 8:3:1132:C:OP2     | 2.21                     | 0.69              |
| 14:9:798:ARG:HH11  | 61:w:21:LYS:CB     | 1.99                     | 0.69              |
| 50:l:32:TYR:HD2    | 50:l:114:MET:CE    | 2.05                     | 0.69              |
| 3:10:227:ILE:HD12  | 6:17:112:VAL:H     | 1.54                     | 0.69              |
| 6:17:698:SER:CB    | 14:9:769:ILE:CG2   | 2.37                     | 0.69              |
| 8:3:1485:A:H2      | 8:3:2710:G:N1      | 1.90                     | 0.69              |
| 66:15:186:TYR:CE1  | 66:15:570:ALA:HA   | 2.27                     | 0.69              |
| 67:18:140:ASP:OD1  | 67:18:177:HIS:HE1  | 1.75                     | 0.69              |
| 6:17:711:PHE:CB    | 14:9:651:HIS:CE1   | 2.67                     | 0.69              |
| 14:9:451:GLN:O     | 62:y:56:ALA:HB3    | 1.91                     | 0.69              |
| 66:15:877:ARG:HH11 | 66:15:1270:ILE:CG2 | 2.03                     | 0.69              |
| 5:12:89:LYS:NZ     | 6:17:612:LYS:CA    | 2.52                     | 0.69              |
| 6:17:712:ILE:N     | 14:9:651:HIS:CE1   | 2.60                     | 0.69              |
| 8:3:1561:G:C8      | 14:9:248:GLU:CD    | 2.70                     | 0.69              |
| 8:3:2481:U:OP1     | 8:3:2483:C:N4      | 2.25                     | 0.69              |
| 14:9:795:GLN:CA    | 61:w:18:LEU:HD21   | 2.22                     | 0.69              |
| 41:c:30:LYS:H      | 41:c:114:THR:HG21  | 1.56                     | 0.69              |
| 64:13:799:LYS:NZ   | 64:13:884:GLU:OE2  | 2.26                     | 0.69              |
| 64:13:1192:LEU:CD1 | 67:18:88:GLN:NE2   | 2.55                     | 0.69              |
| 6:17:690:LEU:C     | 14:9:682:VAL:HG21  | 2.18                     | 0.69              |
| 6:17:707:GLN:O     | 14:9:670:PRO:HA    | 1.93                     | 0.69              |
| 7:2:4:ARG:NH2      | 8:3:2485:U:O2      | 2.26                     | 0.69              |
| 10:5:399:C:H5'     | 19:C:132:PRO:HD2   | 1.75                     | 0.69              |
| 13:8:35:U:C2       | 17:AB:44:A:H2      | 2.10                     | 0.69              |
| 14:9:798:ARG:NH2   | 61:w:18:LEU:CD2    | 2.49                     | 0.69              |
| 64:13:344:LYS:HE3  | 64:13:363:GLU:HG3  | 1.75                     | 0.69              |
| 6:17:426:LYS:HZ1   | 66:15:183:LEU:HB3  | 1.50                     | 0.69              |
| 8:3:2060:G:O2'     | 40:b:157:GLN:NE2   | 2.25                     | 0.69              |
| 45:g:37:ALA:O      | 45:g:40:ILE:HG22   | 1.94                     | 0.69              |
| 56:r:12:ILE:HG12   | 56:r:43:ALA:HB2    | 1.75                     | 0.69              |
| 5:12:96:LEU:HD22   | 6:17:661:LEU:CA    | 2.22                     | 0.68              |
| 6:17:700:LEU:O     | 14:9:661:GLU:HB3   | 1.93                     | 0.68              |
| 26:K:57:LYS:HD2    | 37:Y:45:A:O5'      | 1.91                     | 0.68              |
| 42:d:38:MET:HE2    | 42:d:150:ARG:HB2   | 1.74                     | 0.68              |
| 65:14:316:LYS:CE   | 65:14:454:GLN:HE22 | 2.06                     | 0.68              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:15:54:GLU:HG2   | 66:15:814:GLN:HE22  | 1.54                     | 0.68              |
| 66:15:981:ILE:HD11 | 66:15:1097:LEU:HD21 | 1.74                     | 0.68              |
| 6:17:703:ASN:HB3   | 14:9:785:LEU:CD1    | 2.23                     | 0.68              |
| 6:17:711:PHE:CD2   | 14:9:649:VAL:O      | 2.46                     | 0.68              |
| 10:5:735:C:OP2     | 20:E:92:ARG:NH2     | 2.26                     | 0.68              |
| 66:15:1154:GLU:CD  | 67:16:71:GLN:O      | 2.37                     | 0.68              |
| 6:17:258:ASN:O     | 65:14:1126:LEU:HD22 | 1.93                     | 0.68              |
| 6:17:703:ASN:CB    | 14:9:785:LEU:HG     | 2.23                     | 0.68              |
| 6:17:955:LYS:NZ    | 14:9:799:GLU:C      | 2.44                     | 0.68              |
| 8:3:1119:A:C8      | 45:g:53:VAL:HG21    | 2.28                     | 0.68              |
| 8:3:2589:G:N2      | 8:3:2589:G:OP2      | 2.24                     | 0.68              |
| 44:f:108:LEU:C     | 44:f:108:LEU:HD13   | 2.18                     | 0.68              |
| 66:15:434:THR:HG22 | 66:15:489:THR:CG2   | 2.24                     | 0.68              |
| 3:10:431:MET:HE3   | 6:17:667:TRP:HH2    | 1.58                     | 0.68              |
| 6:17:709:ASP:OD2   | 14:9:671:LYS:HG3    | 1.93                     | 0.68              |
| 6:17:711:PHE:C     | 14:9:651:HIS:CE1    | 2.70                     | 0.68              |
| 10:5:521:A:N6      | 26:K:102:ASP:OD1    | 2.24                     | 0.68              |
| 10:5:1467:A:H2     | 37:Y:44:A:H2        | 1.35                     | 0.68              |
| 24:I:23:LEU:HD13   | 36:W:217:ARG:HH21   | 1.59                     | 0.68              |
| 65:14:209:VAL:HG23 | 65:14:467:HIS:CE1   | 2.28                     | 0.68              |
| 6:17:262:SER:N     | 65:14:1097:GLN:C    | 2.51                     | 0.68              |
| 6:17:696:ASN:H     | 14:9:633:VAL:HG13   | 1.57                     | 0.68              |
| 8:3:648:G:O6       | 41:c:181:LYS:NZ     | 2.26                     | 0.68              |
| 6:17:430:PRO:HG3   | 66:15:556:GLN:HG3   | 1.75                     | 0.68              |
| 8:3:101:C:O2'      | 14:9:699:VAL:HG11   | 1.93                     | 0.68              |
| 8:3:519:A:N3       | 14:9:165:LEU:HD11   | 2.06                     | 0.68              |
| 8:3:1561:G:H4'     | 14:9:299:LYS:CG     | 2.22                     | 0.68              |
| 9:4:83:U:H5'       | 9:4:84:C:H5'        | 1.74                     | 0.68              |
| 59:u:99:LYS:HE3    | 59:u:101:LYS:HE2    | 1.74                     | 0.68              |
| 60:v:16:ASN:HD22   | 60:v:24:ILE:HG23    | 1.58                     | 0.68              |
| 66:15:961:THR:CG2  | 66:15:1269:LEU:HD21 | 2.23                     | 0.68              |
| 6:17:390:ALA:CB    | 66:15:71:ARG:HH12   | 1.96                     | 0.68              |
| 10:5:787:A:N7      | 12:7:37:MIA:S10     | 2.66                     | 0.68              |
| 10:5:1468:A:N1     | 13:8:36:U:H2'       | 2.07                     | 0.68              |
| 26:K:29:ASN:HD22   | 26:K:32:ASN:HB3     | 1.56                     | 0.68              |
| 36:W:140:SER:HA    | 36:W:143:LYS:HE3    | 1.74                     | 0.68              |
| 42:d:110:ARG:NH2   | 42:d:137:ILE:HA     | 2.09                     | 0.68              |
| 65:14:316:LYS:HG2  | 65:14:454:GLN:NE2   | 2.07                     | 0.68              |
| 65:14:975:SER:HB3  | 65:14:1003:ALA:HA   | 1.75                     | 0.68              |
| 6:17:373:VAL:CG1   | 66:15:171:LYS:O     | 2.41                     | 0.68              |
| 6:17:387:VAL:CA    | 66:15:68:ILE:HG13   | 2.24                     | 0.68              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:17:706:ILE:HD11   | 14:9:668:ILE:CD1    | 2.20                     | 0.68              |
| 6:17:706:ILE:HG12   | 14:9:668:ILE:HB     | 1.76                     | 0.68              |
| 10:5:469:C:O2'      | 30:O:80:LYS:NZ      | 2.26                     | 0.68              |
| 24:I:23:LEU:HD21    | 24:I:99:PRO:HB2     | 1.76                     | 0.68              |
| 66:15:865:ASP:HB3   | 66:15:1262:LYS:NZ   | 2.08                     | 0.68              |
| 9:4:55:A:C4         | 42:d:26:MET:HE1     | 2.28                     | 0.68              |
| 45:g:25:VAL:HG11    | 45:g:93:LEU:HD21    | 1.76                     | 0.68              |
| 64:13:1062:ARG:CZ   | 67:18:73:VAL:HG23   | 2.23                     | 0.68              |
| 66:15:1149:THR:CG2  | 66:15:1154:GLU:OE2  | 2.41                     | 0.68              |
| 66:15:1154:GLU:CD   | 67:16:71:GLN:C      | 2.62                     | 0.68              |
| 8:3:1920:A:N7       | 10:5:1469:G:H4'     | 2.08                     | 0.68              |
| 14:9:165:LEU:HA     | 58:t:62:LYS:NZ      | 2.08                     | 0.68              |
| 17:AB:45:A:P        | 37:Y:45:A:C8        | 2.87                     | 0.68              |
| 40:b:47:TYR:HB2     | 40:b:85:ARG:HH21    | 1.58                     | 0.68              |
| 44:f:8:ASP:OD1      | 44:f:14:LYS:HG3     | 1.94                     | 0.68              |
| 8:3:487:C:N4        | 8:3:490:A:OP2       | 2.25                     | 0.67              |
| 8:3:1561:G:O3'      | 14:9:299:LYS:CA     | 2.42                     | 0.67              |
| 65:14:605:GLU:HA    | 66:15:248:THR:HG22  | 1.74                     | 0.67              |
| 6:17:429:ASP:OD1    | 66:15:555:PHE:CZ    | 2.47                     | 0.67              |
| 8:3:1559:A:H1'      | 14:9:247:LYS:CE     | 2.24                     | 0.67              |
| 15:A:181:PRO:HD3    | 15:A:200:ALA:HB1    | 1.75                     | 0.67              |
| 33:R:22:MET:HE1     | 33:R:29:ARG:HG2     | 1.75                     | 0.67              |
| 64:13:1192:LEU:HD21 | 67:18:88:GLN:HG3    | 1.68                     | 0.67              |
| 6:17:264:GLU:HB3    | 65:14:1094:ASN:O    | 1.94                     | 0.67              |
| 6:17:385:ASP:CB     | 66:15:64:LYS:HB3    | 2.23                     | 0.67              |
| 8:3:421:A:N6        | 8:3:424:G:OP2       | 2.26                     | 0.67              |
| 10:5:136:U:H3       | 10:5:157:A:H62      | 1.40                     | 0.67              |
| 10:5:1468:A:N6      | 13:8:36:U:O2'       | 2.26                     | 0.67              |
| 17:AB:45:A:P        | 37:Y:45:A:H8        | 2.15                     | 0.67              |
| 23:H:86:VAL:HG23    | 23:H:100:LEU:HD13   | 1.76                     | 0.67              |
| 66:15:1107:THR:HG23 | 67:16:256:HIS:NE2   | 2.09                     | 0.67              |
| 3:10:275:SER:OG     | 6:17:970:SER:OG     | 1.92                     | 0.67              |
| 6:17:429:ASP:OD2    | 66:15:184:GLN:HB3   | 1.91                     | 0.67              |
| 41:c:113:HIS:HA     | 41:c:211:PHE:CZ     | 2.29                     | 0.67              |
| 41:c:115:VAL:HG21   | 41:c:188:VAL:HG13   | 1.75                     | 0.67              |
| 48:j:89:GLU:CD      | 48:j:89:GLU:H       | 2.02                     | 0.67              |
| 64:13:397:ALA:O     | 64:13:414:LYS:NZ    | 2.25                     | 0.67              |
| 64:13:1062:ARG:HH11 | 67:18:73:VAL:CG2    | 2.06                     | 0.67              |
| 66:15:962:LEU:CB    | 66:15:1269:LEU:HD13 | 2.24                     | 0.67              |
| 66:15:979:GLN:O     | 67:16:258:VAL:HG11  | 1.94                     | 0.67              |
| 66:15:1149:THR:HG23 | 66:15:1154:GLU:OE2  | 1.95                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:9:G:H2'        | 8:3:10:U:C6        | 2.30                     | 0.67              |
| 14:9:451:GLN:CD    | 62:y:57:TYR:OXT    | 2.37                     | 0.67              |
| 15:A:28:THR:O      | 15:A:61:GLN:NE2    | 2.27                     | 0.67              |
| 46:h:24:ALA:O      | 46:h:27:SER:OG     | 2.11                     | 0.67              |
| 60:v:4:LYS:HD2     | 60:v:9:LEU:HD13    | 1.75                     | 0.67              |
| 64:13:356:VAL:HG21 | 64:13:362:VAL:HG21 | 1.76                     | 0.67              |
| 64:13:997:LYS:HB3  | 64:13:999:GLN:HG3  | 1.75                     | 0.67              |
| 65:14:226:LYS:HD3  | 66:15:212:ASP:HB3  | 1.75                     | 0.67              |
| 65:14:605:GLU:OE1  | 66:15:247:LYS:HB3  | 1.93                     | 0.67              |
| 65:14:1183:ARG:NH1 | 65:14:1243:ASN:CB  | 2.57                     | 0.67              |
| 3:10:316:TRP:HH2   | 65:14:88:ARG:O     | 1.77                     | 0.67              |
| 5:12:88:SER:OG     | 6:17:615:PHE:HZ    | 1.77                     | 0.67              |
| 6:17:81:ASN:O      | 65:14:1293:GLN:NE2 | 2.28                     | 0.67              |
| 6:17:251:ASP:OD1   | 65:14:1105:LEU:HA  | 1.94                     | 0.67              |
| 6:17:710:PHE:CE2   | 14:9:673:PHE:CB    | 2.77                     | 0.67              |
| 8:3:195:A:H3'      | 8:3:196:G:H21      | 1.59                     | 0.67              |
| 10:5:9:A:N6        | 19:C:198:GLU:OE2   | 2.27                     | 0.67              |
| 14:9:795:GLN:CD    | 61:w:18:LEU:CD1    | 2.67                     | 0.67              |
| 17:AB:45:A:H62     | 37:Y:45:A:H61      | 1.39                     | 0.67              |
| 30:O:39:LEU:HD22   | 30:O:72:LEU:HD11   | 1.77                     | 0.67              |
| 48:j:93:PRO:HG3    | 48:j:114:ILE:HG12  | 1.77                     | 0.67              |
| 64:13:10:GLN:HG2   | 67:18:197:ASN:HD22 | 0.85                     | 0.67              |
| 65:14:605:GLU:CG   | 66:15:248:THR:CG2  | 2.62                     | 0.67              |
| 6:17:374:ALA:O     | 66:15:172:PRO:O    | 2.13                     | 0.67              |
| 6:17:386:VAL:HG13  | 66:15:177:GLY:N    | 1.98                     | 0.67              |
| 6:17:430:PRO:HD2   | 66:15:137:ILE:HD13 | 1.77                     | 0.67              |
| 6:17:709:ASP:O     | 14:9:674:GLU:HB2   | 1.95                     | 0.67              |
| 10:5:1473:U:C5     | 37:Y:41:U:C4'      | 2.77                     | 0.67              |
| 14:9:162:ALA:HA    | 58:t:60:THR:O      | 1.95                     | 0.67              |
| 14:9:798:ARG:HH21  | 61:w:18:LEU:CG     | 2.07                     | 0.67              |
| 23:H:86:VAL:O      | 23:H:90:LEU:HD23   | 1.94                     | 0.67              |
| 42:d:5:LYS:HD3     | 42:d:97:TRP:CD1    | 2.29                     | 0.67              |
| 66:15:467:LEU:HD23 | 66:15:468:PRO:HD3  | 1.75                     | 0.67              |
| 66:15:1105:VAL:HA  | 67:16:254:LYS:HB3  | 1.76                     | 0.67              |
| 66:15:1106:SER:CA  | 67:16:254:LYS:HB2  | 2.24                     | 0.67              |
| 22:G:104:LEU:O     | 22:G:129:ARG:NH2   | 2.28                     | 0.67              |
| 65:14:610:ILE:CG2  | 66:15:248:THR:OG1  | 2.42                     | 0.67              |
| 66:15:839:TRP:CD1  | 66:15:843:ASN:ND2  | 2.63                     | 0.67              |
| 66:15:1106:SER:HA  | 67:16:256:HIS:ND1  | 1.61                     | 0.67              |
| 26:K:115:LEU:HG    | 26:K:116:ASP:H     | 1.60                     | 0.67              |
| 42:d:70:ALA:HB2    | 42:d:85:ILE:HD11   | 1.76                     | 0.67              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 44:f:97:ILE:HA      | 44:f:100:GLN:HB2   | 1.75                     | 0.67              |
| 57:s:39:ARG:HG2     | 57:s:39:ARG:HH11   | 1.58                     | 0.67              |
| 66:15:900:GLN:HE22  | 66:15:934:GLU:HA   | 1.60                     | 0.67              |
| 66:15:1154:GLU:OE1  | 67:16:71:GLN:C     | 2.38                     | 0.67              |
| 6:17:698:SER:HB3    | 14:9:769:ILE:HG21  | 1.68                     | 0.67              |
| 6:17:703:ASN:CB     | 14:9:663:ASN:CB    | 2.73                     | 0.67              |
| 17:AB:41:U:C3'      | 37:Y:42:C:C6       | 2.77                     | 0.67              |
| 65:14:197:ILE:HD13  | 65:14:489:LYS:HA   | 1.77                     | 0.67              |
| 66:15:71:ARG:HH12   | 66:15:132:LEU:HD21 | 1.60                     | 0.67              |
| 66:15:1107:THR:HG22 | 67:16:253:VAL:HG13 | 1.77                     | 0.67              |
| 6:17:277:SER:CB     | 65:14:1124:LYS:O   | 2.42                     | 0.66              |
| 8:3:102:A:C8        | 14:9:786:MET:HG2   | 2.29                     | 0.66              |
| 45:g:25:VAL:HG23    | 45:g:83:ALA:HB3    | 1.77                     | 0.66              |
| 65:14:316:LYS:HE2   | 65:14:454:GLN:HE22 | 1.60                     | 0.66              |
| 67:18:105:TRP:HZ3   | 67:18:152:TYR:CD2  | 2.13                     | 0.66              |
| 5:12:96:LEU:CD2     | 6:17:661:LEU:N     | 2.58                     | 0.66              |
| 5:12:97:LEU:HD21    | 6:17:664:ILE:HG23  | 1.70                     | 0.66              |
| 6:17:258:ASN:OD1    | 65:14:1126:LEU:HA  | 1.95                     | 0.66              |
| 20:E:90:LEU:HA      | 20:E:93:GLU:HG2    | 1.77                     | 0.66              |
| 26:K:57:LYS:O       | 37:Y:45:A:H4'      | 1.95                     | 0.66              |
| 46:h:122:LYS:HA     | 46:h:125:LEU:CD1   | 2.17                     | 0.66              |
| 18:x:14:PHE:O       | 18:x:22:SER:HA     | 1.96                     | 0.66              |
| 65:14:495:ARG:HD2   | 65:14:510:TYR:OH   | 1.95                     | 0.66              |
| 66:15:330:LEU:HD21  | 66:15:488:GLN:HB3  | 1.77                     | 0.66              |
| 8:3:1698:A:H2       | 48:j:1:MET:HE1     | 1.61                     | 0.66              |
| 46:h:120:ALA:O      | 46:h:123:MET:HG2   | 1.95                     | 0.66              |
| 64:13:1062:ARG:HH12 | 67:18:73:VAL:HA    | 1.59                     | 0.66              |
| 6:17:600:ASN:H      | 14:9:641:ARG:HD2   | 1.61                     | 0.66              |
| 10:5:416:U:O2'      | 10:5:421:G:N2      | 2.28                     | 0.66              |
| 47:i:7:LEU:HD23     | 47:i:7:LEU:H       | 1.60                     | 0.66              |
| 64:13:81:TYR:CZ     | 64:13:111:GLU:HG3  | 2.31                     | 0.66              |
| 65:14:605:GLU:HG2   | 66:15:247:LYS:C    | 2.20                     | 0.66              |
| 66:15:1071:PHE:CE1  | 66:15:1209:GLU:HB3 | 2.31                     | 0.66              |
| 6:17:275:ASN:OD1    | 65:14:1126:LEU:HB3 | 1.96                     | 0.66              |
| 6:17:384:ALA:HB1    | 66:15:64:LYS:N     | 2.11                     | 0.66              |
| 6:17:693:THR:CB     | 14:9:637:CYS:HB3   | 2.12                     | 0.66              |
| 14:9:451:GLN:C      | 62:y:56:ALA:HB3    | 2.19                     | 0.66              |
| 20:E:49:ILE:HD13    | 20:E:84:ARG:HH21   | 1.60                     | 0.66              |
| 54:p:105:PHE:O      | 54:p:109:VAL:HG13  | 1.96                     | 0.66              |
| 64:13:1044:LYS:NZ   | 64:13:1111:ASP:OD1 | 2.28                     | 0.66              |
| 1:0:1:MET:HE3       | 8:3:788:G:H5'      | 1.78                     | 0.66              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:261:LYS:HG2   | 65:14:1096:ILE:HG21 | 1.78                     | 0.66              |
| 8:3:1560:U:O5'     | 14:9:248:GLU:HB2    | 1.95                     | 0.66              |
| 8:3:1568:C:H3'     | 8:3:1569:A:C8       | 2.31                     | 0.66              |
| 10:5:1473:U:N1     | 37:Y:41:U:OP1       | 2.27                     | 0.66              |
| 12:7:29:G:P        | 27:L:117:ALA:HB1    | 2.35                     | 0.66              |
| 65:14:1028:ARG:NH1 | 65:14:1032:GLN:O    | 2.28                     | 0.66              |
| 66:15:192:VAL:O    | 66:15:516:ARG:NH2   | 2.29                     | 0.66              |
| 6:17:699:ILE:H     | 14:9:689:ILE:CG2    | 2.04                     | 0.66              |
| 10:5:195:U:H2'     | 10:5:196:G:H8       | 1.60                     | 0.66              |
| 14:9:798:ARG:HE    | 61:w:18:LEU:HD22    | 1.58                     | 0.66              |
| 46:h:112:LEU:HD22  | 46:h:123:MET:SD     | 2.36                     | 0.66              |
| 6:17:703:ASN:HB3   | 14:9:785:LEU:CG     | 2.26                     | 0.66              |
| 10:5:1009:G:H21    | 10:5:1012:A:H2      | 1.43                     | 0.66              |
| 14:9:801:HIS:HD2   | 61:w:24:GLY:C       | 1.83                     | 0.66              |
| 21:F:112:GLU:HG3   | 21:F:113:LYS:H      | 1.59                     | 0.66              |
| 45:g:110:CYS:HA    | 45:g:123:LEU:HD11   | 1.78                     | 0.66              |
| 6:17:279:GLN:CG    | 65:14:1122:LYS:CB   | 2.51                     | 0.66              |
| 6:17:386:VAL:N     | 66:15:175:PRO:CA    | 2.56                     | 0.66              |
| 6:17:432:LYS:HD2   | 66:15:134:PHE:C     | 2.21                     | 0.66              |
| 8:3:2502:G:H4'     | 50:l:80:GLU:HG2     | 1.77                     | 0.66              |
| 8:3:2863:G:H2'     | 8:3:2864:A:C8       | 2.31                     | 0.66              |
| 10:5:1473:U:OP1    | 37:Y:40:U:C4'       | 2.42                     | 0.66              |
| 6:17:376:LYS:HE2   | 66:15:178:GLU:CB    | 2.14                     | 0.66              |
| 6:17:422:ASP:C     | 66:15:136:ASN:HA    | 2.20                     | 0.66              |
| 6:17:690:LEU:HA    | 14:9:682:VAL:CG2    | 2.22                     | 0.66              |
| 6:17:702:GLU:HG2   | 14:9:663:ASN:HD22   | 0.94                     | 0.66              |
| 53:o:36:LYS:HB3    | 53:o:85:ASN:HB2     | 1.76                     | 0.66              |
| 65:14:68:ARG:HD2   | 65:14:130:ARG:NH2   | 2.11                     | 0.66              |
| 66:15:1091:PHE:HZ  | 66:15:1247:ARG:HD2  | 1.60                     | 0.66              |
| 67:16:140:ASP:OD1  | 67:16:177:HIS:HE1   | 1.79                     | 0.66              |
| 6:17:79:SER:OG     | 65:14:1270:LEU:HB3  | 1.96                     | 0.65              |
| 6:17:258:ASN:OD1   | 65:14:1126:LEU:CA   | 2.44                     | 0.65              |
| 6:17:701:THR:O     | 14:9:662:LEU:HA     | 1.87                     | 0.65              |
| 8:3:1420:A:N6      | 14:9:241:ARG:HH12   | 1.94                     | 0.65              |
| 43:e:112:TYR:HB2   | 43:e:116:ILE:HD11   | 1.78                     | 0.65              |
| 66:15:148:ASP:OD1  | 66:15:166:LYS:NZ    | 2.21                     | 0.65              |
| 6:17:81:ASN:ND2    | 65:14:1293:GLN:HA   | 2.11                     | 0.65              |
| 8:3:619:A:H62      | 8:3:1281:A:H2       | 1.40                     | 0.65              |
| 8:3:1786:U:OP2     | 8:3:1791:A:N6       | 2.23                     | 0.65              |
| 64:13:1020:MET:CB  | 67:18:256:HIS:CG    | 2.73                     | 0.65              |
| 14:9:798:ARG:HH22  | 61:w:18:LEU:N       | 1.93                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:10:435:ARG:NH2    | 6:17:671:SER:OG     | 2.29                     | 0.65              |
| 6:17:430:PRO:HB2    | 66:15:550:GLU:CA    | 1.93                     | 0.65              |
| 41:c:24:LEU:HD11    | 41:c:208:GLU:HB2    | 1.78                     | 0.65              |
| 43:e:25:ILE:HG13    | 43:e:38:LEU:HD21    | 1.79                     | 0.65              |
| 66:15:1170:THR:HB   | 66:15:1173:LEU:HD12 | 1.78                     | 0.65              |
| 5:12:96:LEU:HD21    | 6:17:661:LEU:N      | 2.11                     | 0.65              |
| 14:9:798:ARG:NH2    | 61:w:18:LEU:CB      | 2.59                     | 0.65              |
| 21:F:25:ILE:HB      | 21:F:100:LEU:HD22   | 1.78                     | 0.65              |
| 66:15:1107:THR:HG23 | 67:16:256:HIS:CD2   | 2.31                     | 0.65              |
| 6:17:706:ILE:N      | 14:9:656:GLU:HA     | 2.11                     | 0.65              |
| 6:17:709:ASP:OD2    | 14:9:671:LYS:CG     | 2.44                     | 0.65              |
| 66:15:1208:PHE:CE2  | 66:15:1216:LYS:CE   | 2.79                     | 0.65              |
| 17:AB:43:A:C2       | 37:Y:44:A:C6        | 2.85                     | 0.65              |
| 17:AB:45:A:O2'      | 37:Y:45:A:O2'       | 2.04                     | 0.65              |
| 3:10:235:ILE:HG12   | 6:17:563:VAL:C      | 2.22                     | 0.65              |
| 5:12:97:LEU:HD21    | 6:17:668:LEU:HG     | 1.77                     | 0.65              |
| 6:17:261:LYS:CG     | 65:14:1096:ILE:CG2  | 2.65                     | 0.65              |
| 8:3:1094:G:OP1      | 46:h:68:LYS:NZ      | 2.26                     | 0.65              |
| 14:9:808:GLN:HA     | 61:w:79:THR:HG21    | 0.66                     | 0.65              |
| 17:AB:40:U:C2       | 37:Y:41:U:C4        | 2.83                     | 0.65              |
| 33:R:50:ALA:HB1     | 33:R:57:PHE:HB3     | 1.78                     | 0.65              |
| 64:13:1204:ILE:HD11 | 64:13:1213:LEU:HD11 | 1.78                     | 0.65              |
| 65:14:730:LEU:HA    | 65:14:735:LEU:HD22  | 1.79                     | 0.65              |
| 65:14:863:LYS:HE3   | 65:14:1224:GLU:HA   | 1.79                     | 0.65              |
| 5:12:89:LYS:HZ3     | 6:17:612:LYS:CA     | 1.96                     | 0.65              |
| 6:17:390:ALA:N      | 66:15:71:ARG:NH1    | 2.44                     | 0.65              |
| 8:3:1123:A:N7       | 46:h:130:GLN:NE2    | 2.44                     | 0.65              |
| 8:3:2805:A:H4'      | 8:3:2807:G:H5''     | 1.79                     | 0.65              |
| 10:5:838:A:OP2      | 20:E:110:GLN:NE2    | 2.29                     | 0.65              |
| 10:5:1473:U:H2'     | 37:Y:40:U:O3'       | 1.96                     | 0.65              |
| 28:M:7:LYS:O        | 28:M:11:THR:HG23    | 1.97                     | 0.65              |
| 64:13:1194:LEU:CD2  | 64:13:1197:ILE:HD11 | 2.27                     | 0.65              |
| 66:15:962:LEU:CA    | 66:15:1269:LEU:HD13 | 2.26                     | 0.65              |
| 66:15:1143:LYS:HE3  | 66:15:1194:VAL:CG1  | 2.26                     | 0.65              |
| 6:17:385:ASP:HA     | 66:15:65:ASP:CA     | 2.25                     | 0.65              |
| 6:17:426:LYS:CG     | 66:15:184:GLN:HB2   | 2.18                     | 0.65              |
| 6:17:429:ASP:OD2    | 66:15:184:GLN:HA    | 1.96                     | 0.65              |
| 10:5:515:G:N2       | 10:5:528:G:OP1      | 2.30                     | 0.65              |
| 14:9:230:LYS:HD2    | 61:w:36:GLY:O       | 1.96                     | 0.65              |
| 42:d:175:LEU:HD12   | 42:d:176:PRO:HD2    | 1.79                     | 0.65              |
| 43:e:100:ASN:O      | 43:e:106:LEU:HD12   | 1.97                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:o:93:ARG:HE      | 53:o:118:LYS:HE2    | 1.62                     | 0.65              |
| 64:13:195:ASP:HA    | 64:13:545:ARG:HH12  | 1.62                     | 0.65              |
| 66:15:1103:GLN:CA   | 67:16:259:GLN:HG3   | 2.25                     | 0.65              |
| 5:12:85:TRP:N       | 6:17:8:SER:N        | 2.44                     | 0.64              |
| 8:3:1560:U:O2'      | 14:9:246:LEU:C      | 2.39                     | 0.64              |
| 10:5:404:A:OP1      | 19:C:111:ARG:NH2    | 2.30                     | 0.64              |
| 10:5:983:G:H21      | 10:5:1012:A:H8      | 1.45                     | 0.64              |
| 15:A:30:VAL:O       | 15:A:218:ASN:ND2    | 2.28                     | 0.64              |
| 15:A:293:ARG:HH21   | 35:T:50:GLN:HG2     | 1.62                     | 0.64              |
| 64:13:355:VAL:HG21  | 64:13:406:LEU:HD12  | 1.79                     | 0.64              |
| 65:14:1122:LYS:N    | 66:15:150:PHE:HE1   | 1.85                     | 0.64              |
| 66:15:865:ASP:HB3   | 66:15:1262:LYS:HZ3  | 1.62                     | 0.64              |
| 66:15:873:THR:HG22  | 66:15:1270:ILE:CD1  | 2.27                     | 0.64              |
| 6:17:708:THR:CA     | 14:9:651:HIS:O      | 2.20                     | 0.64              |
| 8:3:1588:A:H2'      | 8:3:1589:A:C8       | 2.32                     | 0.64              |
| 14:9:787:LYS:CE     | 61:w:2:THR:OG1      | 2.37                     | 0.64              |
| 33:R:9:ALA:HB1      | 33:R:39:THR:HG21    | 1.79                     | 0.64              |
| 3:10:235:ILE:HG21   | 6:17:37:LEU:HD11    | 1.79                     | 0.64              |
| 5:12:87:THR:CA      | 6:17:14:LYS:HB2     | 2.06                     | 0.64              |
| 6:17:429:ASP:C      | 66:15:549:LEU:CD2   | 2.71                     | 0.64              |
| 14:9:184:PHE:HB2    | 58:t:57:LYS:NZ      | 2.13                     | 0.64              |
| 46:h:120:ALA:HA     | 46:h:123:MET:SD     | 2.36                     | 0.64              |
| 64:13:986:ILE:HG13  | 64:13:1130:PRO:CB   | 2.26                     | 0.64              |
| 5:12:85:TRP:CG      | 6:17:12:LEU:N       | 2.60                     | 0.64              |
| 5:12:88:SER:OG      | 6:17:615:PHE:CZ     | 2.50                     | 0.64              |
| 6:17:430:PRO:CD     | 66:15:137:ILE:HD13  | 2.27                     | 0.64              |
| 8:3:1096:U:H1'      | 8:3:1105:A:H1'      | 1.80                     | 0.64              |
| 8:3:1111:C:H2'      | 8:3:1112:A:O4'      | 1.98                     | 0.64              |
| 8:3:1561:G:O3'      | 14:9:299:LYS:CB     | 2.46                     | 0.64              |
| 24:I:15:LYS:HB3     | 24:I:105:ARG:HB3    | 1.79                     | 0.64              |
| 5:12:96:LEU:CD2     | 6:17:661:LEU:HA     | 2.26                     | 0.64              |
| 6:17:264:GLU:CA     | 65:14:1096:ILE:C    | 2.69                     | 0.64              |
| 6:17:429:ASP:O      | 66:15:549:LEU:HB3   | 1.78                     | 0.64              |
| 6:17:800:LEU:HD12   | 6:17:839:ILE:HD11   | 1.80                     | 0.64              |
| 8:3:2342:U:C4       | 52:n:10:LEU:HD21    | 2.33                     | 0.64              |
| 20:E:99:SER:O       | 20:E:105:GLN:NE2    | 2.26                     | 0.64              |
| 24:I:32:VAL:HG13    | 24:I:36:LYS:HD2     | 1.79                     | 0.64              |
| 46:h:100:LYS:HA     | 46:h:103:GLU:OE2    | 1.97                     | 0.64              |
| 64:13:997:LYS:C     | 64:13:999:GLN:H     | 2.05                     | 0.64              |
| 65:14:65:ILE:HG12   | 65:14:130:ARG:NH1   | 2.11                     | 0.64              |
| 66:15:1270:ILE:HG23 | 66:15:1274:LEU:HD12 | 1.80                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:17:426:LYS:HD3    | 66:15:183:LEU:N     | 2.12                     | 0.64              |
| 8:3:102:A:H1'       | 14:9:782:ASP:C      | 2.23                     | 0.64              |
| 10:5:787:A:C1'      | 12:7:38:A:H4'       | 2.27                     | 0.64              |
| 17:AB:44:A:N1       | 37:Y:45:A:N1        | 2.46                     | 0.64              |
| 23:H:12:ARG:NH2     | 23:H:109:ASP:OD2    | 2.31                     | 0.64              |
| 42:d:25:ILE:H       | 42:d:25:ILE:HD12    | 1.63                     | 0.64              |
| 64:13:66:ILE:HG12   | 64:13:130:ARG:NH1   | 2.12                     | 0.64              |
| 65:14:806:VAL:CG1   | 65:14:818:GLY:HA2   | 2.21                     | 0.64              |
| 6:17:711:PHE:HB2    | 14:9:651:HIS:HE1    | 1.58                     | 0.64              |
| 6:17:955:LYS:HZ2    | 14:9:799:GLU:CA     | 1.76                     | 0.64              |
| 9:4:2:U:O2          | 9:4:107:G:N2        | 2.30                     | 0.64              |
| 15:A:249:LYS:HG3    | 15:A:250:PRO:HD2    | 1.80                     | 0.64              |
| 21:F:44:GLY:HA3     | 21:F:116:LEU:HD11   | 1.80                     | 0.64              |
| 64:13:897:HIS:NE2   | 64:13:901:ILE:HD11  | 2.13                     | 0.64              |
| 64:13:899:ARG:HG2   | 64:13:1194:LEU:HD11 | 1.80                     | 0.64              |
| 8:3:102:A:C8        | 14:9:786:MET:CG     | 2.80                     | 0.64              |
| 8:3:1029:A:OP2      | 54:p:50:ARG:NH2     | 2.31                     | 0.64              |
| 43:e:92:LEU:CD2     | 43:e:97:TYR:HB3     | 2.26                     | 0.64              |
| 52:n:57:SER:OG      | 52:n:64:ASN:OD1     | 2.15                     | 0.64              |
| 55:q:6:VAL:HG22     | 55:q:11:GLN:HG2     | 1.80                     | 0.64              |
| 64:13:765:LEU:CD1   | 64:13:781:LEU:HD11  | 2.28                     | 0.64              |
| 66:15:168:VAL:HG13  | 66:15:625:LYS:HE3   | 1.80                     | 0.64              |
| 6:17:261:LYS:HB2    | 65:14:1126:LEU:HD11 | 0.69                     | 0.64              |
| 6:17:693:THR:O      | 14:9:633:VAL:CG1    | 2.45                     | 0.64              |
| 8:3:901:C:H4'       | 8:3:902:U:C5'       | 2.27                     | 0.64              |
| 8:3:925:C:OP1       | 27:L:92:ARG:HD2     | 1.98                     | 0.64              |
| 9:4:31:G:O6         | 9:4:48:A:N6         | 2.31                     | 0.64              |
| 14:9:454:ASN:HA     | 62:y:56:ALA:HB2     | 1.79                     | 0.64              |
| 17:AB:49:U:H4'      | 17:AB:50:U:O5'      | 1.97                     | 0.64              |
| 21:F:83:ASN:O       | 21:F:85:GLN:NE2     | 2.31                     | 0.64              |
| 32:Q:53:LEU:HD11    | 32:Q:96:LEU:HD12    | 1.80                     | 0.64              |
| 64:13:1047:LEU:HD23 | 64:13:1110:LEU:HD21 | 1.79                     | 0.64              |
| 64:13:1062:ARG:NH1  | 67:18:72:ALA:O      | 2.30                     | 0.64              |
| 66:15:1208:PHE:CD2  | 66:15:1216:LYS:CE   | 2.81                     | 0.64              |
| 67:18:109:ASP:OD2   | 67:18:144:ARG:HD2   | 1.96                     | 0.64              |
| 5:12:97:LEU:CD2     | 6:17:668:LEU:HG     | 2.28                     | 0.64              |
| 6:17:595:ARG:NE     | 14:9:644:LYS:H      | 1.96                     | 0.64              |
| 8:3:1125:U:H2'      | 8:3:1126:G:C8       | 2.33                     | 0.64              |
| 8:3:1560:U:H5''     | 14:9:249:ASP:CA     | 2.25                     | 0.64              |
| 8:3:1617:U:H5''     | 8:3:1619:A:C4       | 2.32                     | 0.64              |
| 10:5:386:U:H4'      | 30:O:28:ARG:HH21    | 1.62                     | 0.64              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 14:9:275:LYS:HB2    | 57:s:22:GLY:CA     | 2.28                     | 0.64              |
| 26:K:57:LYS:HG3     | 37:Y:45:A:C4'      | 2.28                     | 0.64              |
| 30:O:40:ASN:HB3     | 30:O:43:LEU:HB2    | 1.78                     | 0.64              |
| 40:b:40:LYS:O       | 40:b:48:SER:HA     | 1.98                     | 0.64              |
| 61:w:80:ASN:O       | 61:w:84:VAL:HG13   | 1.98                     | 0.64              |
| 64:13:1194:LEU:HD23 | 64:13:1197:ILE:CD1 | 2.27                     | 0.64              |
| 1:0:24:THR:HG23     | 1:0:27:GLY:H       | 1.62                     | 0.63              |
| 6:17:277:SER:HA     | 65:14:1125:THR:HA  | 1.78                     | 0.63              |
| 8:3:354:C:O2        | 41:c:174:ASN:ND2   | 2.30                     | 0.63              |
| 8:3:1137:C:H2'      | 8:3:1138:A:H8      | 1.61                     | 0.63              |
| 12:7:28:G:O3'       | 27:L:117:ALA:HB1   | 1.98                     | 0.63              |
| 20:E:4:ASN:HB2      | 20:E:90:LEU:HD11   | 1.79                     | 0.63              |
| 6:17:388:ALA:HB2    | 66:15:180:PHE:CZ   | 2.32                     | 0.63              |
| 6:17:429:ASP:O      | 66:15:137:ILE:CG1  | 2.27                     | 0.63              |
| 6:17:709:ASP:O      | 14:9:674:GLU:CB    | 2.45                     | 0.63              |
| 8:3:1518:C:N4       | 8:3:2220:A:OP1     | 2.31                     | 0.63              |
| 14:9:802:GLU:CD     | 61:w:20:ILE:HD12   | 2.22                     | 0.63              |
| 16:AA:219:LEU:OXT   | 22:G:126:LYS:NZ    | 2.31                     | 0.63              |
| 43:e:47:GLU:OE1     | 43:e:49:LYS:HG3    | 1.97                     | 0.63              |
| 64:13:1192:LEU:HD23 | 67:18:88:GLN:HG2   | 0.64                     | 0.63              |
| 67:16:109:ASP:OD2   | 67:16:144:ARG:HD2  | 1.98                     | 0.63              |
| 6:17:709:ASP:OD1    | 14:9:670:PRO:CB    | 2.38                     | 0.63              |
| 8:3:788:G:H2'       | 8:3:789:A:H8       | 1.62                     | 0.63              |
| 8:3:2538:A:N7       | 43:e:175:LYS:NZ    | 2.47                     | 0.63              |
| 8:3:2823:A:O2'      | 8:3:2825:A:N7      | 2.31                     | 0.63              |
| 10:5:1467:A:O2'     | 37:Y:44:A:C1'      | 2.46                     | 0.63              |
| 27:L:52:GLU:OE1     | 27:L:52:GLU:N      | 2.25                     | 0.63              |
| 6:17:386:VAL:H      | 66:15:175:PRO:C    | 2.06                     | 0.63              |
| 8:3:1561:G:C4'      | 14:9:299:LYS:CD    | 2.45                     | 0.63              |
| 13:8:20:U:H4'       | 13:8:20:U:OP1      | 1.97                     | 0.63              |
| 21:F:115:MET:HA     | 21:F:118:LYS:HB2   | 1.81                     | 0.63              |
| 46:h:41:GLU:HG3     | 46:h:42:LYS:HG3    | 1.80                     | 0.63              |
| 67:16:105:TRP:HZ3   | 67:16:152:TYR:CD2  | 2.13                     | 0.63              |
| 6:17:701:THR:OG1    | 14:9:773:ALA:HB3   | 1.91                     | 0.63              |
| 19:C:97:LEU:HD12    | 19:C:136:LEU:HD21  | 1.79                     | 0.63              |
| 20:E:16:GLU:OE1     | 20:E:16:GLU:N      | 2.28                     | 0.63              |
| 27:L:71:ARG:HH22    | 42:d:112:ARG:HE    | 1.45                     | 0.63              |
| 8:3:1055:A:N1       | 8:3:1176:U:O2'     | 2.31                     | 0.63              |
| 8:3:1798:A:O2'      | 39:a:213:ILE:O     | 2.15                     | 0.63              |
| 8:3:2299:U:H2'      | 8:3:2300:A:C8      | 2.34                     | 0.63              |
| 8:3:2799:U:OP1      | 8:3:2896:G:N1      | 2.23                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 41:c:41:GLU:OE1    | 41:c:41:GLU:HA      | 1.98                     | 0.63              |
| 65:14:764:GLN:HE21 | 65:14:776:ASN:HB2   | 1.63                     | 0.63              |
| 6:17:693:THR:CG2   | 14:9:682:VAL:CA     | 2.75                     | 0.63              |
| 8:3:223:A:N3       | 8:3:238:U:O2'       | 2.31                     | 0.63              |
| 10:5:787:A:C8      | 12:7:37:MIA:H111    | 2.33                     | 0.63              |
| 12:7:52:G:N1       | 12:7:62:C:N3        | 2.33                     | 0.63              |
| 14:9:163:PRO:HB2   | 58:t:63:VAL:N       | 2.13                     | 0.63              |
| 67:18:18:VAL:HG12  | 67:18:87:LYS:HE3    | 1.81                     | 0.63              |
| 6:17:261:LYS:HA    | 65:14:1130:LYS:NZ   | 2.14                     | 0.63              |
| 8:3:499:G:N2       | 8:3:502:A:OP2       | 2.27                     | 0.63              |
| 14:9:798:ARG:NE    | 61:w:18:LEU:HD22    | 2.10                     | 0.63              |
| 6:17:831:PHE:CE1   | 6:17:913:VAL:HG11   | 2.34                     | 0.63              |
| 26:K:59:ASN:ND2    | 26:K:102:ASP:OD2    | 2.32                     | 0.63              |
| 46:h:14:LEU:HD13   | 46:h:19:ALA:HB1     | 1.80                     | 0.63              |
| 47:i:80:HIS:HD2    | 47:i:87:ILE:HB      | 1.64                     | 0.63              |
| 64:13:47:ALA:HB1   | 64:13:120:LEU:CD2   | 2.29                     | 0.63              |
| 65:14:947:SER:HG   | 66:15:247:LYS:NZ    | 1.94                     | 0.63              |
| 65:14:1280:LYS:HE3 | 65:14:1296:ARG:HH21 | 1.63                     | 0.63              |
| 6:17:373:VAL:CB    | 66:15:172:PRO:HG2   | 2.19                     | 0.62              |
| 6:17:386:VAL:CG1   | 66:15:177:GLY:H     | 1.88                     | 0.62              |
| 6:17:781:SER:HB2   | 6:17:789:TYR:CE1    | 2.34                     | 0.62              |
| 8:3:102:A:C4       | 14:9:782:ASP:O      | 2.43                     | 0.62              |
| 8:3:1118:U:O2'     | 8:3:1120:A:N7       | 2.31                     | 0.62              |
| 8:3:2254:G:H2'     | 8:3:2255:A:H8       | 1.64                     | 0.62              |
| 41:c:20:LEU:HD21   | 41:c:204:LEU:HD11   | 1.81                     | 0.62              |
| 41:c:116:TRP:CE2   | 41:c:191:LEU:HD11   | 2.33                     | 0.62              |
| 52:n:107:GLU:OE1   | 52:n:107:GLU:HA     | 1.98                     | 0.62              |
| 64:13:972:ASN:CG   | 67:18:256:HIS:CE1   | 2.75                     | 0.62              |
| 64:13:1062:ARG:HD2 | 67:18:73:VAL:CG2    | 2.19                     | 0.62              |
| 65:14:247:SER:O    | 65:14:254:ASN:ND2   | 2.33                     | 0.62              |
| 65:14:263:LEU:HD21 | 65:14:468:LEU:HD21  | 1.81                     | 0.62              |
| 65:14:605:GLU:OE1  | 66:15:247:LYS:CB    | 2.47                     | 0.62              |
| 6:17:261:LYS:HG3   | 65:14:1130:LYS:CG   | 2.29                     | 0.62              |
| 6:17:693:THR:CG2   | 14:9:682:VAL:N      | 2.51                     | 0.62              |
| 8:3:50:G:H22       | 8:3:180:A:H5''      | 1.64                     | 0.62              |
| 8:3:1806:G:OP1     | 39:a:268:ARG:NH1    | 2.29                     | 0.62              |
| 10:5:373:A:H2'     | 10:5:374:G:H8       | 1.62                     | 0.62              |
| 64:13:7:SER:N      | 67:18:198:LEU:CD1   | 2.62                     | 0.62              |
| 6:17:261:LYS:HE3   | 65:14:1130:LYS:CG   | 2.22                     | 0.62              |
| 6:17:261:LYS:CA    | 65:14:1130:LYS:CE   | 2.73                     | 0.62              |
| 10:5:403:A:H5''    | 19:C:111:ARG:NH1    | 2.14                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:9:163:PRO:HG2   | 58:t:63:VAL:CG2    | 2.27                     | 0.62              |
| 14:9:228:PRO:HG3   | 58:t:53:LYS:H      | 1.64                     | 0.62              |
| 14:9:795:GLN:NE2   | 61:w:18:LEU:HD11   | 2.15                     | 0.62              |
| 44:f:108:LEU:HD13  | 44:f:109:GLN:N     | 2.15                     | 0.62              |
| 54:p:70:GLU:OE1    | 54:p:70:GLU:N      | 2.32                     | 0.62              |
| 8:3:1559:A:C1'     | 14:9:247:LYS:HD3   | 2.29                     | 0.62              |
| 10:5:1468:A:O2'    | 37:Y:43:A:N3       | 2.31                     | 0.62              |
| 14:9:795:GLN:HE21  | 61:w:18:LEU:HD12   | 1.58                     | 0.62              |
| 42:d:63:GLN:HG2    | 42:d:95:ARG:HH21   | 1.65                     | 0.62              |
| 64:13:1217:LYS:CE  | 67:18:274:PRO:HB2  | 2.29                     | 0.62              |
| 65:14:173:LYS:HA   | 65:14:550:TYR:CD1  | 2.34                     | 0.62              |
| 16:AA:143:ARG:NH2  | 16:AA:145:GLY:O    | 2.32                     | 0.62              |
| 35:T:6:VAL:HG12    | 35:T:8:ASN:H       | 1.64                     | 0.62              |
| 53:o:27:ALA:HB3    | 53:o:96:VAL:HG21   | 1.80                     | 0.62              |
| 6:17:260:GLN:N     | 65:14:1098:THR:HA  | 2.03                     | 0.62              |
| 6:17:426:LYS:HG3   | 66:15:184:GLN:CD   | 2.24                     | 0.62              |
| 8:3:1561:G:O3'     | 14:9:299:LYS:HB3   | 1.99                     | 0.62              |
| 8:3:2299:U:H2'     | 8:3:2300:A:H8      | 1.64                     | 0.62              |
| 10:5:543:C:OP1     | 19:C:57:LYS:NZ     | 2.31                     | 0.62              |
| 10:5:662:G:H1'     | 10:5:730:G:H5'     | 1.81                     | 0.62              |
| 10:5:1332:U:OP1    | 28:M:35:SER:OG     | 2.17                     | 0.62              |
| 13:8:34:U8U:O4     | 17:AB:44:A:C6      | 2.51                     | 0.62              |
| 22:G:11:HIS:ND1    | 22:G:13:ASP:OD1    | 2.33                     | 0.62              |
| 44:f:87:ARG:HB2    | 44:f:88:PRO:HD3    | 1.82                     | 0.62              |
| 64:13:868:ASN:HD22 | 64:13:1002:GLN:NE2 | 1.97                     | 0.62              |
| 64:13:1062:ARG:NE  | 67:18:73:VAL:HG23  | 2.15                     | 0.62              |
| 65:14:260:ALA:HA   | 65:14:263:LEU:HD12 | 1.81                     | 0.62              |
| 5:12:96:LEU:CG     | 6:17:661:LEU:HA    | 2.15                     | 0.62              |
| 49:k:117:HIS:ND1   | 49:k:117:HIS:O     | 2.33                     | 0.62              |
| 18:x:32:LYS:CE     | 18:x:34:ILE:HD13   | 2.29                     | 0.62              |
| 64:13:290:ASP:HB2  | 64:13:511:SER:HG   | 1.63                     | 0.62              |
| 64:13:1217:LYS:HZ3 | 67:18:274:PRO:CA   | 2.13                     | 0.62              |
| 66:15:322:ALA:HB1  | 66:15:491:VAL:HG11 | 1.80                     | 0.62              |
| 5:12:88:SER:H      | 6:17:14:LYS:HB3    | 1.65                     | 0.62              |
| 6:17:685:LYS:O     | 14:9:679:ASP:HB2   | 1.99                     | 0.62              |
| 14:9:227:GLY:HA2   | 58:t:53:LYS:O      | 1.97                     | 0.62              |
| 18:AC:73:LEU:O     | 18:AC:76:LYS:HG2   | 2.00                     | 0.62              |
| 26:K:57:LYS:NZ     | 37:Y:45:A:OP1      | 2.31                     | 0.62              |
| 36:W:48:TYR:OH     | 36:W:87:LYS:HE3    | 2.00                     | 0.62              |
| 66:15:979:GLN:C    | 67:16:258:VAL:HG11 | 2.25                     | 0.62              |
| 5:12:88:SER:N      | 6:17:14:LYS:HB3    | 2.14                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:2145:A:N6      | 8:3:2161:G:O6      | 2.32                     | 0.62              |
| 17:AB:44:A:O2'     | 37:Y:45:A:O4'      | 2.16                     | 0.62              |
| 17:AB:45:A:H62     | 37:Y:45:A:N6       | 1.93                     | 0.62              |
| 6:17:591:GLU:CD    | 14:9:646:GLN:HE22  | 2.00                     | 0.62              |
| 6:17:692:LYS:HB2   | 14:9:679:ASP:O     | 2.00                     | 0.62              |
| 8:3:2266:C:O2'     | 8:3:2435:C:OP2     | 2.18                     | 0.62              |
| 10:5:874:C:OP1     | 26:K:9:ARG:NH2     | 2.33                     | 0.62              |
| 14:9:165:LEU:HG    | 58:t:62:LYS:CD     | 2.29                     | 0.62              |
| 18:AC:94:LEU:O     | 24:I:94:LYS:NZ     | 2.33                     | 0.62              |
| 19:C:68:ASP:OD1    | 19:C:69:LYS:N      | 2.32                     | 0.62              |
| 64:13:1020:MET:HB3 | 67:18:256:HIS:O    | 2.00                     | 0.62              |
| 66:15:965:LEU:HD12 | 66:15:1269:LEU:CG  | 2.28                     | 0.62              |
| 6:17:685:LYS:O     | 14:9:679:ASP:CB    | 2.48                     | 0.61              |
| 6:17:955:LYS:NZ    | 14:9:799:GLU:CD    | 2.55                     | 0.61              |
| 50:l:78:PRO:HG2    | 50:l:81:VAL:HG21   | 1.82                     | 0.61              |
| 56:r:51:LEU:O      | 56:r:55:ILE:HG13   | 1.99                     | 0.61              |
| 8:3:892:G:H2'      | 8:3:893:A:C8       | 2.34                     | 0.61              |
| 10:5:1468:A:C1'    | 37:Y:43:A:N3       | 2.62                     | 0.61              |
| 22:G:44:ILE:HD12   | 22:G:138:LEU:HD23  | 1.82                     | 0.61              |
| 42:d:148:ARG:NE    | 42:d:149:ILE:H     | 1.97                     | 0.61              |
| 3:10:238:PHE:HE1   | 6:17:563:VAL:HG22  | 1.53                     | 0.61              |
| 5:12:96:LEU:HD22   | 6:17:661:LEU:CD1   | 2.30                     | 0.61              |
| 6:17:256:THR:O     | 65:14:1099:GLN:CG  | 2.48                     | 0.61              |
| 6:17:261:LYS:CA    | 65:14:1130:LYS:HE3 | 2.28                     | 0.61              |
| 6:17:702:GLU:OE1   | 14:9:786:MET:SD    | 2.58                     | 0.61              |
| 40:b:110:VAL:HG11  | 40:b:197:ILE:HD12  | 1.81                     | 0.61              |
| 66:15:961:THR:HG22 | 66:15:1269:LEU:CD2 | 2.29                     | 0.61              |
| 67:16:255:ARG:NH1  | 67:16:259:GLN:HE21 | 1.87                     | 0.61              |
| 6:17:600:ASN:HB3   | 14:9:634:GLU:O     | 1.99                     | 0.61              |
| 6:17:689:ALA:O     | 14:9:682:VAL:CG2   | 2.49                     | 0.61              |
| 6:17:710:PHE:O     | 14:9:649:VAL:C     | 2.42                     | 0.61              |
| 8:3:1798:A:C2      | 8:3:1836:A:H4'     | 2.35                     | 0.61              |
| 8:3:2688:C:H5'     | 40:b:198:ALA:HA    | 1.81                     | 0.61              |
| 10:5:535:A:H5''    | 26:K:123:ARG:HH12  | 1.65                     | 0.61              |
| 30:O:5:ARG:HA      | 30:O:69:VAL:HG21   | 1.82                     | 0.61              |
| 61:w:49:ARG:HG3    | 61:w:49:ARG:HH11   | 1.66                     | 0.61              |
| 6:17:79:SER:OG     | 65:14:1270:LEU:CB  | 2.47                     | 0.61              |
| 6:17:691:THR:O     | 14:9:682:VAL:HG12  | 1.97                     | 0.61              |
| 14:9:274:PHE:HA    | 57:s:21:MET:SD     | 2.39                     | 0.61              |
| 61:w:23:LYS:HD2    | 61:w:51:LEU:HD21   | 1.82                     | 0.61              |
| 64:13:166:PHE:HB2  | 64:13:184:SER:HB2  | 1.83                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:13:997:LYS:C     | 64:13:999:GLN:N     | 2.59                     | 0.61              |
| 65:14:1090:LYS:NZ   | 65:14:1138:ASP:OD1  | 2.28                     | 0.61              |
| 8:3:1000:U:O2'      | 8:3:2281:A:N3       | 2.34                     | 0.61              |
| 27:L:71:ARG:CZ      | 42:d:113:ASP:OD2    | 2.49                     | 0.61              |
| 6:17:432:LYS:HG3    | 66:15:556:GLN:HE22  | 1.56                     | 0.61              |
| 8:3:1600:A:N3       | 39:a:62:ASN:ND2     | 2.49                     | 0.61              |
| 48:j:27:SER:OG      | 48:j:28:THR:N       | 2.33                     | 0.61              |
| 64:13:984:GLN:HG3   | 64:13:1133:THR:N    | 1.77                     | 0.61              |
| 66:15:558:TRP:O     | 66:15:566:LYS:NZ    | 2.33                     | 0.61              |
| 66:15:888:PHE:HB3   | 66:15:935:LEU:HD22  | 1.81                     | 0.61              |
| 6:17:711:PHE:CE2    | 14:9:649:VAL:C      | 2.77                     | 0.61              |
| 6:17:955:LYS:CD     | 14:9:803:LYS:HE3    | 2.30                     | 0.61              |
| 8:3:316:C:H2'       | 8:3:392:A:N6        | 2.15                     | 0.61              |
| 14:9:798:ARG:NH2    | 61:w:18:LEU:CG      | 2.64                     | 0.61              |
| 64:13:61:ASN:HA     | 64:13:608:ALA:HB2   | 1.83                     | 0.61              |
| 65:14:101:THR:CG2   | 65:14:703:GLN:HE21  | 2.14                     | 0.61              |
| 65:14:605:GLU:O     | 66:15:247:LYS:O     | 2.18                     | 0.61              |
| 65:14:605:GLU:HA    | 66:15:248:THR:CG2   | 2.31                     | 0.61              |
| 66:15:1116:ILE:HG21 | 66:15:1248:LEU:HD11 | 1.83                     | 0.61              |
| 6:17:695:SER:O      | 14:9:689:ILE:HB     | 2.00                     | 0.61              |
| 57:s:52:PRO:HB3     | 57:s:83:ILE:HG23    | 1.82                     | 0.61              |
| 64:13:1213:LEU:CB   | 67:18:276:ASN:CG    | 2.71                     | 0.61              |
| 65:14:391:ASP:OD2   | 65:14:398:LYS:NZ    | 2.34                     | 0.61              |
| 8:3:1117:U:H2'      | 8:3:1118:U:O4'      | 2.00                     | 0.61              |
| 9:4:11:A:H2'        | 9:4:12:U:H5''       | 1.82                     | 0.61              |
| 10:5:1264:G:OP1     | 21:F:34:LYS:NZ      | 2.34                     | 0.61              |
| 14:9:313:LYS:HD3    | 38:Z:2:UNK:O        | 2.01                     | 0.61              |
| 45:g:24:PHE:N       | 45:g:112:TYR:O      | 2.30                     | 0.61              |
| 18:x:6:HIS:ND1      | 18:x:7:PHE:HE1      | 1.90                     | 0.61              |
| 64:13:238:GLU:OE1   | 64:13:253:LYS:HD2   | 2.01                     | 0.61              |
| 66:15:1035:ASP:HB2  | 66:15:1058:LEU:O    | 2.01                     | 0.61              |
| 6:17:699:ILE:CG2    | 14:9:689:ILE:O      | 2.50                     | 0.60              |
| 6:17:700:LEU:CD2    | 14:9:658:LEU:CA     | 2.75                     | 0.60              |
| 8:3:620:G:H1        | 49:k:34:ARG:HH11    | 1.48                     | 0.60              |
| 10:5:1153:G:N2      | 10:5:1156:G:OP2     | 2.35                     | 0.60              |
| 10:5:1508:C:H42     | 15:A:294:GLU:HA     | 1.66                     | 0.60              |
| 22:G:13:ASP:OD2     | 22:G:16:ALA:HB3     | 2.01                     | 0.60              |
| 24:I:24:LEU:HD21    | 24:I:78:ARG:HG2     | 1.83                     | 0.60              |
| 64:13:986:ILE:CD1   | 64:13:1130:PRO:CB   | 2.73                     | 0.60              |
| 6:17:595:ARG:HH22   | 14:9:644:LYS:NZ     | 1.93                     | 0.60              |
| 8:3:147:C:H4'       | 61:w:66:GLN:NE2     | 2.16                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 14:9:163:PRO:HB2    | 58:t:63:VAL:HG23   | 1.82                     | 0.60              |
| 27:L:71:ARG:NH2     | 42:d:113:ASP:OD2   | 2.34                     | 0.60              |
| 44:f:96:GLN:NE2     | 44:f:121:PHE:HB3   | 2.15                     | 0.60              |
| 61:w:16:VAL:HG11    | 61:w:68:GLU:HG2    | 1.83                     | 0.60              |
| 66:15:839:TRP:NE1   | 66:15:843:ASN:HD21 | 1.97                     | 0.60              |
| 67:18:202:SER:OG    | 67:18:204:HIS:HE1  | 1.83                     | 0.60              |
| 8:3:410:G:H4'       | 8:3:411:U:O5'      | 2.01                     | 0.60              |
| 8:3:477:U:O2        | 41:c:47:GLN:NE2    | 2.33                     | 0.60              |
| 8:3:615:G:H2'       | 8:3:616:G:H8       | 1.65                     | 0.60              |
| 8:3:880:C:H41       | 8:3:968:U:H2'      | 1.66                     | 0.60              |
| 10:5:528:G:C6       | 13:8:35:U:O2       | 2.53                     | 0.60              |
| 10:5:1022:G:H21     | 10:5:1026:A:H62    | 1.47                     | 0.60              |
| 17:AB:41:U:C3'      | 37:Y:42:C:H6       | 2.14                     | 0.60              |
| 42:d:34:ILE:CD1     | 42:d:96:MET:HB2    | 2.31                     | 0.60              |
| 66:15:1106:SER:O    | 67:16:254:LYS:CG   | 2.49                     | 0.60              |
| 8:3:2098:U:H3'      | 8:3:2099:U:H5''    | 1.83                     | 0.60              |
| 10:5:1468:A:H4'     | 37:Y:43:A:HO2'     | 1.61                     | 0.60              |
| 14:9:795:GLN:HG3    | 61:w:18:LEU:HD11   | 1.82                     | 0.60              |
| 22:G:123:MET:HG3    | 22:G:127:VAL:HG13  | 1.83                     | 0.60              |
| 64:13:62:GLU:HB2    | 64:13:174:THR:HG21 | 1.83                     | 0.60              |
| 64:13:1062:ARG:HH11 | 67:18:73:VAL:HG23  | 1.66                     | 0.60              |
| 5:12:88:SER:CA      | 6:17:615:PHE:HE2   | 2.14                     | 0.60              |
| 6:17:258:ASN:OD1    | 65:14:1126:LEU:CD1 | 2.47                     | 0.60              |
| 6:17:261:LYS:CG     | 65:14:1102:PHE:HB2 | 2.19                     | 0.60              |
| 6:17:263:VAL:C      | 65:14:1095:GLY:O   | 2.44                     | 0.60              |
| 6:17:426:LYS:HZ2    | 66:15:183:LEU:N    | 1.90                     | 0.60              |
| 6:17:704:ASN:C      | 14:9:665:HIS:CE1   | 2.79                     | 0.60              |
| 8:3:2667:G:N2       | 8:3:2670:A:OP2     | 2.29                     | 0.60              |
| 10:5:293:G:N2       | 10:5:296:A:OP2     | 2.34                     | 0.60              |
| 14:9:228:PRO:C      | 58:t:53:LYS:HD2    | 2.26                     | 0.60              |
| 14:9:804:SER:CB     | 57:s:96:GLU:O      | 2.50                     | 0.60              |
| 15:A:45:ILE:HD11    | 15:A:204:THR:HG23  | 1.83                     | 0.60              |
| 17:AB:43:A:H2'      | 37:Y:43:A:C4       | 2.35                     | 0.60              |
| 46:h:57:ALA:HA      | 46:h:63:PHE:CE2    | 2.36                     | 0.60              |
| 48:j:85:VAL:HG21    | 48:j:114:ILE:HD13  | 1.84                     | 0.60              |
| 5:12:96:LEU:CD2     | 6:17:661:LEU:CB    | 2.77                     | 0.60              |
| 6:17:432:LYS:HE2    | 66:15:556:GLN:CD   | 2.27                     | 0.60              |
| 8:3:2475:C:O2       | 50:l:124:LYS:NZ    | 2.32                     | 0.60              |
| 14:9:313:LYS:HE2    | 38:Z:1:UNK:O       | 2.02                     | 0.60              |
| 66:15:71:ARG:HH11   | 66:15:132:LEU:HD21 | 1.64                     | 0.60              |
| 5:12:84:VAL:CA      | 6:17:8:SER:N       | 2.65                     | 0.60              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:386:VAL:CG2   | 66:15:174:ASP:O     | 2.32                     | 0.60              |
| 6:17:422:ASP:OD2   | 66:15:135:SER:CB    | 2.44                     | 0.60              |
| 8:3:1561:G:O2'     | 14:9:299:LYS:NZ     | 2.35                     | 0.60              |
| 14:9:313:LYS:CD    | 38:Z:2:UNK:O        | 2.50                     | 0.60              |
| 45:g:29:TYR:HB2    | 45:g:79:LYS:HD3     | 1.81                     | 0.60              |
| 46:h:25:LEU:HB3    | 46:h:30:ILE:HD12    | 1.83                     | 0.60              |
| 6:17:259:GLY:CA    | 65:14:1098:THR:CA   | 2.73                     | 0.60              |
| 6:17:261:LYS:CB    | 65:14:1126:LEU:HD21 | 2.31                     | 0.60              |
| 6:17:432:LYS:HG3   | 66:15:556:GLN:NE2   | 2.12                     | 0.60              |
| 8:3:1833:G:O2'     | 8:3:1978:U:OP2      | 2.20                     | 0.60              |
| 14:9:798:ARG:NE    | 61:w:18:LEU:O       | 2.33                     | 0.60              |
| 23:H:12:ARG:HH22   | 23:H:111:ARG:HH21   | 1.47                     | 0.60              |
| 48:j:86:LEU:HB3    | 48:j:94:ARG:HD2     | 1.83                     | 0.60              |
| 64:13:53:ALA:C     | 64:13:612:LEU:HD12  | 2.26                     | 0.60              |
| 6:17:430:PRO:HD2   | 66:15:555:PHE:CE1   | 2.37                     | 0.60              |
| 8:3:2328:A:HO2'    | 8:3:2341:G:N2       | 2.00                     | 0.60              |
| 14:9:807:GLY:C     | 61:w:79:THR:HG23    | 2.25                     | 0.60              |
| 15:A:99:ILE:HD13   | 15:A:233:ALA:HB2    | 1.82                     | 0.60              |
| 46:h:76:LEU:HD11   | 46:h:127:THR:HG23   | 1.83                     | 0.60              |
| 64:13:765:LEU:HD11 | 64:13:781:LEU:HD11  | 1.83                     | 0.60              |
| 65:14:16:SER:HB3   | 65:14:1282:GLY:HA3  | 1.82                     | 0.60              |
| 8:3:1919:A:C2      | 10:5:1382:C:O2'     | 2.54                     | 0.60              |
| 17:AB:43:A:N3      | 37:Y:44:A:N7        | 2.49                     | 0.60              |
| 42:d:108:LEU:HB3   | 42:d:114:PHE:HE2    | 1.67                     | 0.60              |
| 44:f:96:GLN:HB3    | 44:f:100:GLN:HE22   | 1.67                     | 0.60              |
| 44:f:130:ILE:HD11  | 44:f:144:PRO:HG3    | 1.84                     | 0.60              |
| 65:14:191:LYS:HG3  | 65:14:537:LEU:HG    | 1.83                     | 0.60              |
| 66:15:239:PRO:HG2  | 66:15:350:ASN:OD1   | 2.01                     | 0.60              |
| 6:17:690:LEU:C     | 14:9:682:VAL:CB     | 2.74                     | 0.59              |
| 6:17:767:MET:HE1   | 6:17:805:PHE:CZ     | 2.36                     | 0.59              |
| 8:3:519:A:C2       | 14:9:165:LEU:HD11   | 2.36                     | 0.59              |
| 8:3:520:C:H5'      | 14:9:160:ASN:O      | 2.01                     | 0.59              |
| 14:9:795:GLN:O     | 61:w:21:LYS:HE2     | 2.02                     | 0.59              |
| 26:K:63:ARG:HG2    | 26:K:79:TYR:HE1     | 1.66                     | 0.59              |
| 65:14:605:GLU:HG2  | 65:14:961:ARG:NH2   | 2.17                     | 0.59              |
| 66:15:1237:PRO:HG2 | 66:15:1239:HIS:CD2  | 2.37                     | 0.59              |
| 6:17:700:LEU:CB    | 14:9:658:LEU:HA     | 2.32                     | 0.59              |
| 8:3:1343:C:O2'     | 8:3:1420:A:N3       | 2.32                     | 0.59              |
| 8:3:1569:A:H2'     | 8:3:1570:A:C2       | 2.37                     | 0.59              |
| 10:5:528:G:C2      | 13:8:35:U:O2        | 2.54                     | 0.59              |
| 52:n:84:LEU:HB3    | 52:n:86:LEU:HD12    | 1.83                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:17:385:ASP:CA     | 66:15:64:LYS:CB     | 2.79                     | 0.59              |
| 10:5:1425:A:H2'     | 10:5:1427:U:H3      | 1.65                     | 0.59              |
| 10:5:1448:A:H2'     | 10:5:1449:G:C8      | 2.37                     | 0.59              |
| 15:A:293:ARG:HE     | 35:T:50:GLN:HG2     | 1.66                     | 0.59              |
| 39:a:128:ILE:CG2    | 39:a:129:ASP:H      | 1.92                     | 0.59              |
| 50:l:35:VAL:HG22    | 50:l:102:VAL:HG22   | 1.84                     | 0.59              |
| 64:13:290:ASP:HB3   | 64:13:511:SER:OG    | 2.01                     | 0.59              |
| 64:13:986:ILE:CG1   | 64:13:1130:PRO:CB   | 2.80                     | 0.59              |
| 65:14:389:ASP:OD2   | 66:15:243:GLN:NE2   | 2.34                     | 0.59              |
| 66:15:965:LEU:CD1   | 66:15:1269:LEU:HG   | 2.31                     | 0.59              |
| 66:15:1154:GLU:OE1  | 67:16:72:ALA:HA     | 2.02                     | 0.59              |
| 6:17:25:GLY:C       | 6:17:652:ILE:HD11   | 2.27                     | 0.59              |
| 6:17:82:ASN:CG      | 65:14:1268:ASN:ND2  | 2.60                     | 0.59              |
| 6:17:251:ASP:C      | 65:14:1100:THR:O    | 2.45                     | 0.59              |
| 6:17:426:LYS:CE     | 66:15:183:LEU:H     | 2.15                     | 0.59              |
| 13:8:35:U:N3        | 17:AB:44:A:H2       | 1.85                     | 0.59              |
| 14:9:225:ILE:HD12   | 58:t:57:LYS:CG      | 2.25                     | 0.59              |
| 28:M:21:TYR:HE1     | 28:M:23:ARG:HE      | 1.50                     | 0.59              |
| 6:17:25:GLY:CA      | 6:17:652:ILE:HD11   | 2.32                     | 0.59              |
| 6:17:260:GLN:CA     | 65:14:1126:LEU:HD23 | 2.33                     | 0.59              |
| 6:17:261:LYS:HG3    | 65:14:1130:LYS:HE3  | 1.79                     | 0.59              |
| 8:3:695:G:H5''      | 41:c:101:LEU:HD22   | 1.83                     | 0.59              |
| 36:W:42:ASN:O       | 36:W:46:VAL:HG22    | 2.03                     | 0.59              |
| 41:c:5:LYS:HD2      | 41:c:13:PHE:CE2     | 2.37                     | 0.59              |
| 6:17:697:TYR:CZ     | 14:9:636:PHE:CE1    | 2.48                     | 0.59              |
| 8:3:13:C:H3'        | 8:3:14:U:H5'        | 1.84                     | 0.59              |
| 8:3:519:A:N3        | 14:9:165:LEU:HD12   | 2.13                     | 0.59              |
| 8:3:1797:C:H2'      | 8:3:1798:A:C8       | 2.37                     | 0.59              |
| 16:AA:212:ARG:NH1   | 22:G:111:LEU:O      | 2.36                     | 0.59              |
| 19:C:179:VAL:HG12   | 19:C:180:ARG:H      | 1.67                     | 0.59              |
| 39:a:41:LEU:HG      | 39:a:66:TYR:HB2     | 1.84                     | 0.59              |
| 66:15:1108:ALA:HB1  | 66:15:1112:LEU:HD23 | 1.85                     | 0.59              |
| 6:17:691:THR:CA     | 14:9:682:VAL:CG1    | 2.80                     | 0.59              |
| 19:C:81:GLN:HB2     | 19:C:85:LEU:HD11    | 1.84                     | 0.59              |
| 19:C:99:ASN:O       | 19:C:103:ARG:HG2    | 2.02                     | 0.59              |
| 39:a:33:PRO:HB2     | 39:a:38:LEU:HD11    | 1.83                     | 0.59              |
| 65:14:1183:ARG:HH21 | 65:14:1222:ASP:CG   | 2.11                     | 0.59              |
| 66:15:1071:PHE:HE1  | 66:15:1209:GLU:HB3  | 1.65                     | 0.59              |
| 66:15:1173:LEU:HD23 | 66:15:1189:LYS:HG2  | 1.83                     | 0.59              |
| 67:16:128:ASN:O     | 67:16:136:LYS:CE    | 2.51                     | 0.59              |
| 5:12:97:LEU:HG      | 6:17:664:ILE:HG23   | 1.83                     | 0.59              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:3:881:A:H1'      | 8:3:882:C:C5'       | 2.32                     | 0.59              |
| 8:3:1246:U:P       | 54:p:7:LYS:HZ1      | 2.26                     | 0.59              |
| 8:3:1618:U:H4'     | 8:3:1619:A:OP2      | 2.01                     | 0.59              |
| 8:3:2026:A:OP2     | 62:y:6:ARG:NH2      | 2.36                     | 0.59              |
| 21:F:117:GLU:OE1   | 21:F:117:GLU:N      | 2.31                     | 0.59              |
| 27:L:50:GLU:OE1    | 27:L:50:GLU:N       | 2.32                     | 0.59              |
| 32:Q:94:ARG:HB3    | 32:Q:101:PHE:CE1    | 2.38                     | 0.59              |
| 39:a:129:ASP:O     | 39:a:136:MET:HE1    | 2.03                     | 0.59              |
| 64:13:52:LYS:HD2   | 64:13:772:VAL:HG21  | 1.85                     | 0.59              |
| 65:14:22:ARG:NE    | 65:14:746:GLU:OE1   | 2.36                     | 0.59              |
| 66:15:991:TRP:CZ2  | 66:15:1260:LEU:HD11 | 2.37                     | 0.59              |
| 66:15:1071:PHE:CE2 | 66:15:1247:ARG:CD   | 2.86                     | 0.59              |
| 6:17:390:ALA:N     | 66:15:71:ARG:HH12   | 2.01                     | 0.59              |
| 8:3:343:A:N3       | 8:3:363:G:O2'       | 2.34                     | 0.59              |
| 10:5:661:G:OP1     | 32:Q:84:ARG:NH1     | 2.36                     | 0.59              |
| 26:K:32:ASN:ND2    | 26:K:32:ASN:O       | 2.36                     | 0.59              |
| 50:l:47:ILE:HD11   | 50:l:68:ILE:HD11    | 1.84                     | 0.59              |
| 56:r:15:GLN:CD     | 62:y:17:ARG:NH1     | 2.60                     | 0.59              |
| 66:15:325:ASP:OD1  | 66:15:432:ARG:NH2   | 2.36                     | 0.59              |
| 6:17:690:LEU:O     | 14:9:682:VAL:CB     | 2.50                     | 0.59              |
| 6:17:698:SER:CA    | 14:9:769:ILE:HG21   | 2.30                     | 0.59              |
| 10:5:354:U:H2'     | 10:5:355:A:H8       | 1.67                     | 0.59              |
| 10:5:577:G:H5'     | 10:5:725:A:H1'      | 1.85                     | 0.59              |
| 17:AB:44:A:N3      | 37:Y:45:A:C5        | 2.71                     | 0.59              |
| 29:N:15:HIS:O      | 29:N:18:ASP:HB3     | 2.02                     | 0.59              |
| 40:b:47:TYR:HD1    | 40:b:85:ARG:NE      | 2.01                     | 0.59              |
| 45:g:119:ASN:H     | 45:g:122:ASP:HB2    | 1.68                     | 0.59              |
| 52:n:31:MET:CE     | 52:n:44:TRP:HB2     | 2.32                     | 0.59              |
| 64:13:20:PHE:HB3   | 64:13:1209:ILE:CD1  | 2.33                     | 0.59              |
| 64:13:398:GLN:HA   | 64:13:414:LYS:HZ3   | 1.67                     | 0.59              |
| 66:15:675:GLN:NE2  | 66:15:711:GLY:O     | 2.35                     | 0.59              |
| 66:15:1105:VAL:C   | 67:16:254:LYS:HB2   | 2.19                     | 0.59              |
| 6:17:429:ASP:N     | 66:15:549:LEU:HD22  | 2.18                     | 0.58              |
| 6:17:916:PHE:O     | 6:17:920:VAL:HG23   | 2.03                     | 0.58              |
| 8:3:1095:U:H1'     | 8:3:1096:U:H3'      | 1.85                     | 0.58              |
| 10:5:787:A:N7      | 12:7:37:MIA:H111    | 2.18                     | 0.58              |
| 10:5:1468:A:N6     | 13:8:36:U:HO2'      | 2.01                     | 0.58              |
| 39:a:65:LYS:O      | 39:a:67:ARG:NH1     | 2.36                     | 0.58              |
| 44:f:68:LEU:HD13   | 44:f:108:LEU:HD21   | 1.84                     | 0.58              |
| 8:3:1559:A:C1'     | 14:9:247:LYS:CE     | 2.81                     | 0.58              |
| 33:R:21:ASP:O      | 33:R:24:LYS:HG2     | 2.03                     | 0.58              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:W:114:LEU:HD23  | 36:W:114:LEU:H      | 1.68                     | 0.58              |
| 54:p:86:ASN:OD1    | 54:p:118:LYS:NZ     | 2.36                     | 0.58              |
| 65:14:343:ASN:OD1  | 65:14:440:ALA:HB2   | 2.04                     | 0.58              |
| 65:14:605:GLU:CA   | 66:15:248:THR:HG22  | 2.33                     | 0.58              |
| 66:15:671:VAL:HG13 | 66:15:717:GLU:HG2   | 1.85                     | 0.58              |
| 8:3:1270:C:H2'     | 8:3:1271:A:H8       | 1.66                     | 0.58              |
| 9:4:40:U:H5''      | 42:d:64:LYS:HD2     | 1.85                     | 0.58              |
| 10:5:1467:A:H1'    | 37:Y:44:A:C2'       | 2.29                     | 0.58              |
| 12:7:35:A:H61      | 17:AB:41:U:H3       | 1.49                     | 0.58              |
| 14:9:784:GLU:O     | 61:w:6:GLU:CD       | 2.46                     | 0.58              |
| 17:AB:41:U:N1      | 37:Y:42:C:C5        | 2.71                     | 0.58              |
| 20:E:6:ILE:HD13    | 32:Q:54:ILE:HD11    | 1.83                     | 0.58              |
| 21:F:128:ASN:O     | 21:F:130:THR:HG23   | 2.03                     | 0.58              |
| 41:c:82:PRO:HB3    | 41:c:90:VAL:HG23    | 1.85                     | 0.58              |
| 65:14:858:ASN:CG   | 65:14:1228:THR:HG23 | 2.29                     | 0.58              |
| 8:3:140:G:N2       | 8:3:143:A:OP2       | 2.26                     | 0.58              |
| 9:4:55:A:C5        | 42:d:26:MET:HE1     | 2.39                     | 0.58              |
| 10:5:1330:A:H2'    | 10:5:1331:A:C8      | 2.39                     | 0.58              |
| 12:7:28:G:O3'      | 27:L:117:ALA:HB2    | 2.03                     | 0.58              |
| 33:R:36:ARG:HB3    | 33:R:72:GLY:HA3     | 1.84                     | 0.58              |
| 42:d:40:VAL:HG21   | 42:d:42:ASP:OD1     | 2.03                     | 0.58              |
| 46:h:58:TYR:CE2    | 46:h:60:ASP:HB3     | 2.38                     | 0.58              |
| 64:13:986:ILE:CG1  | 64:13:1130:PRO:HB3  | 2.34                     | 0.58              |
| 65:14:316:LYS:HG2  | 65:14:454:GLN:HE22  | 1.67                     | 0.58              |
| 6:17:387:VAL:CA    | 66:15:68:ILE:CG1    | 2.74                     | 0.58              |
| 8:3:201:A:N6       | 8:3:2438:A:O2'      | 2.37                     | 0.58              |
| 8:3:1031:U:O2'     | 47:i:4:THR:HG21     | 2.03                     | 0.58              |
| 8:3:1559:A:O2'     | 14:9:247:LYS:HD3    | 2.03                     | 0.58              |
| 8:3:2308:U:H2'     | 8:3:2309:A:C8       | 2.36                     | 0.58              |
| 8:3:2311:G:H21     | 42:d:129:THR:HG21   | 1.68                     | 0.58              |
| 30:O:59:LEU:HD11   | 30:O:73:PHE:HE2     | 1.68                     | 0.58              |
| 39:a:154:PRO:HB3   | 39:a:195:GLU:HG3    | 1.85                     | 0.58              |
| 64:13:1035:LYS:C   | 64:13:1070:LEU:HD23 | 2.29                     | 0.58              |
| 65:14:68:ARG:HD2   | 65:14:130:ARG:HH21  | 1.66                     | 0.58              |
| 66:15:954:LYS:HB3  | 66:15:1274:LEU:CD2  | 2.34                     | 0.58              |
| 6:17:385:ASP:CB    | 66:15:64:LYS:CB     | 2.81                     | 0.58              |
| 8:3:1909:C:O2'     | 39:a:251:ARG:O      | 2.19                     | 0.58              |
| 31:P:8:VAL:HG12    | 31:P:64:VAL:HG12    | 1.86                     | 0.58              |
| 43:e:92:LEU:HD21   | 43:e:97:TYR:CB      | 2.29                     | 0.58              |
| 65:14:80:PHE:HB2   | 65:14:114:TRP:CZ3   | 2.39                     | 0.58              |
| 6:17:397:LYS:HE2   | 66:15:67:ASN:CB     | 2.34                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:17:691:THR:HG1    | 14:9:683:HIS:HE1    | 1.50                     | 0.58              |
| 10:5:164:C:H2'      | 10:5:165:A:H8       | 1.68                     | 0.58              |
| 10:5:373:A:H2'      | 10:5:374:G:C8       | 2.38                     | 0.58              |
| 16:AA:177:ASP:OD1   | 16:AA:177:ASP:N     | 2.36                     | 0.58              |
| 36:W:48:TYR:CE1     | 36:W:88:ILE:HG22    | 2.38                     | 0.58              |
| 36:W:158:GLY:HA3    | 36:W:199:ILE:HD13   | 1.85                     | 0.58              |
| 51:m:50:THR:HA      | 51:m:53:LYS:HE3     | 1.85                     | 0.58              |
| 52:n:29:VAL:HG11    | 52:n:46:PHE:CE1     | 2.37                     | 0.58              |
| 66:15:153:THR:O     | 66:15:536:ASN:ND2   | 2.37                     | 0.58              |
| 66:15:286:GLY:HA2   | 66:15:487:LEU:HD22  | 1.83                     | 0.58              |
| 3:10:238:PHE:CB     | 6:17:562:ALA:HB1    | 2.34                     | 0.58              |
| 6:17:710:PHE:CD2    | 14:9:654:LEU:CD2    | 2.85                     | 0.58              |
| 6:17:874:ARG:HH12   | 14:9:647:ASN:HD21   | 0.64                     | 0.58              |
| 8:3:1386:G:O2'      | 8:3:1401:A:N6       | 2.36                     | 0.58              |
| 10:5:1078:G:H5'     | 10:5:1078:G:H8      | 1.69                     | 0.58              |
| 36:W:37:ASP:HB2     | 36:W:58:ILE:HD12    | 1.86                     | 0.58              |
| 64:13:921:THR:HG21  | 67:18:84:THR:HG23   | 1.84                     | 0.58              |
| 65:14:1218:VAL:HG13 | 65:14:1242:LEU:HD22 | 1.85                     | 0.58              |
| 8:3:1119:A:H2'      | 8:3:1120:A:C8       | 2.39                     | 0.58              |
| 10:5:181:G:O2'      | 31:P:3:ARG:NH1      | 2.36                     | 0.58              |
| 10:5:1332:U:H3      | 10:5:1338:A:N6      | 2.02                     | 0.58              |
| 64:13:982:THR:O     | 64:13:1134:GLY:HA3  | 2.04                     | 0.58              |
| 67:16:195:LYS:HE2   | 67:16:199:ASP:OD1   | 2.03                     | 0.58              |
| 8:3:583:U:O4        | 47:i:3:LYS:HD3      | 2.03                     | 0.58              |
| 8:3:622:U:H2'       | 8:3:623:A:C8        | 2.39                     | 0.58              |
| 20:E:112:ARG:NH1    | 32:Q:46:ILE:HG23    | 2.19                     | 0.58              |
| 41:c:132:LEU:HA     | 41:c:135:LYS:HB2    | 1.86                     | 0.58              |
| 45:g:10:GLN:O       | 45:g:14:VAL:HG13    | 2.03                     | 0.58              |
| 64:13:373:TYR:HE1   | 64:13:375:ASP:OD1   | 1.87                     | 0.58              |
| 65:14:87:LEU:HD11   | 65:14:103:ILE:HD12  | 1.86                     | 0.58              |
| 65:14:209:VAL:HG21  | 65:14:467:HIS:CE1   | 2.39                     | 0.58              |
| 66:15:40:GLU:CD     | 66:15:829:TRP:HZ2   | 2.12                     | 0.58              |
| 66:15:1104:SER:CB   | 67:16:256:HIS:HA    | 2.31                     | 0.58              |
| 6:17:695:SER:O      | 14:9:633:VAL:CG2    | 2.16                     | 0.57              |
| 8:3:585:U:H2'       | 8:3:586:G:H8        | 1.68                     | 0.57              |
| 17:AB:43:A:C2       | 37:Y:44:A:C5        | 2.92                     | 0.57              |
| 44:f:103:THR:HG21   | 44:f:110:LYS:HD3    | 1.86                     | 0.57              |
| 53:o:54:ARG:HB2     | 53:o:100:TYR:CD1    | 2.39                     | 0.57              |
| 64:13:251:ARG:NH1   | 64:13:300:ASP:HA    | 2.18                     | 0.57              |
| 64:13:332:VAL:HG12  | 64:13:514:LEU:HD13  | 1.86                     | 0.57              |
| 65:14:38:ARG:NH2    | 65:14:578:ALA:HA    | 2.19                     | 0.57              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:955:LYS:NZ    | 14:9:799:GLU:CB     | 0.43                     | 0.57              |
| 8:3:1246:U:P       | 54:p:7:LYS:NZ       | 2.76                     | 0.57              |
| 27:L:73:ILE:O      | 27:L:77:ILE:HG12    | 2.05                     | 0.57              |
| 50:l:116:LYS:HD3   | 50:l:120:ARG:NH2    | 2.19                     | 0.57              |
| 18:x:14:PHE:CE2    | 18:x:34:ILE:HB      | 2.39                     | 0.57              |
| 65:14:397:TYR:CE2  | 65:14:615:LEU:HD11  | 2.38                     | 0.57              |
| 66:15:1143:LYS:CE  | 66:15:1194:VAL:HG13 | 2.32                     | 0.57              |
| 6:17:955:LYS:HD3   | 14:9:803:LYS:CD     | 2.33                     | 0.57              |
| 8:3:720:A:OP1      | 8:3:721:G:N2        | 2.37                     | 0.57              |
| 8:3:1670:U:H2'     | 8:3:1671:C:C6       | 2.38                     | 0.57              |
| 14:9:163:PRO:HD2   | 58:t:46:LYS:HG3     | 1.86                     | 0.57              |
| 14:9:165:LEU:HG    | 58:t:62:LYS:HG2     | 1.87                     | 0.57              |
| 15:A:147:LYS:O     | 15:A:151:MET:HG3    | 2.04                     | 0.57              |
| 64:13:277:THR:OG1  | 64:13:450:PHE:HE2   | 1.87                     | 0.57              |
| 66:15:4:LEU:HD11   | 66:15:99:PRO:HD2    | 1.87                     | 0.57              |
| 8:3:102:A:N6       | 14:9:785:LEU:HD23   | 2.19                     | 0.57              |
| 8:3:2797:C:O2      | 8:3:2895:A:O2'      | 2.22                     | 0.57              |
| 8:3:2813:A:H2'     | 8:3:2814:A:C8       | 2.39                     | 0.57              |
| 10:5:424:U:OP1     | 19:C:12:ARG:NH2     | 2.38                     | 0.57              |
| 13:8:31:A:N1       | 13:8:38:A:N6        | 2.52                     | 0.57              |
| 38:Z:20:UNK:CB     | 56:r:95:MET:HE1     | 2.33                     | 0.57              |
| 44:f:4:ILE:HG22    | 44:f:18:VAL:HG22    | 1.87                     | 0.57              |
| 65:14:200:GLU:OE2  | 65:14:291:LYS:HB3   | 2.03                     | 0.57              |
| 65:14:753:ILE:HG21 | 65:14:782:TRP:CZ2   | 2.38                     | 0.57              |
| 66:15:1139:LYS:HE2 | 66:15:1198:ASP:HA   | 1.86                     | 0.57              |
| 14:9:199:LYS:NZ    | 58:t:59:SER:HB2     | 2.20                     | 0.57              |
| 14:9:787:LYS:HG2   | 61:w:3:VAL:HG13     | 1.86                     | 0.57              |
| 40:b:45:ASP:O      | 40:b:46:LYS:HB2     | 2.05                     | 0.57              |
| 42:d:100:LEU:O     | 42:d:104:ILE:HG22   | 2.04                     | 0.57              |
| 45:g:27:PHE:O      | 45:g:81:ALA:N       | 2.37                     | 0.57              |
| 57:s:8:LEU:HB2     | 57:s:30:VAL:HG23    | 1.86                     | 0.57              |
| 66:15:386:LYS:HE3  | 66:15:424:HIS:CG    | 2.39                     | 0.57              |
| 6:17:258:ASN:C     | 65:14:1126:LEU:HD22 | 2.29                     | 0.57              |
| 6:17:259:GLY:O     | 65:14:1098:THR:N    | 2.36                     | 0.57              |
| 8:3:180:A:H5'      | 8:3:181:G:C8        | 2.40                     | 0.57              |
| 8:3:916:U:H2'      | 8:3:917:G:C8        | 2.39                     | 0.57              |
| 8:3:1564:U:OP2     | 14:9:302:GLU:OE2    | 2.22                     | 0.57              |
| 42:d:110:ARG:HH21  | 42:d:137:ILE:C      | 2.13                     | 0.57              |
| 42:d:148:ARG:HE    | 42:d:149:ILE:N      | 2.02                     | 0.57              |
| 65:14:152:LYS:NZ   | 65:14:505:ASP:OD1   | 2.37                     | 0.57              |
| 66:15:1104:SER:HG  | 67:16:256:HIS:HA    | 1.65                     | 0.57              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 67:18:30:GLU:HG2  | 67:18:44:TYR:CE2    | 2.40                     | 0.57              |
| 67:18:128:ASN:O   | 67:18:136:LYS:CE    | 2.53                     | 0.57              |
| 6:17:80:GLY:O     | 65:14:1268:ASN:CG   | 2.48                     | 0.57              |
| 6:17:797:LEU:HD12 | 6:17:836:GLN:HE22   | 1.68                     | 0.57              |
| 10:5:1019:G:O2'   | 10:5:1020:G:OP2     | 2.21                     | 0.57              |
| 10:5:1123:G:O2'   | 10:5:1124:U:O5'     | 2.22                     | 0.57              |
| 14:9:551:ALA:HB3  | 14:9:555:ILE:HD12   | 1.87                     | 0.57              |
| 14:9:798:ARG:HH11 | 61:w:21:LYS:N       | 2.03                     | 0.57              |
| 46:h:105:ALA:HA   | 46:h:123:MET:HE1    | 1.87                     | 0.57              |
| 64:13:602:LEU:CD1 | 64:13:612:LEU:HD23  | 2.34                     | 0.57              |
| 64:13:868:ASN:ND2 | 64:13:1002:GLN:HE21 | 2.02                     | 0.57              |
| 65:14:605:GLU:HG2 | 66:15:247:LYS:O     | 2.04                     | 0.57              |
| 65:14:1209:LYS:NZ | 66:15:250:PHE:CZ    | 2.73                     | 0.57              |
| 6:17:259:GLY:HA2  | 65:14:1098:THR:HB   | 1.85                     | 0.57              |
| 6:17:260:GLN:CA   | 65:14:1126:LEU:CD2  | 2.83                     | 0.57              |
| 6:17:422:ASP:C    | 66:15:135:SER:O     | 2.21                     | 0.57              |
| 6:17:703:ASN:CA   | 14:9:665:HIS:HD2    | 2.16                     | 0.57              |
| 8:3:1292:A:H61    | 8:3:2024:C:H42      | 1.52                     | 0.57              |
| 43:e:147:PHE:HA   | 43:e:150:GLU:OE1    | 2.04                     | 0.57              |
| 64:13:10:GLN:CA   | 67:18:197:ASN:HD22  | 2.16                     | 0.57              |
| 6:17:256:THR:O    | 65:14:1099:GLN:CD   | 2.48                     | 0.57              |
| 6:17:256:THR:C    | 65:14:1099:GLN:CG   | 2.64                     | 0.57              |
| 6:17:396:ARG:HD2  | 6:17:399:ARG:HH21   | 1.69                     | 0.57              |
| 8:3:1106:G:N2     | 8:3:1124:G:O2'      | 2.38                     | 0.57              |
| 8:3:2623:U:H1'    | 62:y:4:GLN:HB3      | 1.87                     | 0.57              |
| 10:5:710:G:H2'    | 10:5:711:G:C8       | 2.40                     | 0.57              |
| 12:7:15:G:N2      | 12:7:21:A:H1'       | 2.19                     | 0.57              |
| 14:9:226:SER:C    | 58:t:53:LYS:O       | 2.45                     | 0.57              |
| 19:C:68:ASP:O     | 19:C:72:ARG:HG3     | 2.04                     | 0.57              |
| 41:c:64:LYS:NZ    | 41:c:68:GLN:OE1     | 2.37                     | 0.57              |
| 44:f:130:ILE:HB   | 44:f:142:VAL:HB     | 1.87                     | 0.57              |
| 47:i:63:ASP:OD2   | 47:i:63:ASP:N       | 2.34                     | 0.57              |
| 51:m:63:VAL:HG12  | 51:m:79:MET:HE2     | 1.86                     | 0.57              |
| 65:14:942:PHE:HZ  | 66:15:247:LYS:O     | 1.86                     | 0.57              |
| 5:12:89:LYS:HA    | 6:17:659:TYR:HE1    | 1.69                     | 0.57              |
| 6:17:259:GLY:O    | 65:14:1097:GLN:O    | 2.16                     | 0.57              |
| 8:3:2059:G:H4'    | 40:b:148:GLN:OE1    | 2.05                     | 0.57              |
| 10:5:197:A:H2'    | 10:5:198:A:C8       | 2.39                     | 0.57              |
| 10:5:452:A:N6     | 10:5:476:U:O2       | 2.37                     | 0.57              |
| 14:9:313:LYS:CD   | 38:Z:2:UNK:CB       | 2.80                     | 0.57              |
| 14:9:795:GLN:NE2  | 61:w:18:LEU:HD12    | 2.15                     | 0.57              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 39:a:124:SER:OG    | 39:a:128:ILE:HD11   | 2.05                     | 0.57              |
| 53:o:36:LYS:HE3    | 53:o:85:ASN:HA      | 1.86                     | 0.57              |
| 64:13:980:LYS:HB2  | 64:13:1007:HIS:NE2  | 2.20                     | 0.57              |
| 66:15:881:ARG:HH22 | 66:15:1274:LEU:HB3  | 1.69                     | 0.57              |
| 66:15:1107:THR:CG2 | 67:16:253:VAL:HG13  | 2.35                     | 0.57              |
| 6:17:382:ASP:CA    | 66:15:64:LYS:HZ1    | 1.63                     | 0.56              |
| 8:3:155:A:H2'      | 8:3:156:A:H8        | 1.70                     | 0.56              |
| 8:3:733:C:O2'      | 8:3:769:A:N6        | 2.36                     | 0.56              |
| 8:3:1648:A:N1      | 56:r:93:SER:OG      | 2.38                     | 0.56              |
| 10:5:358:G:OP1     | 26:K:71:THR:OG1     | 2.22                     | 0.56              |
| 12:7:35:A:N1       | 17:AB:41:U:C2       | 2.73                     | 0.56              |
| 53:o:24:GLU:HA     | 53:o:55:ARG:HH12    | 1.70                     | 0.56              |
| 64:13:235:PHE:HE2  | 64:13:354:ILE:HD11  | 1.69                     | 0.56              |
| 65:14:58:GLU:O     | 65:14:66:LYS:HE3    | 2.05                     | 0.56              |
| 6:17:25:GLY:HA3    | 6:17:652:ILE:HD11   | 1.86                     | 0.56              |
| 6:17:362:TYR:CE1   | 65:14:1098:THR:HG22 | 2.26                     | 0.56              |
| 6:17:426:LYS:HD3   | 66:15:184:GLN:H     | 1.58                     | 0.56              |
| 6:17:697:TYR:H     | 14:9:633:VAL:CG2    | 2.13                     | 0.56              |
| 6:17:838:ARG:NH2   | 6:17:879:GLY:HA3    | 2.21                     | 0.56              |
| 10:5:172:C:O2'     | 34:S:48:TYR:OH      | 2.15                     | 0.56              |
| 14:9:798:ARG:NH1   | 61:w:18:LEU:C       | 2.62                     | 0.56              |
| 52:n:64:ASN:ND2    | 52:n:65:GLY:H       | 2.03                     | 0.56              |
| 64:13:211:GLN:OE1  | 64:13:215:GLN:NE2   | 2.38                     | 0.56              |
| 66:15:872:GLN:HG3  | 66:15:897:VAL:HG21  | 1.87                     | 0.56              |
| 3:10:253:PHE:CE2   | 6:17:15:ILE:HD12    | 2.26                     | 0.56              |
| 3:10:316:TRP:CH2   | 65:14:88:ARG:O      | 2.58                     | 0.56              |
| 6:17:386:VAL:CA    | 66:15:176:ASN:CG    | 2.67                     | 0.56              |
| 6:17:386:VAL:C     | 66:15:176:ASN:HB2   | 1.93                     | 0.56              |
| 8:3:880:C:N4       | 8:3:968:U:H2'       | 2.20                     | 0.56              |
| 8:3:1949:C:OP2     | 8:3:1950:U:O2'      | 2.17                     | 0.56              |
| 10:5:520:C:H41     | 26:K:63:ARG:HH21    | 1.54                     | 0.56              |
| 10:5:787:A:N7      | 12:7:37:MIA:C11     | 2.68                     | 0.56              |
| 21:F:25:ILE:O      | 21:F:29:ILE:HG12    | 2.05                     | 0.56              |
| 23:H:30:ILE:HG13   | 23:H:65:ILE:HG13    | 1.85                     | 0.56              |
| 32:Q:94:ARG:HB3    | 32:Q:101:PHE:HE1    | 1.70                     | 0.56              |
| 36:W:11:ARG:NH1    | 36:W:180:THR:O      | 2.38                     | 0.56              |
| 42:d:49:PHE:CZ     | 42:d:147:LYS:HB2    | 2.38                     | 0.56              |
| 43:e:142:GLU:N     | 43:e:142:GLU:OE2    | 2.38                     | 0.56              |
| 50:l:63:LYS:HG2    | 50:l:65:TRP:CH2     | 2.39                     | 0.56              |
| 56:r:41:LYS:HE3    | 62:y:22:LEU:HD11    | 1.87                     | 0.56              |
| 64:13:171:PHE:CB   | 66:15:1183:LEU:CD1  | 2.72                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:13:415:LYS:NZ    | 64:13:436:GLN:OE1   | 2.38                     | 0.56              |
| 65:14:849:TYR:CE1   | 65:14:1270:LEU:HB2  | 2.41                     | 0.56              |
| 66:15:321:THR:HB    | 66:15:705:TYR:CE2   | 2.41                     | 0.56              |
| 66:15:1115:GLN:HG3  | 66:15:1123:LEU:HD11 | 1.86                     | 0.56              |
| 67:16:115:TRP:HH2   | 67:16:179:GLN:O     | 1.88                     | 0.56              |
| 10:5:250:G:H2'      | 10:5:251:G:H8       | 1.70                     | 0.56              |
| 12:7:34:G:N1        | 17:AB:42:C:C2       | 2.62                     | 0.56              |
| 14:9:787:LYS:HE2    | 61:w:3:VAL:HG22     | 1.86                     | 0.56              |
| 30:O:23:ASP:HB3     | 30:O:26:VAL:HG23    | 1.88                     | 0.56              |
| 31:P:64:VAL:HG23    | 31:P:76:ARG:HG2     | 1.86                     | 0.56              |
| 39:a:128:ILE:CG2    | 39:a:129:ASP:N      | 2.54                     | 0.56              |
| 53:o:92:ARG:HH12    | 53:o:116:GLU:HG3    | 1.70                     | 0.56              |
| 5:12:88:SER:CA      | 6:17:615:PHE:CE2    | 2.89                     | 0.56              |
| 6:17:800:LEU:HD21   | 6:17:920:VAL:HG22   | 1.86                     | 0.56              |
| 8:3:622:U:H2'       | 8:3:623:A:H8        | 1.70                     | 0.56              |
| 8:3:755:C:H2'       | 8:3:756:A:H8        | 1.71                     | 0.56              |
| 8:3:1098:G:O2'      | 46:h:84:LYS:NZ      | 2.38                     | 0.56              |
| 8:3:2028:G:OP1      | 62:y:9:SER:OG       | 2.23                     | 0.56              |
| 8:3:2335:A:H2'      | 8:3:2336:A:C8       | 2.40                     | 0.56              |
| 10:5:36:G:H21       | 26:K:128:SER:HG     | 1.52                     | 0.56              |
| 10:5:1138:U:H3      | 10:5:1149:G:H1      | 1.53                     | 0.56              |
| 39:a:81:ALA:HB1     | 39:a:99:ILE:HD13    | 1.86                     | 0.56              |
| 49:k:102:GLN:OE1    | 49:k:102:GLN:HA     | 2.05                     | 0.56              |
| 51:m:60:ARG:O       | 51:m:79:MET:HE1     | 2.06                     | 0.56              |
| 18:x:6:HIS:ND1      | 18:x:7:PHE:HD1      | 2.01                     | 0.56              |
| 5:12:96:LEU:HD22    | 6:17:661:LEU:HA     | 1.85                     | 0.56              |
| 10:5:1467:A:C1'     | 37:Y:44:A:HO2'      | 2.14                     | 0.56              |
| 12:7:51:U:H2'       | 12:7:52:G:H8        | 1.70                     | 0.56              |
| 17:AB:40:U:N3       | 37:Y:41:U:C4        | 2.73                     | 0.56              |
| 23:H:93:ASN:OD1     | 23:H:96:LEU:HD13    | 2.05                     | 0.56              |
| 40:b:21:ASN:OD1     | 48:j:73:ASP:HB3     | 2.06                     | 0.56              |
| 53:o:25:PHE:HB3     | 53:o:90:LEU:HD13    | 1.86                     | 0.56              |
| 64:13:10:GLN:HA     | 67:18:197:ASN:HD22  | 1.70                     | 0.56              |
| 64:13:22:ASN:ND2    | 64:13:1203:ASN:HD22 | 2.04                     | 0.56              |
| 66:15:1124:VAL:HG13 | 66:15:1129:LYS:HA   | 1.87                     | 0.56              |
| 6:17:92:PHE:CZ      | 6:17:96:ILE:HD11    | 2.40                     | 0.56              |
| 6:17:703:ASN:C      | 14:9:663:ASN:CA     | 2.73                     | 0.56              |
| 16:AA:166:ILE:H     | 16:AA:166:ILE:HD12  | 1.71                     | 0.56              |
| 18:AC:66:PHE:HZ     | 33:R:68:GLY:HA2     | 1.71                     | 0.56              |
| 47:i:3:LYS:HG3      | 47:i:4:THR:N        | 2.20                     | 0.56              |
| 65:14:931:ASP:HA    | 65:14:1198:TYR:CZ   | 2.41                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:15:234:PRO:HD2  | 66:15:699:LEU:HD12  | 1.86                     | 0.56              |
| 66:15:966:VAL:HG22 | 66:15:1265:LEU:HD13 | 1.88                     | 0.56              |
| 67:16:194:ARG:HD2  | 67:16:271:VAL:O     | 2.06                     | 0.56              |
| 6:17:711:PHE:CZ    | 14:9:650:ASN:N      | 2.73                     | 0.56              |
| 8:3:118:G:OP2      | 8:3:120:A:O2'       | 2.24                     | 0.56              |
| 8:3:316:C:C2'      | 8:3:392:A:H61       | 2.17                     | 0.56              |
| 8:3:1691:U:H2'     | 8:3:1692:A:H8       | 1.69                     | 0.56              |
| 8:3:2196:G:H2'     | 8:3:2197:U:C6       | 2.41                     | 0.56              |
| 10:5:305:A:O2'     | 10:5:605:A:N1       | 2.37                     | 0.56              |
| 10:5:1127:A:H5''   | 24:I:50:THR:HG23    | 1.87                     | 0.56              |
| 10:5:1270:C:H5'    | 27:L:14:ARG:NH1     | 2.21                     | 0.56              |
| 64:13:1020:MET:HB3 | 67:18:256:HIS:HB3   | 1.87                     | 0.56              |
| 5:12:93:THR:O      | 6:17:664:ILE:CG1    | 2.51                     | 0.56              |
| 6:17:698:SER:HB3   | 14:9:632:PHE:CB     | 2.29                     | 0.56              |
| 6:17:706:ILE:CD1   | 14:9:659:ASN:H      | 2.02                     | 0.56              |
| 8:3:154:U:H2'      | 8:3:155:A:H8        | 1.70                     | 0.56              |
| 8:3:1002:A:H4'     | 8:3:2279:G:H22      | 1.70                     | 0.56              |
| 8:3:1544:G:H2'     | 8:3:1545:A:H8       | 1.71                     | 0.56              |
| 8:3:2323:U:O2      | 42:d:125:ARG:NH1    | 2.38                     | 0.56              |
| 10:5:80:U:H2'      | 10:5:81:A:H8        | 1.71                     | 0.56              |
| 10:5:452:A:OP1     | 30:O:70:ARG:NH1     | 2.38                     | 0.56              |
| 33:R:30:PRO:HA     | 33:R:48:THR:HG23    | 1.88                     | 0.56              |
| 62:y:39:PHE:O      | 62:y:41:ARG:NH1     | 2.36                     | 0.56              |
| 66:15:873:THR:CG2  | 66:15:1270:ILE:CD1  | 2.84                     | 0.56              |
| 67:16:128:ASN:O    | 67:16:136:LYS:HE2   | 2.06                     | 0.56              |
| 6:17:703:ASN:HB3   | 14:9:785:LEU:HD11   | 1.87                     | 0.56              |
| 6:17:770:VAL:HG13  | 6:17:832:TRP:CE2    | 2.41                     | 0.56              |
| 8:3:700:U:H2'      | 8:3:701:A:H8        | 1.71                     | 0.56              |
| 8:3:1091:G:H4'     | 8:3:1121:A:H8       | 1.71                     | 0.56              |
| 8:3:1306:G:H2'     | 8:3:1307:G:H8       | 1.71                     | 0.56              |
| 8:3:2352:U:OP1     | 63:z:35:ASN:ND2     | 2.39                     | 0.56              |
| 9:4:11:A:O2'       | 9:4:12:U:H3'        | 2.06                     | 0.56              |
| 10:5:1022:G:O2'    | 10:5:1023:G:O4'     | 2.23                     | 0.56              |
| 15:A:20:LEU:HG     | 15:A:62:ARG:HH21    | 1.71                     | 0.56              |
| 20:E:142:ARG:O     | 20:E:144:SER:N      | 2.39                     | 0.56              |
| 30:O:39:LEU:HD12   | 30:O:40:ASN:H       | 1.70                     | 0.56              |
| 47:i:78:TYR:CE1    | 47:i:89:LYS:HB3     | 2.41                     | 0.56              |
| 64:13:238:GLU:OE1  | 64:13:253:LYS:CD    | 2.54                     | 0.56              |
| 8:3:917:G:H2'      | 8:3:918:G:H8        | 1.71                     | 0.55              |
| 8:3:1098:G:H1'     | 46:h:131:MET:HE1    | 1.88                     | 0.55              |
| 16:AA:215:ASN:HB2  | 16:AA:218:GLU:HB3   | 1.88                     | 0.55              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 41:c:194:ALA:C      | 41:c:196:ALA:H      | 2.13                     | 0.55              |
| 66:15:141:VAL:HG21  | 66:15:549:LEU:CD1   | 2.36                     | 0.55              |
| 66:15:961:THR:CG2   | 66:15:1269:LEU:HD23 | 2.36                     | 0.55              |
| 6:17:259:GLY:O      | 65:14:1097:GLN:C    | 2.49                     | 0.55              |
| 8:3:86:A:N6         | 8:3:101:C:O4'       | 2.39                     | 0.55              |
| 8:3:1564:U:H2'      | 8:3:1565:G:C8       | 2.40                     | 0.55              |
| 8:3:2223:C:H2'      | 8:3:2224:A:H8       | 1.71                     | 0.55              |
| 10:5:787:A:H5'      | 12:7:39:PSU:H5''    | 1.88                     | 0.55              |
| 15:A:181:PRO:HG2    | 15:A:206:THR:HG21   | 1.89                     | 0.55              |
| 58:t:94:ASP:OD2     | 58:t:94:ASP:N       | 2.40                     | 0.55              |
| 64:13:1126:ARG:NH1  | 65:14:152:LYS:NZ    | 2.51                     | 0.55              |
| 65:14:1043:VAL:HG21 | 65:14:1073:ASN:OD1  | 2.05                     | 0.55              |
| 65:14:1122:LYS:HB2  | 66:15:150:PHE:HZ    | 1.67                     | 0.55              |
| 66:15:1103:GLN:HA   | 67:16:259:GLN:CG    | 2.36                     | 0.55              |
| 66:15:1210:GLY:HA2  | 66:15:1219:MET:HG2  | 1.87                     | 0.55              |
| 6:17:426:LYS:CA     | 66:15:140:ASN:HD22  | 2.16                     | 0.55              |
| 8:3:1559:A:H1'      | 14:9:247:LYS:HD3    | 1.88                     | 0.55              |
| 8:3:1568:C:H3'      | 8:3:1569:A:H8       | 1.69                     | 0.55              |
| 43:e:18:LEU:HD12    | 43:e:20:PHE:CZ      | 2.41                     | 0.55              |
| 64:13:190:TRP:CZ2   | 64:13:196:PRO:HB3   | 2.41                     | 0.55              |
| 64:13:984:GLN:OE1   | 64:13:1132:GLY:C    | 2.49                     | 0.55              |
| 64:13:1217:LYS:HE2  | 67:18:275:LEU:C     | 2.31                     | 0.55              |
| 66:15:59:TRP:HB2    | 66:15:640:PHE:CD2   | 2.42                     | 0.55              |
| 66:15:995:TYR:CE1   | 66:15:997:ASP:OD1   | 2.59                     | 0.55              |
| 67:16:206:TYR:HB2   | 67:16:267:PHE:CE1   | 2.41                     | 0.55              |
| 8:3:174:A:H2'       | 8:3:175:A:H8        | 1.72                     | 0.55              |
| 10:5:398:G:OP1      | 19:C:73:ARG:NH1     | 2.40                     | 0.55              |
| 10:5:1009:G:N2      | 10:5:1012:A:OP2     | 2.27                     | 0.55              |
| 36:W:47:ASN:OD1     | 36:W:48:TYR:HD2     | 1.88                     | 0.55              |
| 40:b:47:TYR:HD1     | 40:b:85:ARG:HE      | 1.54                     | 0.55              |
| 6:17:711:PHE:CB     | 14:9:651:HIS:HE1    | 2.16                     | 0.55              |
| 8:3:569:U:H2'       | 8:3:570:C:C6        | 2.41                     | 0.55              |
| 8:3:2160:U:H2'      | 8:3:2161:G:H8       | 1.72                     | 0.55              |
| 8:3:2376:C:H2'      | 8:3:2377:A:H8       | 1.70                     | 0.55              |
| 10:5:1468:A:HO2'    | 37:Y:43:A:C1'       | 2.09                     | 0.55              |
| 17:AB:49:U:H3       | 36:W:167:ARG:HD2    | 1.72                     | 0.55              |
| 42:d:33:LYS:HE2     | 42:d:157:VAL:HG21   | 1.88                     | 0.55              |
| 42:d:135:GLN:HG3    | 42:d:136:ILE:HD12   | 1.87                     | 0.55              |
| 45:g:18:LEU:HD13    | 45:g:68:PHE:HE2     | 1.71                     | 0.55              |
| 52:n:64:ASN:CG      | 52:n:65:GLY:H       | 2.14                     | 0.55              |
| 65:14:22:ARG:HD2    | 65:14:746:GLU:OE1   | 2.07                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:15:33:VAL:HA    | 66:15:832:ILE:HD11  | 1.88                     | 0.55              |
| 6:17:261:LYS:CG    | 65:14:1096:ILE:HG21 | 2.34                     | 0.55              |
| 8:3:817:A:C2       | 39:a:233:MET:HG2    | 2.41                     | 0.55              |
| 8:3:2797:C:H5'     | 8:3:2798:A:O5'      | 2.07                     | 0.55              |
| 8:3:2854:A:N7      | 8:3:2872:A:O2'      | 2.31                     | 0.55              |
| 21:F:39:GLN:HE22   | 23:H:45:LEU:HD22    | 1.70                     | 0.55              |
| 48:j:17:LYS:N      | 48:j:45:ASP:O       | 2.34                     | 0.55              |
| 5:12:92:ILE:HG21   | 6:17:660:GLY:N      | 2.21                     | 0.55              |
| 6:17:80:GLY:N      | 65:14:1271:ILE:HD12 | 2.22                     | 0.55              |
| 6:17:389:VAL:N     | 66:15:132:LEU:CD2   | 2.60                     | 0.55              |
| 8:3:1460:G:H2'     | 8:3:1461:A:C8       | 2.41                     | 0.55              |
| 14:9:795:GLN:CG    | 61:w:18:LEU:HG      | 2.33                     | 0.55              |
| 19:C:96:ARG:HB2    | 19:C:99:ASN:HB3     | 1.87                     | 0.55              |
| 36:W:46:VAL:HG23   | 36:W:47:ASN:N       | 2.22                     | 0.55              |
| 36:W:133:LEU:HD11  | 36:W:137:MET:HE2    | 1.89                     | 0.55              |
| 66:15:396:GLN:HE22 | 66:15:412:GLY:HA2   | 1.67                     | 0.55              |
| 6:17:710:PHE:CD2   | 14:9:673:PHE:HB2    | 2.39                     | 0.55              |
| 8:3:680:A:H2'      | 8:3:682:A:N7        | 2.21                     | 0.55              |
| 8:3:703:A:H2'      | 8:3:705:A:H62       | 1.72                     | 0.55              |
| 10:5:195:U:H2'     | 10:5:196:G:C8       | 2.42                     | 0.55              |
| 10:5:435:U:O2'     | 10:5:437:U:O4       | 2.20                     | 0.55              |
| 14:9:165:LEU:CD2   | 58:t:62:LYS:HZ1     | 1.89                     | 0.55              |
| 16:AA:127:HIS:ND1  | 16:AA:200:LEU:HD21  | 2.22                     | 0.55              |
| 41:c:187:SER:OG    | 41:c:190:ASP:OD1    | 2.18                     | 0.55              |
| 61:w:49:ARG:HG3    | 61:w:49:ARG:NH1     | 2.22                     | 0.55              |
| 65:14:1032:GLN:CD  | 66:15:540:ASN:CG    | 2.74                     | 0.55              |
| 6:17:703:ASN:CG    | 14:9:663:ASN:CG     | 2.74                     | 0.55              |
| 8:3:193:G:OP2      | 60:v:26:ARG:NH1     | 2.40                     | 0.55              |
| 8:3:831:U:H2'      | 8:3:832:C:C6        | 2.41                     | 0.55              |
| 8:3:2071:C:H2'     | 8:3:2072:C:H6       | 1.72                     | 0.55              |
| 8:3:2862:U:H2'     | 8:3:2863:G:C8       | 2.42                     | 0.55              |
| 14:9:313:LYS:HE3   | 38:Z:2:UNK:O        | 2.06                     | 0.55              |
| 14:9:313:LYS:CE    | 38:Z:2:UNK:O        | 2.55                     | 0.55              |
| 15:A:234:ASP:OD1   | 15:A:245:MET:N      | 2.26                     | 0.55              |
| 20:E:90:LEU:HD12   | 20:E:90:LEU:H       | 1.72                     | 0.55              |
| 44:f:23:ASP:N      | 44:f:23:ASP:OD1     | 2.39                     | 0.55              |
| 53:o:54:ARG:HB2    | 53:o:100:TYR:HD1    | 1.71                     | 0.55              |
| 56:r:7:GLN:HB2     | 56:r:50:LEU:HD11    | 1.88                     | 0.55              |
| 58:t:52:THR:H      | 58:t:55:ALA:HB3     | 1.70                     | 0.55              |
| 65:14:52:VAL:HG23  | 65:14:563:ILE:HD12  | 1.87                     | 0.55              |
| 6:17:261:LYS:CE    | 65:14:1130:LYS:HG2  | 2.25                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:262:SER:CB    | 65:14:1098:THR:H    | 2.20                     | 0.55              |
| 6:17:599:ASN:CA    | 14:9:641:ARG:H      | 2.14                     | 0.55              |
| 6:17:696:ASN:N     | 14:9:633:VAL:HG13   | 2.17                     | 0.55              |
| 8:3:299:A:H2'      | 8:3:300:G:H8        | 1.71                     | 0.55              |
| 8:3:2254:G:H2'     | 8:3:2255:A:C8       | 2.41                     | 0.55              |
| 9:4:7:G:H2'        | 9:4:8:C:O4'         | 2.07                     | 0.55              |
| 10:5:447:G:H5''    | 10:5:448:A:H3'      | 1.89                     | 0.55              |
| 10:5:1438:U:OP1    | 53:o:110:LYS:CD     | 2.56                     | 0.55              |
| 12:7:16:U:OP2      | 12:7:16:U:H6        | 1.90                     | 0.55              |
| 16:AA:140:VAL:HG22 | 16:AA:201:LYS:HE3   | 1.89                     | 0.55              |
| 64:13:344:LYS:CE   | 64:13:363:GLU:HG3   | 2.37                     | 0.55              |
| 65:14:316:LYS:CG   | 65:14:454:GLN:HE22  | 2.20                     | 0.55              |
| 6:17:258:ASN:O     | 65:14:1126:LEU:CD2  | 2.55                     | 0.54              |
| 6:17:386:VAL:HG13  | 66:15:174:ASP:OD2   | 2.05                     | 0.54              |
| 6:17:390:ALA:HB3   | 66:15:71:ARG:NH2    | 0.30                     | 0.54              |
| 6:17:594:LEU:O     | 14:9:641:ARG:NH1    | 2.40                     | 0.54              |
| 8:3:849:C:H2'      | 8:3:850:G:H8        | 1.72                     | 0.54              |
| 8:3:1563:G:N2      | 8:3:1566:A:OP2      | 2.31                     | 0.54              |
| 8:3:2477:A:H2'     | 8:3:2478:G:O4'      | 2.07                     | 0.54              |
| 10:5:350:G:O2'     | 10:5:385:A:OP1      | 2.17                     | 0.54              |
| 64:13:912:LEU:CD2  | 64:13:1180:LEU:HD11 | 2.37                     | 0.54              |
| 64:13:984:GLN:CD   | 64:13:1133:THR:CG2  | 2.64                     | 0.54              |
| 64:13:1213:LEU:CG  | 67:18:276:ASN:HB3   | 2.32                     | 0.54              |
| 65:14:205:VAL:HG21 | 65:14:290:LEU:HD13  | 1.88                     | 0.54              |
| 66:15:958:PHE:CE2  | 66:15:1270:ILE:CG1  | 2.86                     | 0.54              |
| 6:17:388:ALA:HB1   | 66:15:132:LEU:CA    | 2.29                     | 0.54              |
| 6:17:701:THR:OG1   | 14:9:773:ALA:C      | 2.48                     | 0.54              |
| 12:7:37:MIA:H112   | 12:7:38:A:H1'       | 1.89                     | 0.54              |
| 15:A:18:VAL:HG11   | 15:A:231:LEU:HD11   | 1.89                     | 0.54              |
| 15:A:127:ILE:HG21  | 15:A:166:VAL:HG12   | 1.89                     | 0.54              |
| 31:P:28:SER:HB3    | 31:P:41:ARG:HD2     | 1.89                     | 0.54              |
| 57:s:3:VAL:HG23    | 61:w:65:TRP:HZ2     | 1.73                     | 0.54              |
| 66:15:877:ARG:NE   | 66:15:1270:ILE:CG2  | 2.69                     | 0.54              |
| 66:15:900:GLN:HE22 | 66:15:934:GLU:CG    | 2.14                     | 0.54              |
| 8:3:12:A:H2'       | 8:3:13:C:O4'        | 2.08                     | 0.54              |
| 8:3:520:C:H5''     | 14:9:160:ASN:CB     | 2.37                     | 0.54              |
| 8:3:2078:A:H2'     | 8:3:2079:G:H8       | 1.72                     | 0.54              |
| 8:3:2260:G:O6      | 59:u:18:LYS:NZ      | 2.33                     | 0.54              |
| 9:4:7:G:H2'        | 9:4:8:C:H6          | 1.73                     | 0.54              |
| 10:5:1438:U:H2'    | 10:5:1439:G:H8      | 1.72                     | 0.54              |
| 21:F:14:ASP:OD2    | 21:F:17:PHE:N       | 2.35                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:G:125:ASP:OD1   | 22:G:126:LYS:N      | 2.41                     | 0.54              |
| 52:n:62:LEU:HD13   | 52:n:69:ASN:HD22    | 1.72                     | 0.54              |
| 65:14:610:ILE:HG22 | 66:15:248:THR:OG1   | 2.07                     | 0.54              |
| 66:15:363:ASP:OD2  | 66:15:424:HIS:CD2   | 2.60                     | 0.54              |
| 6:17:699:ILE:H     | 14:9:689:ILE:HG21   | 1.59                     | 0.54              |
| 8:3:1132:C:H3'     | 8:3:1133:A:H8       | 1.72                     | 0.54              |
| 8:3:2009:U:OP1     | 51:m:14:ARG:NH1     | 2.37                     | 0.54              |
| 8:3:2813:A:H2'     | 8:3:2814:A:H8       | 1.72                     | 0.54              |
| 10:5:145:G:N2      | 10:5:148:A:OP2      | 2.35                     | 0.54              |
| 15:A:244:THR:OG1   | 15:A:249:LYS:NZ     | 2.31                     | 0.54              |
| 19:C:148:THR:O     | 19:C:151:ILE:HG22   | 2.08                     | 0.54              |
| 22:G:31:MET:HE3    | 22:G:73:ASN:HD22    | 1.72                     | 0.54              |
| 23:H:6:TYR:HB2     | 23:H:21:LEU:HB2     | 1.89                     | 0.54              |
| 42:d:31:LEU:HD23   | 42:d:96:MET:CE      | 2.38                     | 0.54              |
| 43:e:159:PRO:HA    | 43:e:172:ILE:HD13   | 1.89                     | 0.54              |
| 45:g:37:ALA:O      | 45:g:41:ARG:HG2     | 2.08                     | 0.54              |
| 51:m:46:ASP:O      | 51:m:50:THR:HG22    | 2.08                     | 0.54              |
| 65:14:173:LYS:HA   | 65:14:550:TYR:CE1   | 2.43                     | 0.54              |
| 8:3:1141:U:O2      | 45:g:79:LYS:NZ      | 2.35                     | 0.54              |
| 8:3:1445:U:H2'     | 8:3:1446:G:O4'      | 2.08                     | 0.54              |
| 10:5:1473:U:C5     | 37:Y:41:U:H4'       | 2.40                     | 0.54              |
| 13:8:5:C:H2'       | 13:8:6:G:H8         | 1.73                     | 0.54              |
| 14:9:188:ARG:HD3   | 58:t:57:LYS:HG2     | 1.80                     | 0.54              |
| 16:AA:156:GLN:O    | 19:C:84:ASN:HB3     | 2.07                     | 0.54              |
| 65:14:870:LEU:HD12 | 65:14:1223:VAL:HG21 | 1.89                     | 0.54              |
| 66:15:786:LEU:HD23 | 66:15:790:TRP:CH2   | 2.43                     | 0.54              |
| 8:3:799:A:H5''     | 39:a:217:GLY:HA3    | 1.90                     | 0.54              |
| 8:3:996:A:H61      | 50:l:83:MET:HE2     | 1.73                     | 0.54              |
| 8:3:1114:C:H3'     | 8:3:1115:G:H8       | 1.72                     | 0.54              |
| 8:3:1529:U:H2'     | 8:3:1530:G:H8       | 1.71                     | 0.54              |
| 10:5:808:C:O2'     | 10:5:895:A:N1       | 2.40                     | 0.54              |
| 14:9:228:PRO:HG3   | 58:t:52:THR:CG2     | 2.32                     | 0.54              |
| 21:F:21:LEU:O      | 21:F:25:ILE:HG22    | 2.08                     | 0.54              |
| 36:W:15:ASN:ND2    | 36:W:181:LEU:O      | 2.40                     | 0.54              |
| 41:c:197:LEU:HD13  | 41:c:199:VAL:HG23   | 1.90                     | 0.54              |
| 44:f:33:LYS:HD3    | 44:f:113:PHE:HB2    | 1.89                     | 0.54              |
| 51:m:63:VAL:CG1    | 51:m:79:MET:HE2     | 2.37                     | 0.54              |
| 65:14:858:ASN:ND2  | 65:14:1228:THR:HG23 | 2.22                     | 0.54              |
| 1:0:1:MET:CE       | 8:3:788:G:H5'       | 2.37                     | 0.54              |
| 6:17:256:THR:O     | 65:14:1103:ASP:OD1  | 2.20                     | 0.54              |
| 6:17:260:GLN:N     | 65:14:1126:LEU:CD2  | 2.70                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:3:615:G:H2'       | 8:3:616:G:C8        | 2.42                     | 0.54              |
| 8:3:652:U:H2'       | 8:3:653:G:H8        | 1.72                     | 0.54              |
| 10:5:408:U:H1'      | 19:C:28:GLY:HA2     | 1.88                     | 0.54              |
| 14:9:243:VAL:HG12   | 14:9:299:LYS:HE2    | 1.90                     | 0.54              |
| 14:9:787:LYS:HG2    | 61:w:3:VAL:CG1      | 2.35                     | 0.54              |
| 19:C:60:MET:HE3     | 19:C:191:ILE:HG12   | 1.89                     | 0.54              |
| 46:h:70:THR:HG22    | 46:h:71:PRO:HD2     | 1.90                     | 0.54              |
| 57:s:59:ILE:O       | 57:s:61:LYS:NZ      | 2.40                     | 0.54              |
| 6:17:384:ALA:CB     | 66:15:64:LYS:N      | 2.71                     | 0.54              |
| 6:17:693:THR:CG2    | 14:9:682:VAL:HG23   | 2.36                     | 0.54              |
| 8:3:518:A:O2'       | 8:3:532:A:N1        | 2.38                     | 0.54              |
| 8:3:2736:U:O2'      | 8:3:2737:G:H8       | 1.90                     | 0.54              |
| 10:5:434:U:H5'      | 19:C:151:ILE:HD11   | 1.89                     | 0.54              |
| 10:5:1064:U:O2'     | 15:A:119:ASN:ND2    | 2.41                     | 0.54              |
| 10:5:1467:A:O2'     | 37:Y:44:A:O4'       | 2.26                     | 0.54              |
| 14:9:798:ARG:CZ     | 61:w:18:LEU:CD2     | 2.76                     | 0.54              |
| 20:E:90:LEU:HB3     | 32:Q:50:ARG:HH22    | 1.72                     | 0.54              |
| 33:R:22:MET:HE3     | 33:R:29:ARG:O       | 2.08                     | 0.54              |
| 50:l:5:LYS:HD2      | 50:l:6:ARG:HH22     | 1.73                     | 0.54              |
| 63:z:10:GLY:HA2     | 63:z:17:ILE:HA      | 1.90                     | 0.54              |
| 66:15:1031:VAL:HG21 | 66:15:1058:LEU:HD11 | 1.90                     | 0.54              |
| 67:18:206:TYR:HB2   | 67:18:267:PHE:CE1   | 2.43                     | 0.54              |
| 5:12:96:LEU:HD12    | 6:17:664:ILE:HG13   | 1.88                     | 0.54              |
| 6:17:424:VAL:C      | 66:15:184:GLN:HE22  | 2.15                     | 0.54              |
| 6:17:707:GLN:C      | 14:9:670:PRO:CB     | 2.81                     | 0.54              |
| 10:5:88:A:OP1       | 34:S:12:ARG:NH2     | 2.37                     | 0.54              |
| 14:9:275:LYS:HB2    | 57:s:22:GLY:N       | 2.23                     | 0.54              |
| 23:H:34:ARG:HG2     | 23:H:34:ARG:HH11    | 1.73                     | 0.54              |
| 31:P:70:SER:O       | 31:P:74:ARG:NH1     | 2.41                     | 0.54              |
| 42:d:14:LYS:HG3     | 42:d:18:LYS:HE2     | 1.90                     | 0.54              |
| 47:i:7:LEU:HD13     | 54:p:60:TRP:HE1     | 1.73                     | 0.54              |
| 49:k:20:LEU:O       | 49:k:32:SER:OG      | 2.20                     | 0.54              |
| 66:15:434:THR:CG2   | 66:15:489:THR:HG21  | 2.37                     | 0.54              |
| 66:15:648:GLN:O     | 66:15:652:LYS:HB2   | 2.08                     | 0.54              |
| 6:17:690:LEU:HG     | 14:9:679:ASP:OD2    | 2.08                     | 0.54              |
| 6:17:698:SER:CA     | 14:9:769:ILE:CG2    | 2.85                     | 0.54              |
| 8:3:1282:G:C2       | 54:p:32:LYS:HB3     | 2.42                     | 0.54              |
| 8:3:1652:A:C4       | 51:m:4:ILE:HD12     | 2.43                     | 0.54              |
| 20:E:25:GLN:HE22    | 20:E:37:THR:HG22    | 1.73                     | 0.54              |
| 29:N:18:ASP:OD2     | 29:N:21:SER:HB2     | 2.08                     | 0.54              |
| 39:a:143:GLU:CD     | 39:a:143:GLU:H      | 2.14                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:13:149:PRO:CB    | 66:15:1168:VAL:HA   | 2.33                     | 0.54              |
| 64:13:196:PRO:HG2   | 64:13:554:LEU:HD11  | 1.90                     | 0.54              |
| 64:13:1068:SER:HA   | 64:13:1083:ILE:HG21 | 1.89                     | 0.54              |
| 64:13:1126:ARG:NH2  | 65:14:156:GLU:OE1   | 2.41                     | 0.54              |
| 66:15:877:ARG:HH11  | 66:15:1270:ILE:HG21 | 1.72                     | 0.54              |
| 66:15:1097:LEU:HD13 | 66:15:1251:MET:HE2  | 1.90                     | 0.54              |
| 3:10:435:ARG:NH1    | 6:17:667:TRP:HZ2    | 2.06                     | 0.53              |
| 5:12:23:LYS:H       | 5:12:23:LYS:HD2     | 1.73                     | 0.53              |
| 6:17:149:PHE:CE2    | 6:17:173:ALA:HB1    | 2.43                     | 0.53              |
| 6:17:428:GLY:HA2    | 66:15:526:LEU:HD21  | 1.90                     | 0.53              |
| 8:3:341:G:N1        | 8:3:344:A:OP2       | 2.30                     | 0.53              |
| 8:3:517:G:O5'       | 58:t:44:ARG:NH1     | 2.41                     | 0.53              |
| 8:3:700:U:H5''      | 49:k:46:LEU:CD2     | 2.38                     | 0.53              |
| 8:3:2098:U:O2       | 60:v:34:GLN:NE2     | 2.41                     | 0.53              |
| 10:5:1330:A:H2'     | 10:5:1331:A:H8      | 1.73                     | 0.53              |
| 30:O:43:LEU:HD23    | 30:O:47:LYS:HA      | 1.90                     | 0.53              |
| 40:b:54:PHE:O       | 40:b:80:HIS:HB2     | 2.08                     | 0.53              |
| 43:e:23:ASP:OD1     | 43:e:23:ASP:N       | 2.40                     | 0.53              |
| 58:t:46:LYS:HE3     | 58:t:63:VAL:HB      | 1.90                     | 0.53              |
| 6:17:386:VAL:N      | 66:15:176:ASN:CG    | 2.66                     | 0.53              |
| 6:17:696:ASN:N      | 14:9:686:HIS:CA     | 2.71                     | 0.53              |
| 6:17:702:GLU:N      | 14:9:662:LEU:C      | 2.57                     | 0.53              |
| 8:3:1099:C:H3'      | 8:3:1100:U:H6       | 1.73                     | 0.53              |
| 8:3:1437:A:H2'      | 8:3:1438:G:H8       | 1.74                     | 0.53              |
| 8:3:2807:G:H2'      | 8:3:2808:A:H8       | 1.74                     | 0.53              |
| 15:A:115:GLY:HA2    | 15:A:118:THR:HG22   | 1.91                     | 0.53              |
| 22:G:26:ARG:HG3     | 22:G:82:PRO:HG3     | 1.90                     | 0.53              |
| 49:k:52:GLU:OE1     | 49:k:57:PRO:HA      | 2.08                     | 0.53              |
| 66:15:83:HIS:NE2    | 66:15:113:GLU:HG3   | 2.23                     | 0.53              |
| 5:12:93:THR:HA      | 6:17:664:ILE:HG13   | 1.90                     | 0.53              |
| 6:17:387:VAL:HG22   | 66:15:68:ILE:HG13   | 1.89                     | 0.53              |
| 10:5:250:G:OP1      | 31:P:70:SER:OG      | 2.26                     | 0.53              |
| 10:5:1088:C:H5''    | 15:A:154:ARG:HH22   | 1.72                     | 0.53              |
| 10:5:1497:U:H2'     | 10:5:1498:G:H8      | 1.72                     | 0.53              |
| 18:AC:73:LEU:HD21   | 33:R:13:ALA:HB2     | 1.91                     | 0.53              |
| 19:C:106:PHE:HD1    | 19:C:157:ALA:HB1    | 1.74                     | 0.53              |
| 21:F:110:ARG:HG2    | 21:F:112:GLU:HB2    | 1.89                     | 0.53              |
| 23:H:103:LYS:HG3    | 23:H:105:LEU:HG     | 1.89                     | 0.53              |
| 27:L:101:ARG:NH1    | 27:L:104:THR:HG22   | 2.23                     | 0.53              |
| 42:d:104:ILE:HG23   | 42:d:105:TYR:CD2    | 2.43                     | 0.53              |
| 61:w:16:VAL:O       | 61:w:19:VAL:HG12    | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:13:1194:LEU:CD2 | 64:13:1197:ILE:CD1 | 2.85                     | 0.53              |
| 65:14:608:ASN:HD22 | 66:15:251:ASP:H    | 1.54                     | 0.53              |
| 6:17:387:VAL:HG21  | 66:15:67:ASN:HB2   | 1.90                     | 0.53              |
| 6:17:700:LEU:O     | 14:9:661:GLU:CA    | 2.56                     | 0.53              |
| 8:3:549:A:N3       | 8:3:614:C:O2'      | 2.40                     | 0.53              |
| 8:3:1485:A:N1      | 8:3:2710:G:C6      | 2.76                     | 0.53              |
| 9:4:104:C:H2'      | 9:4:105:A:C8       | 2.43                     | 0.53              |
| 10:5:520:C:H41     | 26:K:63:ARG:NH2    | 2.07                     | 0.53              |
| 14:9:795:GLN:HA    | 61:w:18:LEU:CD2    | 2.38                     | 0.53              |
| 18:AC:69:GLY:HA3   | 33:R:9:ALA:H       | 1.74                     | 0.53              |
| 46:h:123:MET:O     | 46:h:127:THR:HG22  | 2.08                     | 0.53              |
| 52:n:9:ARG:HH11    | 52:n:9:ARG:HG3     | 1.74                     | 0.53              |
| 18:x:14:PHE:HE2    | 18:x:34:ILE:HB     | 1.73                     | 0.53              |
| 66:15:51:ASN:HB3   | 66:15:647:ILE:HG12 | 1.90                     | 0.53              |
| 6:17:388:ALA:HB3   | 66:15:132:LEU:CD2  | 1.96                     | 0.53              |
| 8:3:102:A:H1'      | 14:9:783:GLU:N     | 2.23                     | 0.53              |
| 8:3:1096:U:H3      | 46:h:13:ASN:HD21   | 1.55                     | 0.53              |
| 8:3:2383:G:N2      | 8:3:2386:A:OP2     | 2.34                     | 0.53              |
| 10:5:550:U:H2'     | 10:5:551:A:H8      | 1.73                     | 0.53              |
| 21:F:74:LEU:HD22   | 21:F:85:GLN:HB2    | 1.89                     | 0.53              |
| 29:N:15:HIS:ND1    | 29:N:16:ASP:O      | 2.36                     | 0.53              |
| 42:d:74:ILE:HG12   | 42:d:79:LEU:HD23   | 1.90                     | 0.53              |
| 46:h:120:ALA:HB1   | 46:h:123:MET:CE    | 2.37                     | 0.53              |
| 6:17:430:PRO:HB2   | 66:15:550:GLU:C    | 2.33                     | 0.53              |
| 6:17:688:GLN:HB3   | 14:9:683:HIS:CD2   | 2.30                     | 0.53              |
| 6:17:704:ASN:ND2   | 14:9:665:HIS:O     | 2.33                     | 0.53              |
| 8:3:299:A:H2'      | 8:3:300:G:C8       | 2.43                     | 0.53              |
| 8:3:1436:C:H2'     | 8:3:1437:A:H8      | 1.74                     | 0.53              |
| 8:3:1562:A:C5'     | 14:9:299:LYS:HA    | 2.39                     | 0.53              |
| 8:3:1906:G:H21     | 8:3:1909:C:H41     | 1.55                     | 0.53              |
| 10:5:22:G:H2'      | 10:5:23:G:C8       | 2.43                     | 0.53              |
| 10:5:941:A:H2'     | 10:5:942:G:C8      | 2.43                     | 0.53              |
| 14:9:353:VAL:HG22  | 58:t:53:LYS:HE2    | 1.91                     | 0.53              |
| 23:H:32:VAL:HA     | 23:H:67:VAL:HB     | 1.90                     | 0.53              |
| 23:H:73:GLY:O      | 23:H:77:GLN:NE2    | 2.42                     | 0.53              |
| 35:T:5:GLU:HG3     | 35:T:7:LYS:H       | 1.73                     | 0.53              |
| 42:d:171:ARG:HD3   | 42:d:180:GLY:HA2   | 1.90                     | 0.53              |
| 49:k:82:LEU:HB2    | 49:k:116:GLY:HA3   | 1.90                     | 0.53              |
| 65:14:345:THR:HG23 | 65:14:380:LYS:NZ   | 2.23                     | 0.53              |
| 66:15:83:HIS:HB2   | 66:15:116:TRP:CZ3  | 2.43                     | 0.53              |
| 66:15:1237:PRO:HG2 | 66:15:1239:HIS:CE1 | 2.42                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:1:15:LYS:HD3      | 8:3:664:G:H5''      | 1.89                     | 0.53              |
| 6:17:80:GLY:O       | 65:14:1268:ASN:OD1  | 2.27                     | 0.53              |
| 6:17:955:LYS:HZ2    | 14:9:799:GLU:CB     | 0.67                     | 0.53              |
| 8:3:26:G:H1'        | 56:r:77:ASN:HB3     | 1.90                     | 0.53              |
| 8:3:890:U:H2'       | 8:3:891:G:C8        | 2.44                     | 0.53              |
| 8:3:1561:G:N7       | 14:9:248:GLU:CG     | 2.70                     | 0.53              |
| 12:7:10:G:O2'       | 12:7:11:C:OP1       | 2.25                     | 0.53              |
| 12:7:34:G:C2        | 17:AB:42:C:O2       | 2.59                     | 0.53              |
| 27:L:25:ILE:HG23    | 27:L:29:ARG:HG2     | 1.90                     | 0.53              |
| 36:W:220:ALA:C      | 36:W:222:ILE:H      | 2.17                     | 0.53              |
| 43:e:39:PRO:HG2     | 43:e:42:LEU:HD13    | 1.90                     | 0.53              |
| 44:f:106:MET:SD     | 44:f:107:ALA:HB2    | 2.49                     | 0.53              |
| 47:i:101:ASP:HB2    | 47:i:127:VAL:HG13   | 1.90                     | 0.53              |
| 64:13:1213:LEU:HB2  | 67:18:276:ASN:ND2   | 2.24                     | 0.53              |
| 66:15:1149:THR:HG21 | 66:15:1154:GLU:CB   | 2.38                     | 0.53              |
| 67:18:105:TRP:CH2   | 67:18:152:TYR:HB2   | 2.44                     | 0.53              |
| 6:17:263:VAL:O      | 65:14:1097:GLN:NE2  | 2.40                     | 0.53              |
| 6:17:706:ILE:H      | 14:9:656:GLU:HA     | 1.73                     | 0.53              |
| 7:2:1:MET:CE        | 8:3:2750:A:H5''     | 2.39                     | 0.53              |
| 8:3:1076:U:H3       | 8:3:1149:G:H1       | 1.57                     | 0.53              |
| 8:3:2122:G:O2'      | 8:3:2175:U:O2       | 2.27                     | 0.53              |
| 10:5:1110:C:H2'     | 10:5:1111:G:H8      | 1.74                     | 0.53              |
| 10:5:1213:A:H5'     | 10:5:1310:C:H41     | 1.74                     | 0.53              |
| 10:5:1290:G:N1      | 10:5:1293:A:OP2     | 2.42                     | 0.53              |
| 10:5:1432:A:H5''    | 34:S:26:THR:HG22    | 1.90                     | 0.53              |
| 14:9:178:THR:OG1    | 14:9:181:GLU:HG3    | 2.08                     | 0.53              |
| 26:K:86:ASN:ND2     | 26:K:118:VAL:HG22   | 2.23                     | 0.53              |
| 40:b:37:ALA:HB3     | 40:b:51:LEU:HD23    | 1.90                     | 0.53              |
| 57:s:4:THR:O        | 57:s:4:THR:HG22     | 2.09                     | 0.53              |
| 65:14:730:LEU:HD22  | 65:14:1286:ILE:HD11 | 1.90                     | 0.53              |
| 66:15:467:LEU:CD2   | 66:15:468:PRO:HD3   | 2.39                     | 0.53              |
| 10:5:670:G:H2'      | 10:5:671:G:C8       | 2.44                     | 0.53              |
| 12:7:51:U:H2'       | 12:7:52:G:C8        | 2.44                     | 0.53              |
| 20:E:52:GLN:OE1     | 20:E:53:LEU:N       | 2.40                     | 0.53              |
| 41:c:154:ASP:OD1    | 41:c:154:ASP:N      | 2.34                     | 0.53              |
| 46:h:121:LEU:O      | 46:h:125:LEU:HD12   | 2.08                     | 0.53              |
| 53:o:76:GLU:OE2     | 53:o:105:ARG:NH1    | 2.42                     | 0.53              |
| 64:13:875:LYS:HE2   | 64:13:879:GLU:OE1   | 2.09                     | 0.53              |
| 66:15:22:PHE:CD1    | 66:15:827:ILE:HD11  | 2.41                     | 0.53              |
| 66:15:1217:VAL:HG21 | 66:15:1237:PRO:HA   | 1.90                     | 0.53              |
| 6:17:426:LYS:CB     | 66:15:184:GLN:CB    | 2.01                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:3:166:A:H1'      | 44:f:105:GLY:HA3    | 1.91                     | 0.53              |
| 8:3:2071:C:H2'     | 8:3:2072:C:C6       | 2.44                     | 0.53              |
| 14:9:784:GLU:OE1   | 61:w:5:LYS:HG2      | 2.09                     | 0.53              |
| 22:G:129:ARG:HG2   | 22:G:129:ARG:HH11   | 1.73                     | 0.53              |
| 39:a:39:VAL:O      | 39:a:66:TYR:N       | 2.42                     | 0.53              |
| 56:r:125:VAL:O     | 56:r:129:VAL:HG23   | 2.09                     | 0.53              |
| 60:v:16:ASN:ND2    | 60:v:24:ILE:HG23    | 2.24                     | 0.53              |
| 66:15:494:ARG:HH11 | 66:15:701:GLN:NE2   | 2.07                     | 0.53              |
| 6:17:252:SER:N     | 65:14:1100:THR:O    | 2.39                     | 0.52              |
| 6:17:693:THR:CG2   | 14:9:682:VAL:CG2    | 2.77                     | 0.52              |
| 8:3:65:A:H2'       | 8:3:66:A:C8         | 2.44                     | 0.52              |
| 8:3:1566:A:H2'     | 8:3:1567:U:O4'      | 2.08                     | 0.52              |
| 10:5:394:U:H2'     | 10:5:395:G:H8       | 1.73                     | 0.52              |
| 10:5:1468:A:O2'    | 37:Y:43:A:C2'       | 2.55                     | 0.52              |
| 64:13:702:TRP:HE1  | 64:13:736:ASN:ND2   | 2.03                     | 0.52              |
| 66:15:707:ARG:NE   | 66:15:711:GLY:HA2   | 2.19                     | 0.52              |
| 67:16:30:GLU:HG2   | 67:16:44:TYR:CE2    | 2.43                     | 0.52              |
| 3:10:238:PHE:CD1   | 6:17:563:VAL:HG23   | 2.41                     | 0.52              |
| 8:3:604:A:O2'      | 8:3:606:G:OP2       | 2.25                     | 0.52              |
| 8:3:1239:G:O2'     | 8:3:1267:A:N1       | 2.37                     | 0.52              |
| 8:3:1557:G:O6      | 8:3:1571:G:O2'      | 2.27                     | 0.52              |
| 16:AA:80:THR:OG1   | 16:AA:81:LYS:N      | 2.42                     | 0.52              |
| 17:AB:44:A:N1      | 37:Y:45:A:C6        | 2.76                     | 0.52              |
| 22:G:90:ILE:HG22   | 22:G:97:ILE:HG13    | 1.90                     | 0.52              |
| 25:J:21:ASN:HD22   | 25:J:21:ASN:C       | 2.12                     | 0.52              |
| 30:O:77:GLY:O      | 30:O:81:LYS:HE3     | 2.10                     | 0.52              |
| 42:d:96:MET:HG3    | 42:d:97:TRP:N       | 2.24                     | 0.52              |
| 53:o:26:SER:N      | 53:o:29:ASP:OD2     | 2.37                     | 0.52              |
| 58:t:28:MET:HE2    | 58:t:31:ARG:HH12    | 1.73                     | 0.52              |
| 64:13:197:THR:OG1  | 64:13:329:LYS:HE3   | 2.07                     | 0.52              |
| 64:13:1151:PHE:CD2 | 64:13:1171:ILE:HD11 | 2.44                     | 0.52              |
| 67:18:15:GLN:NE2   | 67:18:90:GLN:OE1    | 2.42                     | 0.52              |
| 2:1:5:SER:HA       | 2:1:8:LYS:HE2       | 1.91                     | 0.52              |
| 6:17:386:VAL:HA    | 66:15:175:PRO:N     | 2.24                     | 0.52              |
| 8:3:340:U:H2'      | 8:3:341:G:O4'       | 2.09                     | 0.52              |
| 8:3:512:G:N1       | 8:3:515:A:OP2       | 2.36                     | 0.52              |
| 8:3:652:U:H2'      | 8:3:653:G:C8        | 2.43                     | 0.52              |
| 8:3:713:C:H2'      | 8:3:714:G:H8        | 1.73                     | 0.52              |
| 8:3:1143:U:H5''    | 45:g:77:LYS:HA      | 1.90                     | 0.52              |
| 8:3:1559:A:H1'     | 14:9:247:LYS:HE2    | 1.87                     | 0.52              |
| 8:3:1583:G:O2'     | 8:3:1584:U:OP1      | 2.25                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:3:1691:U:H2'      | 8:3:1692:A:C8       | 2.44                     | 0.52              |
| 10:5:55:C:OP1       | 10:5:347:G:N2       | 2.42                     | 0.52              |
| 26:K:50:VAL:HG21    | 26:K:87:LEU:HB3     | 1.91                     | 0.52              |
| 32:Q:72:PRO:HD2     | 32:Q:75:ILE:HD12    | 1.91                     | 0.52              |
| 41:c:24:LEU:O       | 41:c:113:HIS:CE1    | 2.58                     | 0.52              |
| 42:d:171:ARG:HA     | 42:d:171:ARG:CZ     | 2.39                     | 0.52              |
| 45:g:25:VAL:HA      | 45:g:111:GLY:HA3    | 1.92                     | 0.52              |
| 52:n:31:MET:HE1     | 52:n:44:TRP:CG      | 2.44                     | 0.52              |
| 56:r:29:THR:HG23    | 56:r:55:ILE:HD13    | 1.91                     | 0.52              |
| 65:14:948:VAL:CG2   | 66:15:247:LYS:HZ2   | 2.19                     | 0.52              |
| 66:15:965:LEU:HB3   | 66:15:1265:LEU:HD21 | 1.89                     | 0.52              |
| 3:10:235:ILE:HG12   | 6:17:564:GLY:N      | 2.25                     | 0.52              |
| 6:17:426:LYS:CD     | 66:15:183:LEU:N     | 2.73                     | 0.52              |
| 8:3:1104:A:H5'      | 8:3:1105:A:C5       | 2.45                     | 0.52              |
| 8:3:1956:G:H2'      | 8:3:1957:G:H8       | 1.74                     | 0.52              |
| 8:3:2228:U:H5'      | 44:f:95:LYS:HG2     | 1.92                     | 0.52              |
| 10:5:836:C:H1'      | 20:E:145:ARG:HG2    | 1.91                     | 0.52              |
| 13:8:74:C:OP1       | 13:8:75:C:H5'       | 2.10                     | 0.52              |
| 15:A:84:PHE:CE1     | 15:A:177:ILE:HD12   | 2.44                     | 0.52              |
| 16:AA:154:ALA:HB1   | 16:AA:158:THR:HG21  | 1.92                     | 0.52              |
| 19:C:172:LYS:O      | 19:C:172:LYS:HG2    | 2.10                     | 0.52              |
| 20:E:170:GLN:HG2    | 22:G:78:GLN:HE22    | 1.74                     | 0.52              |
| 29:N:77:ASN:O       | 29:N:81:THR:HG23    | 2.09                     | 0.52              |
| 42:d:60:ILE:HD12    | 42:d:138:PHE:HD1    | 1.75                     | 0.52              |
| 66:15:343:LYS:HE3   | 66:15:439:MET:CB    | 2.39                     | 0.52              |
| 66:15:839:TRP:CD1   | 66:15:843:ASN:HD21  | 2.26                     | 0.52              |
| 66:15:1107:THR:HG23 | 66:15:1271:ARG:NH2  | 2.24                     | 0.52              |
| 6:17:699:ILE:O      | 14:9:692:LYS:HD2    | 2.09                     | 0.52              |
| 6:17:706:ILE:CA     | 14:9:656:GLU:HA     | 2.34                     | 0.52              |
| 8:3:890:U:H2'       | 8:3:891:G:H8        | 1.73                     | 0.52              |
| 8:3:1092:A:N6       | 8:3:1122:G:OP1      | 2.38                     | 0.52              |
| 8:3:2060:G:H4'      | 40:b:157:GLN:HG2    | 1.91                     | 0.52              |
| 10:5:250:G:H2'      | 10:5:251:G:C8       | 2.45                     | 0.52              |
| 10:5:1158:A:O2'     | 10:5:1159:A:OP1     | 2.28                     | 0.52              |
| 14:9:275:LYS:HD3    | 57:s:22:GLY:CA      | 2.31                     | 0.52              |
| 15:A:158:ARG:O      | 15:A:161:LYS:HG2    | 2.09                     | 0.52              |
| 21:F:130:THR:O      | 21:F:130:THR:OG1    | 2.26                     | 0.52              |
| 27:L:69:LEU:O       | 27:L:73:ILE:HG13    | 2.09                     | 0.52              |
| 58:t:28:MET:HE1     | 58:t:68:PRO:HB3     | 1.92                     | 0.52              |
| 66:15:869:LEU:HD22  | 66:15:1262:LYS:HB3  | 1.92                     | 0.52              |
| 66:15:1149:THR:HG21 | 66:15:1154:GLU:HB3  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:17:80:GLY:HA3   | 65:14:1268:ASN:CB  | 2.39                     | 0.52              |
| 6:17:386:VAL:CG1  | 66:15:174:ASP:OD2  | 2.57                     | 0.52              |
| 6:17:388:ALA:CA   | 66:15:132:LEU:CD2  | 2.21                     | 0.52              |
| 6:17:647:MET:HE1  | 6:17:833:LEU:HD13  | 1.91                     | 0.52              |
| 8:3:925:C:H4'     | 8:3:926:U:O4'      | 2.08                     | 0.52              |
| 8:3:1440:U:H2'    | 8:3:1441:A:C8      | 2.45                     | 0.52              |
| 10:5:923:G:O2'    | 10:5:1508:C:OP1    | 2.26                     | 0.52              |
| 10:5:1022:G:O2'   | 10:5:1023:G:O5'    | 2.28                     | 0.52              |
| 10:5:1295:U:O3'   | 33:R:78:ARG:NH2    | 2.43                     | 0.52              |
| 44:f:97:ILE:O     | 44:f:101:ALA:N     | 2.43                     | 0.52              |
| 54:p:73:MET:HE3   | 54:p:78:PHE:HD2    | 1.75                     | 0.52              |
| 64:13:253:LYS:HE3 | 64:13:348:GLU:OE2  | 2.10                     | 0.52              |
| 64:13:984:GLN:CD  | 64:13:1132:GLY:C   | 2.70                     | 0.52              |
| 6:17:107:GLN:OE1  | 6:17:176:ALA:HB1   | 2.09                     | 0.52              |
| 6:17:262:SER:HB2  | 65:14:1098:THR:CB  | 2.40                     | 0.52              |
| 6:17:703:ASN:O    | 14:9:664:MET:N     | 2.43                     | 0.52              |
| 8:3:756:A:H2'     | 8:3:757:A:H8       | 1.75                     | 0.52              |
| 8:3:881:A:O4'     | 8:3:882:C:H6       | 1.92                     | 0.52              |
| 10:5:1144:A:H2'   | 10:5:1145:A:C8     | 2.45                     | 0.52              |
| 19:C:14:LEU:O     | 19:C:59:ARG:NH2    | 2.43                     | 0.52              |
| 20:E:161:GLN:HB3  | 22:G:59:VAL:HG12   | 1.92                     | 0.52              |
| 21:F:68:VAL:HG21  | 21:F:103:ILE:HD11  | 1.91                     | 0.52              |
| 30:O:66:THR:H     | 30:O:69:VAL:HB     | 1.75                     | 0.52              |
| 30:O:66:THR:HG22  | 30:O:67:ASP:H      | 1.75                     | 0.52              |
| 61:w:12:SER:O     | 61:w:16:VAL:HG13   | 2.10                     | 0.52              |
| 65:14:730:LEU:HA  | 65:14:735:LEU:CD2  | 2.40                     | 0.52              |
| 66:15:1091:PHE:CZ | 66:15:1247:ARG:CD  | 2.89                     | 0.52              |
| 6:17:429:ASP:C    | 66:15:549:LEU:CG   | 2.82                     | 0.52              |
| 6:17:432:LYS:HG2  | 66:15:556:GLN:CD   | 2.35                     | 0.52              |
| 6:17:698:SER:N    | 14:9:689:ILE:HD13  | 2.25                     | 0.52              |
| 8:3:1683:G:O2'    | 51:m:109:ASP:OD2   | 2.28                     | 0.52              |
| 8:3:2644:U:H4'    | 40:b:83:GLU:OE2    | 2.10                     | 0.52              |
| 10:5:409:G:H22    | 10:5:425:G:H1'     | 1.75                     | 0.52              |
| 10:5:1062:C:H2'   | 10:5:1063:G:H8     | 1.74                     | 0.52              |
| 14:9:184:PHE:CB   | 58:t:57:LYS:NZ     | 2.73                     | 0.52              |
| 16:AA:70:ILE:HD12 | 16:AA:92:VAL:HG22  | 1.91                     | 0.52              |
| 24:I:31:ILE:HD12  | 24:I:96:ILE:HD13   | 1.91                     | 0.52              |
| 24:I:83:VAL:HG23  | 24:I:84:ASP:H      | 1.74                     | 0.52              |
| 25:J:22:ASN:OD1   | 25:J:23:THR:N      | 2.38                     | 0.52              |
| 46:h:14:LEU:HD22  | 46:h:19:ALA:HA     | 1.92                     | 0.52              |
| 64:13:355:VAL:CG2 | 64:13:406:LEU:HD12 | 2.39                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 64:13:1035:LYS:O   | 64:13:1070:LEU:HD23 | 2.09                     | 0.52              |
| 65:14:942:PHE:CZ   | 66:15:247:LYS:O     | 2.63                     | 0.52              |
| 66:15:271:GLN:HB2  | 66:15:437:GLN:OE1   | 2.09                     | 0.52              |
| 66:15:1139:LYS:CE  | 66:15:1197:VAL:O    | 2.53                     | 0.52              |
| 66:15:1139:LYS:NZ  | 66:15:1200:LEU:O    | 2.23                     | 0.52              |
| 5:12:89:LYS:N      | 6:17:615:PHE:HE2    | 2.07                     | 0.52              |
| 6:17:261:LYS:CG    | 65:14:1096:ILE:HB   | 2.31                     | 0.52              |
| 6:17:702:GLU:CD    | 14:9:781:PHE:CZ     | 2.86                     | 0.52              |
| 8:3:1961:A:O2'     | 8:3:1963:U:O4       | 2.21                     | 0.52              |
| 8:3:2054:C:H2'     | 8:3:2055:A:H8       | 1.75                     | 0.52              |
| 10:5:1126:U:O4     | 10:5:1127:A:N6      | 2.42                     | 0.52              |
| 15:A:107:PHE:HD2   | 15:A:109:THR:HG23   | 1.75                     | 0.52              |
| 16:AA:87:ARG:HG2   | 16:AA:109:LEU:HD22  | 1.92                     | 0.52              |
| 50:l:41:TRP:HE1    | 50:l:96:VAL:HG22    | 1.75                     | 0.52              |
| 18:x:37:ASP:OD2    | 18:x:38:ILE:HG13    | 2.09                     | 0.52              |
| 65:14:677:LYS:HE2  | 65:14:681:GLU:OE1   | 2.10                     | 0.52              |
| 66:15:1071:PHE:HE2 | 66:15:1247:ARG:CD   | 2.21                     | 0.52              |
| 6:17:955:LYS:HD3   | 14:9:799:GLU:HB3    | 1.89                     | 0.52              |
| 8:3:2094:A:H2'     | 8:3:2095:A:H8       | 1.75                     | 0.52              |
| 10:5:576:A:O2'     | 10:5:725:A:N3       | 2.41                     | 0.52              |
| 10:5:1068:G:N2     | 10:5:1071:A:OP2     | 2.28                     | 0.52              |
| 14:9:788:ALA:N     | 61:w:6:GLU:CD       | 2.64                     | 0.52              |
| 27:L:50:GLU:O      | 27:L:54:VAL:HG22    | 2.09                     | 0.52              |
| 32:Q:36:ARG:HB2    | 32:Q:38:LYS:HG2     | 1.92                     | 0.52              |
| 39:a:132:PRO:HD2   | 39:a:132:PRO:O      | 2.09                     | 0.52              |
| 44:f:68:LEU:HB3    | 44:f:108:LEU:HD21   | 1.92                     | 0.52              |
| 51:m:120:ASP:OD2   | 51:m:120:ASP:N      | 2.42                     | 0.52              |
| 64:13:46:ILE:HD12  | 64:13:591:LEU:HD23  | 1.92                     | 0.52              |
| 67:18:194:ARG:HD2  | 67:18:271:VAL:O     | 2.10                     | 0.52              |
| 6:17:952:GLN:OE1   | 61:w:74:LEU:HB2     | 2.10                     | 0.51              |
| 8:3:1562:A:C3'     | 14:9:302:GLU:OE1    | 2.34                     | 0.51              |
| 10:5:403:A:H2'     | 10:5:404:A:C8       | 2.45                     | 0.51              |
| 10:5:460:A:H2'     | 10:5:461:G:C8       | 2.46                     | 0.51              |
| 10:5:1468:A:H1'    | 37:Y:43:A:C2        | 2.45                     | 0.51              |
| 31:P:53:VAL:O      | 31:P:55:ALA:N       | 2.42                     | 0.51              |
| 41:c:41:GLU:OE1    | 41:c:41:GLU:CA      | 2.58                     | 0.51              |
| 6:17:179:HIS:CD2   | 6:17:293:GLY:HA2    | 2.46                     | 0.51              |
| 8:3:858:A:H2'      | 8:3:859:G:H8        | 1.76                     | 0.51              |
| 8:3:1009:A:H5''    | 55:q:77:LYS:HD2     | 1.91                     | 0.51              |
| 8:3:1559:A:C1'     | 14:9:247:LYS:CD     | 2.88                     | 0.51              |
| 8:3:1665:G:N1      | 8:3:1668:G:OP2      | 2.34                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:3:2634:C:H2'      | 8:3:2635:G:H8       | 1.75                     | 0.51              |
| 9:4:7:G:O2'         | 9:4:8:C:H5'         | 2.10                     | 0.51              |
| 10:5:257:U:OP1      | 34:S:64:ARG:NH1     | 2.43                     | 0.51              |
| 10:5:977:U:OP2      | 28:M:23:ARG:NH2     | 2.44                     | 0.51              |
| 12:7:34:G:O6        | 17:AB:42:C:C4       | 2.59                     | 0.51              |
| 13:8:61:C:H2'       | 13:8:62:C:H6        | 1.75                     | 0.51              |
| 46:h:96:ILE:HG23    | 46:h:100:LYS:HG3    | 1.91                     | 0.51              |
| 51:m:106:ARG:HG3    | 51:m:113:MET:SD     | 2.50                     | 0.51              |
| 65:14:242:LYS:NZ    | 65:14:396:GLU:CD    | 2.69                     | 0.51              |
| 65:14:1188:ILE:HG12 | 65:14:1192:LYS:HG3  | 1.92                     | 0.51              |
| 6:17:427:ASN:HD21   | 66:15:168:VAL:CG2   | 2.16                     | 0.51              |
| 6:17:598:LYS:O      | 14:9:678:PHE:CD2    | 2.60                     | 0.51              |
| 8:3:225:A:C4        | 8:3:237:A:H1'       | 2.45                     | 0.51              |
| 8:3:1536:C:H2'      | 8:3:1537:A:H8       | 1.76                     | 0.51              |
| 8:3:2032:G:H2'      | 8:3:2033:G:C8       | 2.45                     | 0.51              |
| 8:3:2802:C:N4       | 8:3:2803:G:H21      | 2.09                     | 0.51              |
| 10:5:1000:A:O2'     | 10:5:1029:C:O2'     | 2.16                     | 0.51              |
| 10:5:1279:G:H21     | 10:5:1306:A:H2      | 1.57                     | 0.51              |
| 12:7:35:A:C2        | 17:AB:41:U:O2       | 2.63                     | 0.51              |
| 12:7:44:G:H2'       | 12:7:45:U:C6        | 2.45                     | 0.51              |
| 14:9:275:LYS:HD3    | 57:s:22:GLY:HA2     | 1.80                     | 0.51              |
| 25:J:16:VAL:HG22    | 25:J:25:VAL:HG13    | 1.92                     | 0.51              |
| 26:K:57:LYS:HG3     | 37:Y:45:A:H4'       | 1.91                     | 0.51              |
| 64:13:6:ASN:C       | 67:18:198:LEU:HD11  | 2.36                     | 0.51              |
| 66:15:1207:LYS:HE2  | 66:15:1252:SER:OG   | 2.11                     | 0.51              |
| 66:15:1212:VAL:CG2  | 66:15:1248:LEU:HD12 | 2.41                     | 0.51              |
| 6:17:259:GLY:C      | 65:14:1098:THR:C    | 2.77                     | 0.51              |
| 6:17:277:SER:HA     | 65:14:1125:THR:CA   | 2.41                     | 0.51              |
| 8:3:756:A:H2'       | 8:3:757:A:C8        | 2.45                     | 0.51              |
| 8:3:899:A:H2'       | 8:3:900:G:C8        | 2.44                     | 0.51              |
| 8:3:1296:G:O2'      | 8:3:2019:G:O6       | 2.27                     | 0.51              |
| 8:3:2251:U:H2'      | 8:3:2252:U:C6       | 2.46                     | 0.51              |
| 8:3:2493:G:O3'      | 50:l:126:PRO:HB3    | 2.11                     | 0.51              |
| 9:4:2:U:H2'         | 9:4:3:U:C6          | 2.45                     | 0.51              |
| 30:O:86:LYS:C       | 30:O:86:LYS:HD3     | 2.36                     | 0.51              |
| 36:W:109:ILE:HD12   | 36:W:222:ILE:HG23   | 1.93                     | 0.51              |
| 43:e:39:PRO:HD3     | 43:e:71:TYR:OH      | 2.11                     | 0.51              |
| 44:f:82:LYS:HE2     | 44:f:125:GLU:CD     | 2.35                     | 0.51              |
| 47:i:75:GLU:OE1     | 47:i:75:GLU:HA      | 2.09                     | 0.51              |
| 54:p:39:ILE:HG22    | 54:p:43:LYS:HE3     | 1.93                     | 0.51              |
| 61:w:63:LEU:HD11    | 61:w:68:GLU:HB2     | 1.92                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:13:29:GLN:NE2    | 64:13:746:LYS:HB2   | 2.25                     | 0.51              |
| 66:15:1103:GLN:OE1  | 67:16:258:VAL:HG12  | 2.09                     | 0.51              |
| 6:17:261:LYS:HA     | 65:14:1130:LYS:HE2  | 1.88                     | 0.51              |
| 6:17:692:LYS:CA     | 14:9:683:HIS:HD1    | 2.18                     | 0.51              |
| 8:3:312:U:H2'       | 8:3:313:G:O4'       | 2.10                     | 0.51              |
| 8:3:567:U:H4'       | 8:3:568:G:C8        | 2.46                     | 0.51              |
| 8:3:917:G:H2'       | 8:3:918:G:C8        | 2.45                     | 0.51              |
| 8:3:1437:A:H2'      | 8:3:1438:G:C8       | 2.45                     | 0.51              |
| 8:3:1536:C:H2'      | 8:3:1537:A:C8       | 2.44                     | 0.51              |
| 8:3:2655:U:H2'      | 8:3:2656:G:H8       | 1.76                     | 0.51              |
| 18:AC:91:HIS:NE2    | 24:I:103:THR:HG21   | 2.24                     | 0.51              |
| 20:E:25:GLN:HG2     | 20:E:35:LEU:HD22    | 1.92                     | 0.51              |
| 39:a:3:ILE:HD13     | 39:a:210:LEU:HB2    | 1.93                     | 0.51              |
| 43:e:12:ASP:OD1     | 43:e:12:ASP:N       | 2.44                     | 0.51              |
| 45:g:97:ASP:HA      | 45:g:100:VAL:CG2    | 2.40                     | 0.51              |
| 50:l:52:ILE:HG22    | 50:l:56:LYS:HE2     | 1.92                     | 0.51              |
| 54:p:64:LEU:CD1     | 54:p:94:LEU:HB3     | 2.40                     | 0.51              |
| 64:13:897:HIS:CE1   | 64:13:901:ILE:HD11  | 2.45                     | 0.51              |
| 66:15:965:LEU:HD12  | 66:15:1269:LEU:CD1  | 2.40                     | 0.51              |
| 3:10:227:ILE:HD12   | 6:17:111:SER:HA     | 1.93                     | 0.51              |
| 6:17:80:GLY:CA      | 65:14:1271:ILE:HD12 | 2.41                     | 0.51              |
| 6:17:955:LYS:HE3    | 14:9:799:GLU:HB2    | 1.76                     | 0.51              |
| 8:3:520:C:H5''      | 14:9:160:ASN:HB2    | 1.93                     | 0.51              |
| 8:3:2081:U:HO2'     | 8:3:2605:G:HO2'     | 1.57                     | 0.51              |
| 10:5:133:G:H2'      | 10:5:134:G:C8       | 2.46                     | 0.51              |
| 10:5:334:A:P        | 48:j:97:ARG:HH12    | 2.34                     | 0.51              |
| 10:5:394:U:H2'      | 10:5:395:G:C8       | 2.46                     | 0.51              |
| 10:5:1193:U:H2'     | 10:5:1194:A:C8      | 2.46                     | 0.51              |
| 10:5:1468:A:O4'     | 37:Y:44:A:O4'       | 2.28                     | 0.51              |
| 19:C:179:VAL:HG12   | 19:C:180:ARG:N      | 2.25                     | 0.51              |
| 23:H:131:LYS:HE3    | 23:H:132:ARG:NH1    | 2.26                     | 0.51              |
| 65:14:1032:GLN:CD   | 66:15:540:ASN:ND2   | 2.69                     | 0.51              |
| 66:15:324:ILE:HG23  | 66:15:719:PHE:HB2   | 1.91                     | 0.51              |
| 66:15:714:PRO:HG2   | 66:15:761:ILE:HG22  | 1.92                     | 0.51              |
| 66:15:857:GLU:OE1   | 66:15:871:LYS:NZ    | 2.23                     | 0.51              |
| 66:15:995:TYR:HE1   | 66:15:997:ASP:OD1   | 1.92                     | 0.51              |
| 66:15:1098:THR:HG23 | 66:15:1106:SER:OG   | 2.10                     | 0.51              |
| 3:10:249:PHE:CZ     | 6:17:656:PHE:CE1    | 2.98                     | 0.51              |
| 6:17:712:ILE:HG13   | 14:9:651:HIS:CE1    | 2.46                     | 0.51              |
| 8:3:984:C:H2'       | 8:3:985:A:H8        | 1.75                     | 0.51              |
| 8:3:1118:U:H5''     | 45:g:41:ARG:CZ      | 2.40                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:2847:C:H2'     | 8:3:2848:A:H8      | 1.75                     | 0.51              |
| 9:4:104:C:H2'      | 9:4:105:A:H8       | 1.75                     | 0.51              |
| 10:5:1351:U:H2'    | 10:5:1352:A:C8     | 2.46                     | 0.51              |
| 29:N:33:ILE:O      | 29:N:37:THR:HG23   | 2.11                     | 0.51              |
| 34:S:56:ARG:HH12   | 34:S:57:LYS:NZ     | 2.09                     | 0.51              |
| 59:u:78:ASP:HB3    | 59:u:100:HIS:NE2   | 2.25                     | 0.51              |
| 65:14:1078:GLY:HA2 | 65:14:1182:SER:O   | 2.11                     | 0.51              |
| 66:15:311:ARG:NH1  | 66:15:673:GLY:HA3  | 2.26                     | 0.51              |
| 67:18:115:TRP:HH2  | 67:18:179:GLN:O    | 1.93                     | 0.51              |
| 8:3:1093:U:H3      | 8:3:1115:G:H22     | 1.57                     | 0.51              |
| 8:3:1561:G:O3'     | 14:9:299:LYS:CD    | 2.57                     | 0.51              |
| 8:3:2137:A:O2'     | 8:3:2165:A:N6      | 2.43                     | 0.51              |
| 8:3:2653:G:OP2     | 8:3:2653:G:N2      | 2.26                     | 0.51              |
| 10:5:192:A:H2'     | 10:5:193:G:H8      | 1.76                     | 0.51              |
| 10:5:510:U:H2'     | 10:5:511:A:H8      | 1.76                     | 0.51              |
| 14:9:84:TYR:H      | 14:9:87:GLN:HE21   | 1.59                     | 0.51              |
| 24:I:23:LEU:HB2    | 36:W:217:ARG:NH2   | 2.26                     | 0.51              |
| 26:K:57:LYS:HD2    | 37:Y:45:A:P        | 2.49                     | 0.51              |
| 40:b:29:ILE:HD13   | 40:b:207:ILE:HD11  | 1.92                     | 0.51              |
| 42:d:42:ASP:O      | 42:d:46:ASP:N      | 2.41                     | 0.51              |
| 64:13:784:LEU:HD11 | 64:13:792:PRO:HG2  | 1.93                     | 0.51              |
| 64:13:798:LEU:HD23 | 64:13:1216:LEU:CD1 | 2.41                     | 0.51              |
| 65:14:296:PHE:CE2  | 65:14:590:VAL:HG22 | 2.45                     | 0.51              |
| 66:15:1097:LEU:CD1 | 66:15:1251:MET:HG3 | 2.41                     | 0.51              |
| 6:17:388:ALA:O     | 66:15:71:ARG:NH1   | 2.44                     | 0.51              |
| 6:17:424:VAL:CG1   | 66:15:140:ASN:HD21 | 2.24                     | 0.51              |
| 6:17:712:ILE:H     | 14:9:651:HIS:CE1   | 2.29                     | 0.51              |
| 8:3:411:U:H2'      | 8:3:412:A:H8       | 1.75                     | 0.51              |
| 8:3:621:U:H2'      | 8:3:622:U:C6       | 2.46                     | 0.51              |
| 8:3:963:U:H2'      | 8:3:964:A:H8       | 1.75                     | 0.51              |
| 8:3:1232:U:H2'     | 8:3:1233:A:H8      | 1.76                     | 0.51              |
| 8:3:1807:C:OP2     | 39:a:190:ARG:NH2   | 2.44                     | 0.51              |
| 8:3:2799:U:H2'     | 8:3:2800:U:C6      | 2.46                     | 0.51              |
| 10:5:1400:A:H2'    | 10:5:1401:A:C8     | 2.46                     | 0.51              |
| 23:H:110:LYS:HG2   | 23:H:110:LYS:O     | 2.10                     | 0.51              |
| 25:J:43:MET:HE1    | 25:J:62:LYS:HD3    | 1.92                     | 0.51              |
| 40:b:17:PHE:O      | 53:o:17:GLN:NE2    | 2.27                     | 0.51              |
| 41:c:153:LEU:HD12  | 41:c:153:LEU:H     | 1.76                     | 0.51              |
| 44:f:88:PRO:HG2    | 44:f:89:TYR:HD1    | 1.75                     | 0.51              |
| 52:n:18:LYS:O      | 52:n:22:THR:HG23   | 2.10                     | 0.51              |
| 65:14:34:SER:O     | 65:14:40:SER:HB2   | 2.09                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:10:435:ARG:NH1   | 6:17:667:TRP:CZ2    | 2.78                     | 0.51              |
| 6:17:79:SER:CB     | 65:14:1269:ALA:C    | 2.68                     | 0.51              |
| 6:17:387:VAL:CG2   | 66:15:68:ILE:HG13   | 2.40                     | 0.51              |
| 6:17:693:THR:CG2   | 14:9:682:VAL:HA     | 2.26                     | 0.51              |
| 10:5:680:G:H21     | 25:J:33:ASN:H       | 1.59                     | 0.51              |
| 27:L:96:PRO:HB3    | 27:L:100:GLN:HB2    | 1.92                     | 0.51              |
| 41:c:6:LEU:HD12    | 41:c:127:LEU:HB3    | 1.91                     | 0.51              |
| 64:13:329:LYS:HD2  | 64:13:692:TYR:CE2   | 2.46                     | 0.51              |
| 64:13:388:ILE:HG23 | 64:13:952:PHE:CE1   | 2.46                     | 0.51              |
| 65:14:1096:ILE:O   | 65:14:1130:LYS:CE   | 2.54                     | 0.51              |
| 66:15:877:ARG:HD2  | 66:15:1270:ILE:CG2  | 2.25                     | 0.51              |
| 8:3:155:A:H2'      | 8:3:156:A:C8        | 2.45                     | 0.50              |
| 8:3:1033:A:OP2     | 54:p:57:ARG:NH1     | 2.44                     | 0.50              |
| 8:3:1124:G:N2      | 8:3:1125:U:O4       | 2.44                     | 0.50              |
| 8:3:2078:A:H2'     | 8:3:2079:G:C8       | 2.46                     | 0.50              |
| 8:3:2713:A:O2'     | 8:3:2856:G:OP1      | 2.28                     | 0.50              |
| 8:3:2764:U:H1'     | 8:3:2765:A:H5''     | 1.92                     | 0.50              |
| 10:5:96:G:H1       | 10:5:326:C:H41      | 1.57                     | 0.50              |
| 10:5:304:U:H2'     | 10:5:305:A:H8       | 1.76                     | 0.50              |
| 30:O:18:ARG:HA     | 30:O:38:HIS:HA      | 1.94                     | 0.50              |
| 64:13:81:TYR:HB2   | 64:13:114:TRP:CZ3   | 2.46                     | 0.50              |
| 65:14:323:SER:HB2  | 65:14:448:LYS:HE3   | 1.93                     | 0.50              |
| 65:14:1184:PHE:CZ  | 65:14:1192:LYS:HG2  | 2.46                     | 0.50              |
| 66:15:977:LEU:HD12 | 66:15:1255:LEU:HD21 | 1.92                     | 0.50              |
| 3:10:227:ILE:HG21  | 6:17:110:SER:O      | 2.11                     | 0.50              |
| 5:12:89:LYS:N      | 6:17:615:PHE:CE2    | 2.80                     | 0.50              |
| 6:17:369:HIS:NE2   | 6:17:396:ARG:CZ     | 2.75                     | 0.50              |
| 6:17:376:LYS:CD    | 66:15:178:GLU:OE2   | 2.57                     | 0.50              |
| 6:17:711:PHE:CZ    | 14:9:649:VAL:C      | 2.89                     | 0.50              |
| 8:3:663:A:N7       | 49:k:81:ASN:ND2     | 2.56                     | 0.50              |
| 8:3:893:A:H61      | 8:3:957:G:H1        | 1.58                     | 0.50              |
| 8:3:1246:U:OP2     | 54:p:7:LYS:NZ       | 2.38                     | 0.50              |
| 8:3:2005:G:OP2     | 40:b:142:ARG:NH2    | 2.44                     | 0.50              |
| 10:5:57:U:H2'      | 10:5:58:G:H8        | 1.77                     | 0.50              |
| 10:5:473:A:H2'     | 10:5:474:G:C8       | 2.46                     | 0.50              |
| 10:5:1261:A:H2'    | 10:5:1262:A:C8      | 2.46                     | 0.50              |
| 14:9:787:LYS:HE2   | 61:w:3:VAL:CG2      | 2.41                     | 0.50              |
| 20:E:114:LYS:O     | 20:E:118:ILE:HD12   | 2.11                     | 0.50              |
| 64:13:356:VAL:HG21 | 64:13:443:LEU:HD11  | 1.93                     | 0.50              |
| 65:14:745:GLN:O    | 65:14:751:LYS:NZ    | 2.44                     | 0.50              |
| 6:17:261:LYS:HB2   | 65:14:1126:LEU:CD2  | 2.40                     | 0.50              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 8:3:918:G:O6      | 8:3:932:U:O2        | 2.29                     | 0.50              |
| 8:3:2565:G:H2'    | 8:3:2566:C:C6       | 2.46                     | 0.50              |
| 14:9:227:GLY:H    | 58:t:53:LYS:CE      | 2.24                     | 0.50              |
| 17:AB:43:A:C2     | 37:Y:44:A:N7        | 2.79                     | 0.50              |
| 20:E:112:ARG:NH1  | 20:E:112:ARG:HA     | 2.25                     | 0.50              |
| 23:H:90:LEU:HD13  | 23:H:97:LYS:HB2     | 1.92                     | 0.50              |
| 32:Q:53:LEU:HG    | 32:Q:54:ILE:HG13    | 1.92                     | 0.50              |
| 46:h:11:LYS:HE3   | 46:h:52:PRO:HB2     | 1.92                     | 0.50              |
| 47:i:43:ASN:O     | 54:p:70:GLU:OE2     | 2.29                     | 0.50              |
| 64:13:171:PHE:CE2 | 66:15:1184:ILE:HG12 | 2.46                     | 0.50              |
| 65:14:242:LYS:HZ3 | 65:14:396:GLU:CD    | 2.19                     | 0.50              |
| 66:15:397:SER:HB3 | 66:15:408:ARG:NH1   | 2.26                     | 0.50              |
| 6:17:576:PHE:CE2  | 6:17:890:TYR:CD2    | 2.99                     | 0.50              |
| 8:3:638:A:H62     | 8:3:660:U:H3        | 1.60                     | 0.50              |
| 8:3:1451:A:H2'    | 8:3:1452:G:H8       | 1.77                     | 0.50              |
| 8:3:1565:G:H2'    | 8:3:1566:A:C8       | 2.46                     | 0.50              |
| 8:3:1814:G:N2     | 8:3:1817:A:OP2      | 2.43                     | 0.50              |
| 10:5:378:A:H2'    | 10:5:379:A:C8       | 2.46                     | 0.50              |
| 19:C:123:LEU:HD21 | 19:C:145:LYS:HE2    | 1.93                     | 0.50              |
| 19:C:155:LYS:O    | 19:C:159:GLU:HG2    | 2.12                     | 0.50              |
| 23:H:12:ARG:HD2   | 23:H:79:GLY:HA3     | 1.93                     | 0.50              |
| 36:W:90:LYS:HA    | 36:W:93:LYS:HE2     | 1.93                     | 0.50              |
| 60:v:14:TYR:CZ    | 60:v:28:LYS:HD3     | 2.46                     | 0.50              |
| 63:z:24:ASN:HD22  | 63:z:27:LYS:HB2     | 1.77                     | 0.50              |
| 64:13:984:GLN:HG3 | 64:13:1133:THR:CB   | 2.41                     | 0.50              |
| 66:15:148:ASP:OD2 | 66:15:626:SER:OG    | 2.20                     | 0.50              |
| 66:15:575:MET:SD  | 66:15:641:LYS:HG3   | 2.51                     | 0.50              |
| 6:17:376:LYS:CD   | 66:15:178:GLU:CD    | 2.79                     | 0.50              |
| 8:3:631:A:H2'     | 8:3:632:A:C8        | 2.47                     | 0.50              |
| 19:C:104:MET:HE2  | 19:C:176:GLY:HA3    | 1.93                     | 0.50              |
| 20:E:24:LYS:HE2   | 20:E:75:THR:HG22    | 1.93                     | 0.50              |
| 20:E:25:GLN:HE21  | 20:E:35:LEU:HB3     | 1.76                     | 0.50              |
| 23:H:61:LYS:HG2   | 23:H:63:PHE:CZ      | 2.46                     | 0.50              |
| 23:H:77:GLN:O     | 23:H:81:ILE:HG12    | 2.12                     | 0.50              |
| 42:d:148:ARG:HH21 | 42:d:149:ILE:HG12   | 1.76                     | 0.50              |
| 44:f:8:ASP:OD1    | 44:f:14:LYS:HA      | 2.11                     | 0.50              |
| 44:f:56:GLU:OE1   | 44:f:56:GLU:N       | 2.36                     | 0.50              |
| 45:g:103:LYS:HD2  | 45:g:106:MET:HG2    | 1.93                     | 0.50              |
| 50:l:32:TYR:CD2   | 50:l:114:MET:HE3    | 2.38                     | 0.50              |
| 59:u:39:LYS:NZ    | 59:u:45:ILE:HG13    | 2.26                     | 0.50              |
| 66:15:888:PHE:CB  | 66:15:935:LEU:HD22  | 2.42                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:426:LYS:N     | 66:15:140:ASN:ND2   | 2.31                     | 0.50              |
| 10:5:1289:U:O2'    | 10:5:1334:A:N3      | 2.38                     | 0.50              |
| 10:5:1406:U:O4     | 10:5:1407:A:N6      | 2.44                     | 0.50              |
| 10:5:1472:G:H1'    | 10:5:1493:MA6:H2    | 1.93                     | 0.50              |
| 20:E:65:ASP:OD1    | 20:E:66:ASN:N       | 2.41                     | 0.50              |
| 41:c:120:LEU:HA    | 41:c:125:THR:HG21   | 1.93                     | 0.50              |
| 43:e:168:PHE:C     | 43:e:169:ASP:OD2    | 2.54                     | 0.50              |
| 46:h:50:MET:HE1    | 46:h:52:PRO:HG3     | 1.93                     | 0.50              |
| 49:k:131:VAL:HG12  | 49:k:148:LEU:HD21   | 1.93                     | 0.50              |
| 64:13:283:ARG:HD3  | 64:13:290:ASP:CG    | 2.35                     | 0.50              |
| 64:13:633:THR:HG23 | 64:13:737:ILE:HD13  | 1.94                     | 0.50              |
| 66:15:161:THR:HG21 | 66:15:283:SER:OG    | 2.11                     | 0.50              |
| 66:15:1071:PHE:HD2 | 66:15:1247:ARG:NH1  | 2.00                     | 0.50              |
| 6:17:710:PHE:CD2   | 14:9:673:PHE:CG     | 3.00                     | 0.50              |
| 8:3:1031:U:HO2'    | 54:p:92:LYS:NZ      | 2.09                     | 0.50              |
| 8:3:2427:U:H5''    | 63:z:20:LEU:HD22    | 1.94                     | 0.50              |
| 8:3:2799:U:O4      | 8:3:2811:G:N2       | 2.45                     | 0.50              |
| 8:3:2803:G:O2'     | 8:3:2804:C:O5'      | 2.30                     | 0.50              |
| 10:5:1467:A:O2'    | 37:Y:44:A:C4'       | 2.60                     | 0.50              |
| 15:A:53:ASN:ND2    | 15:A:279:SER:O      | 2.43                     | 0.50              |
| 16:AA:72:LYS:HD2   | 16:AA:74:LYS:HG3    | 1.93                     | 0.50              |
| 24:I:49:PRO:O      | 24:I:77:LYS:NZ      | 2.45                     | 0.50              |
| 42:d:117:LEU:HD23  | 42:d:118:SER:N      | 2.26                     | 0.50              |
| 44:f:11:ASN:HB3    | 44:f:12:LEU:HG      | 1.93                     | 0.50              |
| 66:15:961:THR:HB   | 66:15:1269:LEU:HD23 | 1.89                     | 0.50              |
| 66:15:1209:GLU:CG  | 66:15:1249:TRP:CD1  | 2.93                     | 0.50              |
| 66:15:1219:MET:CE  | 66:15:1247:ARG:HH21 | 2.19                     | 0.50              |
| 8:3:339:U:H2'      | 8:3:340:U:C6        | 2.46                     | 0.50              |
| 8:3:408:G:OP2      | 8:3:459:A:N6        | 2.45                     | 0.50              |
| 8:3:848:U:H2'      | 8:3:849:C:C6        | 2.47                     | 0.50              |
| 8:3:2224:A:H2'     | 8:3:2225:G:H8       | 1.76                     | 0.50              |
| 8:3:2324:A:H2'     | 8:3:2325:U:C6       | 2.47                     | 0.50              |
| 10:5:528:G:C6      | 13:8:35:U:H1'       | 2.46                     | 0.50              |
| 10:5:1049:G:H5''   | 36:W:189:LEU:HD11   | 1.93                     | 0.50              |
| 17:AB:43:A:H2'     | 37:Y:44:A:H8        | 1.76                     | 0.50              |
| 36:W:156:VAL:HG22  | 36:W:201:VAL:HG12   | 1.93                     | 0.50              |
| 42:d:96:MET:HE3    | 42:d:97:TRP:CD1     | 2.47                     | 0.50              |
| 55:q:55:VAL:HG22   | 55:q:97:PHE:CE1     | 2.47                     | 0.50              |
| 64:13:803:ASP:O    | 64:13:809:LYS:HE3   | 2.11                     | 0.50              |
| 66:15:1116:ILE:CG2 | 66:15:1248:LEU:HD11 | 2.41                     | 0.50              |
| 6:17:699:ILE:O     | 14:9:692:LYS:CD     | 2.60                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:941:VAL:HG13  | 6:17:945:ILE:CD1    | 2.42                     | 0.50              |
| 8:3:1005:G:H2'     | 8:3:1006:U:C6       | 2.46                     | 0.50              |
| 8:3:1485:A:H4'     | 8:3:1486:U:C4       | 2.47                     | 0.50              |
| 8:3:1837:C:H2'     | 8:3:1838:A:H8       | 1.77                     | 0.50              |
| 9:4:106:A:H2'      | 9:4:107:G:C8        | 2.47                     | 0.50              |
| 10:5:998:G:H5'     | 10:5:999:C:C4       | 2.47                     | 0.50              |
| 17:AB:41:U:C3'     | 37:Y:42:C:C5        | 2.95                     | 0.50              |
| 17:AB:47:U:H3'     | 17:AB:48:C:H6       | 1.77                     | 0.50              |
| 20:E:49:ILE:HD13   | 20:E:84:ARG:NH2     | 2.25                     | 0.50              |
| 41:c:183:LEU:HD12  | 41:c:203:VAL:HG13   | 1.94                     | 0.50              |
| 65:14:138:GLU:OE2  | 65:14:501:TYR:OH    | 2.22                     | 0.50              |
| 65:14:311:TYR:CE2  | 65:14:478:LEU:HD21  | 2.47                     | 0.50              |
| 66:15:991:TRP:HA   | 66:15:1093:GLY:O    | 2.12                     | 0.50              |
| 67:18:62:ILE:HG22  | 67:18:68:SER:HB2    | 1.94                     | 0.50              |
| 6:17:80:GLY:HA2    | 65:14:1271:ILE:HD12 | 1.93                     | 0.49              |
| 6:17:429:ASP:CG    | 66:15:184:GLN:HB3   | 2.36                     | 0.49              |
| 6:17:595:ARG:NE    | 14:9:644:LYS:N      | 2.50                     | 0.49              |
| 6:17:598:LYS:HG3   | 14:9:641:ARG:HH21   | 0.46                     | 0.49              |
| 8:3:230:G:O2'      | 8:3:232:A:N6        | 2.45                     | 0.49              |
| 8:3:340:U:H1'      | 8:3:1241:U:H5       | 1.77                     | 0.49              |
| 8:3:1391:U:O2'     | 8:3:1816:A:N3       | 2.34                     | 0.49              |
| 8:3:2299:U:OP1     | 8:3:2388:C:O2'      | 2.29                     | 0.49              |
| 24:I:48:LEU:HD11   | 24:I:79:LEU:HD12    | 1.94                     | 0.49              |
| 31:P:18:ASN:HB2    | 31:P:21:THR:OG1     | 2.12                     | 0.49              |
| 46:h:112:LEU:HG    | 46:h:114:ALA:H      | 1.76                     | 0.49              |
| 59:u:61:PRO:HB3    | 59:u:65:VAL:HG12    | 1.94                     | 0.49              |
| 64:13:1020:MET:CB  | 67:18:256:HIS:HB3   | 2.38                     | 0.49              |
| 65:14:1032:GLN:OE1 | 66:15:540:ASN:ND2   | 2.45                     | 0.49              |
| 66:15:343:LYS:CE   | 66:15:439:MET:HB3   | 2.41                     | 0.49              |
| 66:15:494:ARG:NH1  | 66:15:701:GLN:NE2   | 2.59                     | 0.49              |
| 2:1:42:ARG:NH1     | 8:3:2358:U:OP2      | 2.45                     | 0.49              |
| 6:17:835:PHE:CE1   | 6:17:920:VAL:HG21   | 2.47                     | 0.49              |
| 8:3:9:G:H5'        | 47:i:135:MET:HE1    | 1.94                     | 0.49              |
| 8:3:102:A:C8       | 14:9:786:MET:HG3    | 2.45                     | 0.49              |
| 8:3:1103:G:O2'     | 8:3:1104:A:H5'      | 2.12                     | 0.49              |
| 8:3:1134:G:H2'     | 8:3:1135:C:C6       | 2.47                     | 0.49              |
| 8:3:1436:C:H2'     | 8:3:1437:A:C8       | 2.47                     | 0.49              |
| 8:3:1529:U:H2'     | 8:3:1530:G:C8       | 2.46                     | 0.49              |
| 8:3:1559:A:O2'     | 14:9:249:ASP:OD1    | 2.30                     | 0.49              |
| 8:3:2452:G:OP2     | 41:c:69:LYS:HD2     | 2.12                     | 0.49              |
| 8:3:2820:G:N3      | 8:3:2887:A:O2'      | 2.44                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:5:55:C:H2'      | 10:5:348:C:H41     | 1.76                     | 0.49              |
| 10:5:190:A:H2'     | 10:5:191:A:H8      | 1.75                     | 0.49              |
| 13:8:4:U:H2'       | 13:8:5:C:C6        | 2.47                     | 0.49              |
| 14:9:795:GLN:HA    | 61:w:18:LEU:HD21   | 1.92                     | 0.49              |
| 17:AB:48:C:H1'     | 36:W:167:ARG:HH21  | 1.75                     | 0.49              |
| 18:AC:94:LEU:O     | 18:AC:98:ASN:ND2   | 2.44                     | 0.49              |
| 19:C:92:VAL:O      | 19:C:96:ARG:NH1    | 2.44                     | 0.49              |
| 42:d:34:ILE:HG23   | 42:d:155:THR:O     | 2.13                     | 0.49              |
| 64:13:134:LYS:C    | 64:13:578:ASN:HD21 | 2.20                     | 0.49              |
| 64:13:1151:PHE:CE2 | 64:13:1171:ILE:CD1 | 2.95                     | 0.49              |
| 65:14:242:LYS:HE2  | 65:14:396:GLU:OE2  | 2.12                     | 0.49              |
| 65:14:948:VAL:HG23 | 66:15:247:LYS:NZ   | 2.21                     | 0.49              |
| 66:15:973:TYR:CE1  | 66:15:977:LEU:HD11 | 2.47                     | 0.49              |
| 66:15:1154:GLU:HG3 | 67:16:70:ASN:O     | 2.12                     | 0.49              |
| 67:16:3:ASN:HB2    | 67:16:154:GLU:OE2  | 2.12                     | 0.49              |
| 8:3:894:G:N3       | 8:3:2276:A:H2'     | 2.27                     | 0.49              |
| 8:3:1045:A:N3      | 8:3:1188:C:O2'     | 2.39                     | 0.49              |
| 8:3:1575:C:H2'     | 8:3:1576:G:O4'     | 2.12                     | 0.49              |
| 8:3:2038:A:N3      | 8:3:2463:G:O2'     | 2.40                     | 0.49              |
| 10:5:1051:U:OP1    | 28:M:45:ARG:NH2    | 2.45                     | 0.49              |
| 10:5:1113:U:O4     | 10:5:1114:A:N6     | 2.45                     | 0.49              |
| 31:P:56:LYS:H      | 31:P:56:LYS:HD2    | 1.78                     | 0.49              |
| 36:W:113:MET:O     | 36:W:115:SER:N     | 2.39                     | 0.49              |
| 42:d:50:LEU:O      | 42:d:53:ALA:HB3    | 2.12                     | 0.49              |
| 55:q:19:THR:HG22   | 55:q:93:LYS:HB2    | 1.94                     | 0.49              |
| 55:q:54:ARG:HB2    | 55:q:98:VAL:HB     | 1.94                     | 0.49              |
| 64:13:6:ASN:CA     | 67:18:198:LEU:HD11 | 2.41                     | 0.49              |
| 65:14:324:LYS:NZ   | 65:14:338:ASN:O    | 2.43                     | 0.49              |
| 65:14:753:ILE:CG2  | 65:14:782:TRP:CE2  | 2.94                     | 0.49              |
| 67:18:167:VAL:CG1  | 67:18:170:LEU:HD21 | 2.42                     | 0.49              |
| 67:16:105:TRP:CH2  | 67:16:152:TYR:HB2  | 2.47                     | 0.49              |
| 2:1:19:ILE:HD12    | 2:1:47:VAL:HG21    | 1.94                     | 0.49              |
| 6:17:275:ASN:HB3   | 65:14:1126:LEU:H   | 1.77                     | 0.49              |
| 6:17:697:TYR:HA    | 14:9:636:PHE:CD1   | 2.46                     | 0.49              |
| 6:17:831:PHE:CZ    | 6:17:913:VAL:HG21  | 2.47                     | 0.49              |
| 8:3:147:C:H5''     | 61:w:66:GLN:HE22   | 1.77                     | 0.49              |
| 8:3:410:G:C8       | 60:v:60:LYS:HD2    | 2.47                     | 0.49              |
| 8:3:631:A:H2'      | 8:3:632:A:H8       | 1.77                     | 0.49              |
| 8:3:900:G:H2'      | 8:3:901:C:C6       | 2.47                     | 0.49              |
| 8:3:1245:G:H1      | 8:3:1264:U:H3      | 1.60                     | 0.49              |
| 8:3:1878:A:H3'     | 8:3:1879:A:C8      | 2.47                     | 0.49              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 10:5:92:G:N7      | 34:S:10:ARG:NH2     | 2.61                     | 0.49              |
| 14:9:163:PRO:CB   | 58:t:63:VAL:CG2     | 2.88                     | 0.49              |
| 14:9:798:ARG:HA   | 61:w:25:GLU:CG      | 2.41                     | 0.49              |
| 28:M:19:ARG:HH11  | 28:M:19:ARG:HG3     | 1.78                     | 0.49              |
| 47:i:78:TYR:HE1   | 47:i:89:LYS:HB3     | 1.77                     | 0.49              |
| 48:j:21:ILE:HA    | 48:j:41:VAL:HG12    | 1.95                     | 0.49              |
| 55:q:27:ALA:O     | 55:q:62:HIS:NE2     | 2.46                     | 0.49              |
| 64:13:80:GLN:HE22 | 64:13:122:GLN:NE2   | 2.09                     | 0.49              |
| 65:14:51:PRO:HB3  | 65:14:714:THR:HG21  | 1.95                     | 0.49              |
| 6:17:261:LYS:H    | 65:14:1126:LEU:HD21 | 0.68                     | 0.49              |
| 6:17:540:LEU:HD23 | 6:17:669:PHE:CZ     | 2.47                     | 0.49              |
| 8:3:901:C:H4'     | 8:3:902:U:O5'       | 2.12                     | 0.49              |
| 8:3:2583:U:H4'    | 40:b:148:GLN:HE21   | 1.77                     | 0.49              |
| 8:3:2630:U:O2'    | 8:3:2829:G:N7       | 2.44                     | 0.49              |
| 10:5:68:C:H2'     | 10:5:69:G:C8        | 2.47                     | 0.49              |
| 15:A:44:PHE:HD1   | 15:A:60:LEU:HD13    | 1.77                     | 0.49              |
| 17:AB:41:U:H3'    | 37:Y:42:C:C5        | 2.46                     | 0.49              |
| 59:u:39:LYS:HZ2   | 59:u:45:ILE:HG13    | 1.77                     | 0.49              |
| 61:w:77:LYS:HG2   | 61:w:78:LYS:H       | 1.76                     | 0.49              |
| 64:13:173:GLU:OE1 | 66:15:1178:SER:CA   | 2.56                     | 0.49              |
| 64:13:907:LEU:O   | 64:13:912:LEU:HA    | 2.13                     | 0.49              |
| 66:15:1173:LEU:O  | 66:15:1189:LYS:CE   | 2.60                     | 0.49              |
| 8:3:51:A:H5''     | 8:3:53:G:O4'        | 2.12                     | 0.49              |
| 8:3:355:A:O2'     | 8:3:374:A:N3        | 2.45                     | 0.49              |
| 8:3:619:A:N1      | 8:3:844:G:O2'       | 2.37                     | 0.49              |
| 8:3:776:U:H2'     | 8:3:777:C:H6        | 1.78                     | 0.49              |
| 8:3:1135:C:H2'    | 8:3:1136:U:O4'      | 2.13                     | 0.49              |
| 8:3:1803:U:H2'    | 8:3:1804:A:C8       | 2.47                     | 0.49              |
| 9:4:105:A:H2'     | 9:4:106:A:C8        | 2.47                     | 0.49              |
| 10:5:259:A:OP1    | 34:S:67:ARG:NH1     | 2.45                     | 0.49              |
| 10:5:516:C:H4'    | 10:5:517:C:H5''     | 1.94                     | 0.49              |
| 16:AA:167:ARG:NH1 | 16:AA:171:GLU:OE2   | 2.42                     | 0.49              |
| 19:C:26:SER:OG    | 19:C:27:LYS:N       | 2.44                     | 0.49              |
| 27:L:68:ASP:HA    | 27:L:71:ARG:HH11    | 1.77                     | 0.49              |
| 39:a:147:VAL:HA   | 39:a:200:VAL:HA     | 1.94                     | 0.49              |
| 41:c:8:LYS:NZ     | 41:c:14:GLU:OE1     | 2.45                     | 0.49              |
| 42:d:2:ASN:HB3    | 42:d:5:LYS:HB2      | 1.95                     | 0.49              |
| 45:g:46:LYS:HG2   | 45:g:48:GLY:H       | 1.78                     | 0.49              |
| 54:p:45:ALA:O     | 54:p:49:ARG:HG3     | 2.12                     | 0.49              |
| 58:t:3:ARG:NH2    | 58:t:74:LEU:O       | 2.46                     | 0.49              |
| 65:14:610:ILE:CA  | 66:15:248:THR:HB    | 2.42                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1:9:LYS:O        | 49:k:65:PHE:N      | 2.40                     | 0.49              |
| 3:10:238:PHE:CG    | 6:17:562:ALA:HB1   | 2.48                     | 0.49              |
| 8:3:916:U:H3       | 8:3:935:U:H3       | 1.60                     | 0.49              |
| 8:3:1246:U:OP1     | 54:p:7:LYS:NZ      | 2.46                     | 0.49              |
| 8:3:1440:U:H2'     | 8:3:1441:A:H8      | 1.78                     | 0.49              |
| 8:3:2031:C:H2'     | 8:3:2032:G:H8      | 1.77                     | 0.49              |
| 10:5:87:G:H2'      | 10:5:88:A:H8       | 1.76                     | 0.49              |
| 30:O:8:ARG:HB2     | 30:O:28:ARG:NH1    | 2.27                     | 0.49              |
| 40:b:50:THR:HB     | 40:b:87:MET:HB3    | 1.94                     | 0.49              |
| 42:d:38:MET:HE2    | 42:d:150:ARG:CB    | 2.39                     | 0.49              |
| 60:v:37:LYS:HB3    | 60:v:45:THR:HG22   | 1.94                     | 0.49              |
| 18:x:40:GLY:O      | 18:x:46:TYR:CD2    | 2.66                     | 0.49              |
| 64:13:984:GLN:NE2  | 64:13:1133:THR:CB  | 2.66                     | 0.49              |
| 66:15:866:PHE:HE1  | 66:15:1262:LYS:HG2 | 1.69                     | 0.49              |
| 67:18:15:GLN:OE1   | 67:18:90:GLN:CG    | 2.61                     | 0.49              |
| 6:17:277:SER:CA    | 65:14:1125:THR:HA  | 2.41                     | 0.49              |
| 6:17:712:ILE:HG13  | 14:9:651:HIS:HE2   | 1.74                     | 0.49              |
| 8:3:253:C:O2'      | 49:k:64:LYS:NZ     | 2.34                     | 0.49              |
| 8:3:1178:A:N7      | 47:i:30:LYS:NZ     | 2.56                     | 0.49              |
| 10:5:9:A:O2'       | 19:C:202:ARG:NH2   | 2.45                     | 0.49              |
| 20:E:94:TYR:HB3    | 32:Q:85:HIS:CD2    | 2.48                     | 0.49              |
| 33:R:69:HIS:HB2    | 33:R:74:PHE:CZ     | 2.47                     | 0.49              |
| 45:g:41:ARG:NH1    | 45:g:51:ILE:O      | 2.45                     | 0.49              |
| 64:13:928:VAL:HG21 | 64:13:1034:THR:CG2 | 2.42                     | 0.49              |
| 6:17:426:LYS:CB    | 66:15:184:GLN:CG   | 2.63                     | 0.49              |
| 6:17:706:ILE:HD13  | 14:9:668:ILE:CD1   | 2.41                     | 0.49              |
| 8:3:1457:A:H2'     | 8:3:1458:A:C8      | 2.48                     | 0.49              |
| 10:5:499:U:H2'     | 10:5:500:G:H8      | 1.78                     | 0.49              |
| 10:5:671:G:H2'     | 10:5:672:A:H8      | 1.78                     | 0.49              |
| 10:5:1316:C:H2'    | 10:5:1317:A:C8     | 2.48                     | 0.49              |
| 10:5:1505:G:H2'    | 10:5:1506:A:C8     | 2.48                     | 0.49              |
| 19:C:94:GLU:HG2    | 19:C:182:PRO:HG2   | 1.94                     | 0.49              |
| 27:L:29:ARG:O      | 27:L:33:ILE:HG13   | 2.13                     | 0.49              |
| 27:L:55:ALA:O      | 27:L:59:VAL:HG23   | 2.12                     | 0.49              |
| 42:d:96:MET:HE3    | 42:d:97:TRP:NE1    | 2.28                     | 0.49              |
| 42:d:118:SER:C     | 42:d:120:LYS:H     | 2.21                     | 0.49              |
| 44:f:3:VAL:HG11    | 44:f:21:VAL:HG12   | 1.94                     | 0.49              |
| 58:t:64:GLN:CD     | 58:t:64:GLN:H      | 2.21                     | 0.49              |
| 64:13:58:TYR:HB3   | 64:13:70:LEU:HB2   | 1.95                     | 0.49              |
| 66:15:44:THR:HG23  | 66:15:655:LEU:CD2  | 2.43                     | 0.49              |
| 66:15:141:VAL:HG21 | 66:15:549:LEU:HD11 | 1.95                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 66:15:1149:THR:HG22 | 66:15:1154:GLU:OE2 | 2.13                     | 0.49              |
| 6:17:386:VAL:HG11   | 66:15:177:GLY:HA2  | 1.90                     | 0.49              |
| 8:3:520:C:H4'       | 14:9:161:LEU:CD2   | 2.43                     | 0.49              |
| 8:3:1282:G:N2       | 54:p:32:LYS:HB3    | 2.28                     | 0.49              |
| 8:3:1369:U:OP2      | 8:3:1422:U:O2'     | 2.30                     | 0.49              |
| 8:3:1559:A:H1'      | 14:9:247:LYS:CD    | 2.43                     | 0.49              |
| 8:3:1797:C:O2'      | 39:a:216:ALA:HB2   | 2.13                     | 0.49              |
| 8:3:2081:U:H2'      | 8:3:2082:U:C6      | 2.48                     | 0.49              |
| 8:3:2372:C:H2'      | 8:3:2373:G:O4'     | 2.13                     | 0.49              |
| 8:3:2561:G:C2       | 8:3:2591:G:H1'     | 2.48                     | 0.49              |
| 8:3:2568:G:H2'      | 8:3:2569:A:C8      | 2.48                     | 0.49              |
| 8:3:2869:U:OP2      | 8:3:2870:U:O2'     | 2.27                     | 0.49              |
| 10:5:426:U:H5'      | 19:C:8:PHE:CG      | 2.47                     | 0.49              |
| 10:5:661:G:H5'      | 32:Q:84:ARG:HH11   | 1.77                     | 0.49              |
| 20:E:3:TYR:HB2      | 20:E:62:PHE:CE1    | 2.48                     | 0.49              |
| 31:P:58:GLY:HA3     | 31:P:85:LYS:HD3    | 1.95                     | 0.49              |
| 43:e:9:ILE:HG21     | 43:e:53:LEU:HB3    | 1.95                     | 0.49              |
| 45:g:40:ILE:HD12    | 45:g:43:LYS:HE3    | 1.94                     | 0.49              |
| 46:h:105:ALA:HA     | 46:h:123:MET:HE2   | 1.91                     | 0.49              |
| 64:13:924:LYS:HG3   | 67:18:74:SER:HB2   | 1.95                     | 0.49              |
| 66:15:993:VAL:HG22  | 66:15:1027:PHE:CE1 | 2.48                     | 0.49              |
| 3:10:253:PHE:CZ     | 6:17:15:ILE:CG2    | 2.57                     | 0.48              |
| 6:17:428:GLY:O      | 66:15:188:PHE:CD2  | 2.66                     | 0.48              |
| 6:17:693:THR:CB     | 14:9:637:CYS:CB    | 2.68                     | 0.48              |
| 8:3:879:U:O4        | 8:3:968:U:O2'      | 2.27                     | 0.48              |
| 8:3:2110:U:H3       | 8:3:2194:G:H1      | 1.62                     | 0.48              |
| 8:3:2336:A:H2'      | 8:3:2337:U:C6      | 2.47                     | 0.48              |
| 10:5:76:G:N2        | 10:5:79:A:OP2      | 2.44                     | 0.48              |
| 10:5:733:A:OP1      | 32:Q:92:ARG:NH1    | 2.46                     | 0.48              |
| 17:AB:44:A:O5'      | 37:Y:44:A:C8       | 2.62                     | 0.48              |
| 36:W:72:ALA:HA      | 36:W:109:ILE:HG22  | 1.95                     | 0.48              |
| 43:e:100:ASN:OD1    | 43:e:107:ASN:ND2   | 2.42                     | 0.48              |
| 43:e:120:ILE:HA     | 43:e:147:PHE:HE1   | 1.78                     | 0.48              |
| 44:f:96:GLN:HE21    | 44:f:121:PHE:CB    | 2.20                     | 0.48              |
| 54:p:86:ASN:HB2     | 55:q:47:ALA:HB1    | 1.94                     | 0.48              |
| 60:v:4:LYS:HG3      | 60:v:5:ASP:O       | 2.12                     | 0.48              |
| 64:13:296:LEU:HD11  | 64:13:572:ALA:O    | 2.13                     | 0.48              |
| 65:14:775:ASN:ND2   | 65:14:1228:THR:O   | 2.46                     | 0.48              |
| 66:15:196:ASN:HA    | 66:15:516:ARG:NH2  | 2.28                     | 0.48              |
| 66:15:1131:GLY:HA3  | 66:15:1208:PHE:HB2 | 1.94                     | 0.48              |
| 6:17:374:ALA:N      | 66:15:172:PRO:O    | 2.46                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:1451:A:H2'     | 8:3:1452:G:C8      | 2.49                     | 0.48              |
| 8:3:1561:G:N7      | 14:9:248:GLU:HG3   | 2.28                     | 0.48              |
| 10:5:433:C:H1'     | 19:C:153:ILE:HD11  | 1.95                     | 0.48              |
| 14:9:163:PRO:HB2   | 58:t:63:VAL:CG2    | 2.43                     | 0.48              |
| 17:AB:41:U:C2      | 37:Y:42:C:N4       | 2.70                     | 0.48              |
| 36:W:61:THR:HB     | 36:W:64:THR:HG22   | 1.95                     | 0.48              |
| 46:h:123:MET:HG2   | 46:h:124:VAL:N     | 2.28                     | 0.48              |
| 64:13:216:ILE:HD12 | 64:13:234:PHE:CE2  | 2.49                     | 0.48              |
| 66:15:961:THR:C    | 66:15:1269:LEU:CD2 | 2.80                     | 0.48              |
| 6:17:386:VAL:CG1   | 66:15:177:GLY:CA   | 2.73                     | 0.48              |
| 6:17:697:TYR:CA    | 14:9:636:PHE:CD1   | 2.78                     | 0.48              |
| 6:17:705:ASP:CA    | 14:9:665:HIS:ND1   | 2.69                     | 0.48              |
| 6:17:795:ILE:HD12  | 6:17:931:ILE:HD11  | 1.94                     | 0.48              |
| 8:3:528:U:H2'      | 8:3:529:G:H8       | 1.78                     | 0.48              |
| 8:3:668:A:H2'      | 8:3:669:A:C8       | 2.48                     | 0.48              |
| 8:3:2853:U:O2'     | 8:3:2870:U:O2      | 2.28                     | 0.48              |
| 8:3:2863:G:H8      | 8:3:2863:G:OP2     | 1.96                     | 0.48              |
| 9:4:3:U:O2'        | 9:4:24:A:N1        | 2.43                     | 0.48              |
| 10:5:1102:A:N1     | 36:W:180:THR:HG22  | 2.29                     | 0.48              |
| 16:AA:78:LYS:HG2   | 16:AA:85:ASN:HB2   | 1.95                     | 0.48              |
| 18:AC:70:LYS:NZ    | 33:R:43:GLU:OE1    | 2.46                     | 0.48              |
| 21:F:19:ASN:OD1    | 21:F:22:VAL:HG23   | 2.14                     | 0.48              |
| 25:J:29:ASP:OD1    | 25:J:30:PRO:HD2    | 2.13                     | 0.48              |
| 39:a:252:ASP:OD2   | 39:a:252:ASP:N     | 2.41                     | 0.48              |
| 44:f:62:LYS:O      | 44:f:66:HIS:ND1    | 2.35                     | 0.48              |
| 65:14:152:LYS:HE2  | 65:14:156:GLU:OE1  | 2.13                     | 0.48              |
| 66:15:547:ASN:OD1  | 66:15:550:GLU:HB2  | 2.13                     | 0.48              |
| 66:15:1149:THR:CG2 | 66:15:1154:GLU:CB  | 2.91                     | 0.48              |
| 6:17:256:THR:N     | 65:14:1100:THR:HA  | 2.21                     | 0.48              |
| 6:17:703:ASN:O     | 14:9:665:HIS:N     | 2.46                     | 0.48              |
| 8:3:881:A:H2       | 8:3:968:U:H3       | 1.57                     | 0.48              |
| 8:3:2490:A:HO2'    | 13:8:63:U:HO2'     | 1.58                     | 0.48              |
| 8:3:2583:U:H4'     | 40:b:148:GLN:NE2   | 2.28                     | 0.48              |
| 15:A:118:THR:HA    | 15:A:194:LEU:HD11  | 1.95                     | 0.48              |
| 30:O:36:ILE:HD12   | 30:O:55:ALA:HB2    | 1.94                     | 0.48              |
| 36:W:159:ARG:HH21  | 36:W:196:TYR:HB3   | 1.77                     | 0.48              |
| 41:c:162:ASN:HB2   | 41:c:203:VAL:HG23  | 1.95                     | 0.48              |
| 53:o:64:PHE:CD1    | 53:o:81:ILE:HG12   | 2.49                     | 0.48              |
| 64:13:684:GLY:HA3  | 64:13:861:ILE:O    | 2.13                     | 0.48              |
| 65:14:700:LEU:HD23 | 65:14:701:TYR:CE2  | 2.48                     | 0.48              |
| 66:15:94:GLU:O     | 66:15:98:TRP:HB3   | 2.14                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:15:689:GLU:OE2  | 66:15:1040:SER:OG   | 2.20                     | 0.48              |
| 66:15:1149:THR:CG2 | 66:15:1154:GLU:HB2  | 2.44                     | 0.48              |
| 5:12:85:TRP:CG     | 6:17:8:SER:N        | 2.81                     | 0.48              |
| 6:17:697:TYR:C     | 14:9:689:ILE:HD13   | 2.37                     | 0.48              |
| 6:17:703:ASN:CB    | 14:9:663:ASN:CG     | 2.87                     | 0.48              |
| 8:3:312:U:H2'      | 8:3:313:G:C8        | 2.48                     | 0.48              |
| 10:5:258:A:O3'     | 34:S:63:ASN:ND2     | 2.45                     | 0.48              |
| 10:5:259:A:H2'     | 10:5:260:C:C6       | 2.47                     | 0.48              |
| 10:5:661:G:H5'     | 32:Q:84:ARG:NH1     | 2.29                     | 0.48              |
| 19:C:166:PHE:CD1   | 19:C:182:PRO:HG3    | 2.48                     | 0.48              |
| 23:H:125:ARG:HG2   | 23:H:126:ALA:H      | 1.77                     | 0.48              |
| 64:13:13:PHE:HE2   | 64:13:1210:GLU:OE1  | 1.95                     | 0.48              |
| 64:13:29:GLN:HE22  | 64:13:746:LYS:HD2   | 1.79                     | 0.48              |
| 6:17:430:PRO:HG2   | 66:15:556:GLN:HE21  | 1.79                     | 0.48              |
| 8:3:1561:G:P       | 14:9:251:TYR:CE2    | 3.05                     | 0.48              |
| 10:5:1468:A:C5     | 13:8:37:T6A:O4'     | 2.67                     | 0.48              |
| 13:8:37:T6A:N1     | 13:8:37:T6A:N11     | 2.56                     | 0.48              |
| 26:K:96:ARG:HG2    | 26:K:111:VAL:HG23   | 1.95                     | 0.48              |
| 27:L:3:ARG:O       | 27:L:57:ARG:NH2     | 2.43                     | 0.48              |
| 36:W:92:ILE:O      | 36:W:95:ILE:HG22    | 2.14                     | 0.48              |
| 59:u:78:ASP:HB3    | 59:u:100:HIS:CD2    | 2.47                     | 0.48              |
| 64:13:870:PHE:HB3  | 64:13:874:PHE:CE2   | 2.49                     | 0.48              |
| 64:13:1062:ARG:CZ  | 67:18:69:ASN:O      | 2.61                     | 0.48              |
| 65:14:531:PHE:CZ   | 65:14:563:ILE:HG21  | 2.42                     | 0.48              |
| 67:18:128:ASN:O    | 67:18:136:LYS:HE2   | 2.12                     | 0.48              |
| 6:17:430:PRO:HG3   | 66:15:553:SER:OG    | 2.14                     | 0.48              |
| 6:17:699:ILE:HG21  | 14:9:689:ILE:C      | 2.27                     | 0.48              |
| 6:17:926:PHE:CE1   | 6:17:930:LEU:HD11   | 2.49                     | 0.48              |
| 8:3:1696:C:O2'     | 8:3:2695:U:OP1      | 2.32                     | 0.48              |
| 8:3:2151:G:H1'     | 8:3:2154:A:H61      | 1.78                     | 0.48              |
| 15:A:221:GLN:NE2   | 15:A:279:SER:HB2    | 2.29                     | 0.48              |
| 29:N:16:ASP:O      | 29:N:17:LYS:HG2     | 2.14                     | 0.48              |
| 52:n:31:MET:HE3    | 52:n:44:TRP:CD1     | 2.49                     | 0.48              |
| 55:q:67:LYS:HD2    | 55:q:86:ARG:HD2     | 1.95                     | 0.48              |
| 65:14:872:ARG:HG2  | 65:14:1220:LEU:HD12 | 1.95                     | 0.48              |
| 66:15:1237:PRO:CG  | 66:15:1239:HIS:NE2  | 2.68                     | 0.48              |
| 67:18:105:TRP:HH2  | 67:18:152:TYR:HB2   | 1.77                     | 0.48              |
| 6:17:260:GLN:C     | 65:14:1126:LEU:HD23 | 2.37                     | 0.48              |
| 8:3:101:C:O2'      | 14:9:699:VAL:HG13   | 2.13                     | 0.48              |
| 8:3:1688:A:N7      | 8:3:2012:A:H2       | 2.11                     | 0.48              |
| 10:5:1022:G:H2'    | 10:5:1023:G:C8      | 2.49                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 15:A:178:VAL:HG13   | 15:A:184:GLU:HG3   | 1.96                     | 0.48              |
| 23:H:121:TYR:HE1    | 23:H:127:PRO:HG3   | 1.78                     | 0.48              |
| 30:O:59:LEU:HD11    | 30:O:73:PHE:CE2    | 2.49                     | 0.48              |
| 39:a:112:PRO:HG2    | 39:a:115:ILE:HG12  | 1.95                     | 0.48              |
| 44:f:68:LEU:CB      | 44:f:108:LEU:HD21  | 2.43                     | 0.48              |
| 51:m:19:ARG:O       | 51:m:23:SER:OG     | 2.31                     | 0.48              |
| 54:p:104:LYS:O      | 54:p:108:ILE:HG13  | 2.13                     | 0.48              |
| 61:w:15:LEU:HG      | 61:w:54:ILE:HG23   | 1.96                     | 0.48              |
| 64:13:811:ALA:CB    | 64:13:901:ILE:HG22 | 2.37                     | 0.48              |
| 65:14:316:LYS:HD2   | 65:14:480:GLU:OE1  | 2.14                     | 0.48              |
| 66:15:965:LEU:O     | 66:15:970:ALA:HA   | 2.14                     | 0.48              |
| 67:16:167:VAL:HG12  | 67:16:170:LEU:HG   | 1.96                     | 0.48              |
| 3:10:275:SER:HG     | 6:17:970:SER:HB2   | 1.34                     | 0.48              |
| 6:17:45:VAL:HG13    | 6:17:505:LEU:HD22  | 1.96                     | 0.48              |
| 6:17:955:LYS:HD3    | 14:9:803:LYS:HD2   | 1.95                     | 0.48              |
| 8:3:799:A:H5''      | 39:a:217:GLY:CA    | 2.44                     | 0.48              |
| 8:3:1414:C:H2'      | 8:3:1415:A:H8      | 1.78                     | 0.48              |
| 8:3:1801:U:H2'      | 8:3:1802:C:C6      | 2.48                     | 0.48              |
| 8:3:2530:U:O2'      | 8:3:2655:U:OP1     | 2.28                     | 0.48              |
| 10:5:409:G:N2       | 10:5:425:G:H1'     | 2.29                     | 0.48              |
| 10:5:499:U:H2'      | 10:5:500:G:C8      | 2.48                     | 0.48              |
| 13:8:63:U:H6        | 13:8:63:U:H5''     | 1.78                     | 0.48              |
| 14:9:199:LYS:HZ2    | 58:t:59:SER:HB2    | 1.78                     | 0.48              |
| 15:A:202:CYS:HB3    | 15:A:206:THR:OG1   | 2.13                     | 0.48              |
| 30:O:23:ASP:OD1     | 30:O:24:SER:N      | 2.47                     | 0.48              |
| 31:P:31:LYS:HE3     | 31:P:36:HIS:HB3    | 1.96                     | 0.48              |
| 39:a:252:ASP:OD1    | 39:a:261:ARG:NH1   | 2.46                     | 0.48              |
| 42:d:132:ILE:HB     | 42:d:152:PHE:HB2   | 1.96                     | 0.48              |
| 64:13:1151:PHE:HE2  | 64:13:1171:ILE:CD1 | 2.27                     | 0.48              |
| 65:14:87:LEU:HD11   | 65:14:103:ILE:CD1  | 2.43                     | 0.48              |
| 65:14:386:ILE:HG12  | 65:14:948:VAL:HG12 | 1.96                     | 0.48              |
| 65:14:1193:VAL:HG11 | 65:14:1197:ASN:O   | 2.14                     | 0.48              |
| 66:15:725:SER:C     | 66:15:727:ALA:H    | 2.22                     | 0.48              |
| 3:10:97:ILE:HD11    | 3:10:293:ILE:HG22  | 1.95                     | 0.48              |
| 6:17:829:TYR:CE1    | 6:17:833:LEU:HD11  | 2.49                     | 0.48              |
| 8:3:548:A:H2'       | 8:3:549:A:C8       | 2.49                     | 0.48              |
| 8:3:818:A:H2'       | 8:3:819:U:H4'      | 1.95                     | 0.48              |
| 8:3:1229:U:H2'      | 8:3:1230:U:C6      | 2.49                     | 0.48              |
| 8:3:2032:G:H2'      | 8:3:2033:G:H8      | 1.79                     | 0.48              |
| 8:3:2077:A:H2'      | 8:3:2078:A:H8      | 1.79                     | 0.48              |
| 8:3:2155:G:H2'      | 8:3:2156:G:H8      | 1.78                     | 0.48              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 8:3:2438:A:H2'    | 8:3:2438:A:N3       | 2.28                     | 0.48              |
| 8:3:2638:G:H2'    | 8:3:2639:G:H8       | 1.78                     | 0.48              |
| 10:5:36:G:N2      | 26:K:128:SER:OG     | 2.33                     | 0.48              |
| 10:5:380:G:H2'    | 10:5:381:C:O4'      | 2.14                     | 0.48              |
| 10:5:433:C:H2'    | 10:5:434:U:C6       | 2.49                     | 0.48              |
| 14:9:788:ALA:CA   | 61:w:6:GLU:CG       | 2.91                     | 0.48              |
| 22:G:118:THR:OG1  | 22:G:119:SER:N      | 2.46                     | 0.48              |
| 27:L:49:THR:OG1   | 27:L:52:GLU:OE1     | 2.24                     | 0.48              |
| 40:b:225:GLN:NE2  | 53:o:19:LYS:HD3     | 2.29                     | 0.48              |
| 49:k:81:ASN:OD1   | 49:k:83:ASN:ND2     | 2.47                     | 0.48              |
| 53:o:31:VAL:HG12  | 53:o:90:LEU:HA      | 1.94                     | 0.48              |
| 54:p:64:LEU:O     | 54:p:68:LEU:HD23    | 2.14                     | 0.48              |
| 56:r:1:MET:HE3    | 56:r:62:HIS:HB3     | 1.95                     | 0.48              |
| 59:u:102:LEU:O    | 59:u:103:ASP:C      | 2.57                     | 0.48              |
| 64:13:1192:LEU:CG | 67:18:88:GLN:HE21   | 2.22                     | 0.48              |
| 65:14:849:TYR:CE2 | 65:14:1270:LEU:HD13 | 2.49                     | 0.48              |
| 66:15:155:LYS:NZ  | 66:15:538:LYS:O     | 2.47                     | 0.48              |
| 66:15:286:GLY:HA2 | 66:15:487:LEU:CD2   | 2.44                     | 0.48              |
| 6:17:264:GLU:N    | 65:14:1095:GLY:O    | 2.44                     | 0.47              |
| 8:3:180:A:H5'     | 8:3:181:G:N7        | 2.28                     | 0.47              |
| 8:3:204:U:H4'     | 60:v:22:LYS:HB2     | 1.96                     | 0.47              |
| 8:3:1120:A:H2'    | 8:3:1121:A:N9       | 2.29                     | 0.47              |
| 8:3:2223:C:H2'    | 8:3:2224:A:C8       | 2.49                     | 0.47              |
| 8:3:2811:G:H2'    | 8:3:2812:U:C6       | 2.49                     | 0.47              |
| 8:3:2813:A:H61    | 8:3:2894:G:H2'      | 1.79                     | 0.47              |
| 10:5:265:U:H2'    | 10:5:266:A:C8       | 2.49                     | 0.47              |
| 10:5:470:U:O4     | 10:5:471:A:N6       | 2.47                     | 0.47              |
| 15:A:171:ARG:HG2  | 15:A:172:LEU:H      | 1.79                     | 0.47              |
| 17:AB:44:A:O3'    | 37:Y:44:A:C2'       | 2.32                     | 0.47              |
| 19:C:165:PRO:HB2  | 19:C:180:ARG:NH2    | 2.29                     | 0.47              |
| 54:p:46:TYR:HA    | 54:p:49:ARG:NH1     | 2.29                     | 0.47              |
| 58:t:38:GLY:C     | 58:t:39:LEU:HD23    | 2.39                     | 0.47              |
| 64:13:161:TRP:HH2 | 64:13:291:PHE:CE1   | 2.31                     | 0.47              |
| 65:14:22:ARG:CD   | 65:14:746:GLU:OE1   | 2.62                     | 0.47              |
| 5:12:85:TRP:CD1   | 6:17:8:SER:N        | 2.51                     | 0.47              |
| 8:3:39:C:H2'      | 8:3:40:A:C8         | 2.49                     | 0.47              |
| 8:3:1638:C:H2'    | 8:3:1639:C:C6       | 2.48                     | 0.47              |
| 8:3:2180:U:H4'    | 8:3:2181:A:OP2      | 2.14                     | 0.47              |
| 8:3:2490:A:O2'    | 13:8:63:U:O2'       | 2.29                     | 0.47              |
| 10:5:473:A:H2'    | 10:5:474:G:H8       | 1.80                     | 0.47              |
| 10:5:492:G:O2'    | 10:5:494:A:H1'      | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:5:1473:U:C6     | 37:Y:41:U:OP1      | 2.66                     | 0.47              |
| 10:5:1490:G:H2'    | 10:5:1491:A:C8     | 2.49                     | 0.47              |
| 13:8:58:A:O2'      | 13:8:60:U:OP2      | 2.32                     | 0.47              |
| 35:T:17:LYS:O      | 35:T:21:VAL:HG23   | 2.14                     | 0.47              |
| 44:f:82:LYS:NZ     | 44:f:125:GLU:OE1   | 2.46                     | 0.47              |
| 47:i:40:ARG:HG2    | 47:i:40:ARG:HH11   | 1.77                     | 0.47              |
| 49:k:90:LEU:HD11   | 49:k:97:SER:HB3    | 1.95                     | 0.47              |
| 54:p:73:MET:HE3    | 54:p:78:PHE:CD2    | 2.48                     | 0.47              |
| 61:w:45:ASN:O      | 61:w:49:ARG:HG2    | 2.14                     | 0.47              |
| 64:13:1041:TYR:CE2 | 64:13:1066:GLN:OE1 | 2.67                     | 0.47              |
| 66:15:795:GLN:CD   | 66:15:807:LYS:HB2  | 2.39                     | 0.47              |
| 1:0:6:GLN:O        | 8:3:721:G:H8       | 1.98                     | 0.47              |
| 8:3:474:U:H2'      | 8:3:475:A:C8       | 2.49                     | 0.47              |
| 8:3:1433:U:H2'     | 8:3:1434:U:C6      | 2.48                     | 0.47              |
| 8:3:1560:U:O3'     | 14:9:251:TYR:CE1   | 2.67                     | 0.47              |
| 8:3:2004:G:OP2     | 70:3:3214:PUT:N2   | 2.47                     | 0.47              |
| 10:5:212:G:O2'     | 10:5:464:A:N6      | 2.31                     | 0.47              |
| 10:5:1272:C:C2     | 21:F:113:LYS:NZ    | 2.80                     | 0.47              |
| 10:5:1387:U:H2'    | 10:5:1388:A:C8     | 2.50                     | 0.47              |
| 15:A:223:GLN:HE22  | 15:A:277:ILE:HD13  | 1.79                     | 0.47              |
| 23:H:86:VAL:CG2    | 23:H:100:LEU:HD13  | 2.44                     | 0.47              |
| 24:I:7:VAL:HG23    | 24:I:8:LYS:N       | 2.29                     | 0.47              |
| 39:a:2:PRO:HD2     | 39:a:25:LEU:HD21   | 1.96                     | 0.47              |
| 40:b:150:GLY:HA3   | 40:b:155:SER:HB3   | 1.95                     | 0.47              |
| 46:h:102:LYS:O     | 46:h:106:GLN:OE1   | 2.32                     | 0.47              |
| 54:p:106:ASN:O     | 54:p:109:VAL:HG22  | 2.15                     | 0.47              |
| 65:14:295:MET:CE   | 65:14:308:ILE:HD11 | 2.44                     | 0.47              |
| 65:14:381:THR:OG1  | 65:14:618:LYS:HG2  | 2.14                     | 0.47              |
| 65:14:1090:LYS:NZ  | 65:14:1138:ASP:CG  | 2.72                     | 0.47              |
| 65:14:1183:ARG:NH2 | 65:14:1222:ASP:OD1 | 2.47                     | 0.47              |
| 66:15:372:SER:C    | 66:15:374:ALA:H    | 2.23                     | 0.47              |
| 66:15:1097:LEU:O   | 67:16:256:HIS:HB3  | 2.13                     | 0.47              |
| 5:12:88:SER:N      | 6:17:615:PHE:CE2   | 2.82                     | 0.47              |
| 6:17:386:VAL:HA    | 66:15:175:PRO:CD   | 2.45                     | 0.47              |
| 6:17:807:ALA:HB1   | 6:17:912:ILE:HG21  | 1.96                     | 0.47              |
| 8:3:700:U:H5''     | 49:k:46:LEU:HD22   | 1.96                     | 0.47              |
| 8:3:1081:A:H2      | 45:g:11:VAL:HG11   | 1.79                     | 0.47              |
| 8:3:2403:C:H2'     | 8:3:2404:G:C8      | 2.49                     | 0.47              |
| 8:3:2755:G:O6      | 8:3:2763:C:H5''    | 2.14                     | 0.47              |
| 8:3:2808:A:H2'     | 8:3:2809:A:C8      | 2.49                     | 0.47              |
| 10:5:111:A:H2'     | 10:5:112:U:O4'     | 2.15                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:9:798:ARG:CD     | 61:w:22:LEU:H       | 1.97                     | 0.47              |
| 17:AB:43:A:H2       | 37:Y:44:A:C6        | 2.31                     | 0.47              |
| 22:G:16:ALA:HB2     | 22:G:89:GLN:OE1     | 2.14                     | 0.47              |
| 36:W:111:SER:HB2    | 36:W:114:LEU:HD21   | 1.95                     | 0.47              |
| 53:o:102:SER:O      | 53:o:105:ARG:HG2    | 2.14                     | 0.47              |
| 65:14:208:VAL:HG13  | 65:14:281:SER:HA    | 1.96                     | 0.47              |
| 65:14:610:ILE:HG13  | 66:15:248:THR:CG2   | 2.33                     | 0.47              |
| 66:15:872:GLN:HG3   | 66:15:897:VAL:CG2   | 2.44                     | 0.47              |
| 66:15:1031:VAL:HG11 | 66:15:1058:LEU:HD12 | 1.97                     | 0.47              |
| 6:17:706:ILE:HD13   | 14:9:668:ILE:HD13   | 1.95                     | 0.47              |
| 8:3:174:A:H2'       | 8:3:175:A:C8        | 2.50                     | 0.47              |
| 8:3:1092:A:H2'      | 8:3:1093:U:C6       | 2.50                     | 0.47              |
| 8:3:1422:U:H2'      | 8:3:1423:A:O4'      | 2.14                     | 0.47              |
| 8:3:1560:U:P        | 14:9:249:ASP:OD1    | 2.72                     | 0.47              |
| 8:3:2641:A:O2'      | 40:b:66:GLN:NE2     | 2.48                     | 0.47              |
| 10:5:991:A:H2'      | 10:5:992:U:C6       | 2.49                     | 0.47              |
| 12:7:34:G:C6        | 17:AB:42:C:N4       | 2.75                     | 0.47              |
| 13:8:63:U:O2'       | 13:8:64:G:H5'       | 2.15                     | 0.47              |
| 20:E:132:VAL:HG12   | 20:E:132:VAL:O      | 2.15                     | 0.47              |
| 21:F:74:LEU:HD22    | 21:F:85:GLN:CB      | 2.44                     | 0.47              |
| 42:d:8:TYR:O        | 42:d:12:ILE:HB      | 2.15                     | 0.47              |
| 64:13:332:VAL:HG12  | 64:13:514:LEU:CD1   | 2.44                     | 0.47              |
| 64:13:868:ASN:ND2   | 64:13:1002:GLN:NE2  | 2.60                     | 0.47              |
| 65:14:217:ASP:HB2   | 65:14:221:ASN:HD22  | 1.80                     | 0.47              |
| 65:14:295:MET:HE3   | 65:14:296:PHE:CE2   | 2.50                     | 0.47              |
| 3:10:289:VAL:HG11   | 3:10:422:ILE:CG1    | 2.45                     | 0.47              |
| 5:12:88:SER:HB3     | 6:17:655:TYR:OH     | 2.15                     | 0.47              |
| 8:3:101:C:OP2       | 14:9:776:ALA:HB1    | 2.14                     | 0.47              |
| 8:3:141:A:H2        | 8:3:1437:A:H1'      | 1.79                     | 0.47              |
| 8:3:164:A:OP2       | 8:3:165:U:O2'       | 2.22                     | 0.47              |
| 8:3:855:A:H4'       | 8:3:871:G:N2        | 2.29                     | 0.47              |
| 8:3:1121:A:H5''     | 8:3:1122:G:H5'      | 1.96                     | 0.47              |
| 8:3:1137:C:H2'      | 8:3:1138:A:C8       | 2.45                     | 0.47              |
| 17:AB:47:U:H3'      | 17:AB:48:C:C6       | 2.50                     | 0.47              |
| 19:C:74:LEU:O       | 19:C:78:VAL:HG12    | 2.14                     | 0.47              |
| 36:W:46:VAL:CG2     | 36:W:47:ASN:H       | 2.26                     | 0.47              |
| 40:b:50:THR:OG1     | 40:b:87:MET:O       | 2.22                     | 0.47              |
| 40:b:84:ILE:HD13    | 40:b:87:MET:SD      | 2.55                     | 0.47              |
| 42:d:155:THR:O      | 42:d:156:LEU:HD13   | 2.15                     | 0.47              |
| 62:y:33:CYS:SG      | 62:y:35:LYS:HG2     | 2.54                     | 0.47              |
| 66:15:168:VAL:CG1   | 66:15:625:LYS:HE3   | 2.43                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:15:727:ALA:C    | 66:15:729:GLY:H     | 2.22                     | 0.47              |
| 66:15:1106:SER:O   | 67:16:254:LYS:HD2   | 2.15                     | 0.47              |
| 1:0:18:PHE:CZ      | 1:0:22:MET:HG3      | 2.49                     | 0.47              |
| 5:12:85:TRP:H      | 6:17:8:SER:N        | 2.11                     | 0.47              |
| 6:17:260:GLN:N     | 65:14:1126:LEU:HD22 | 2.30                     | 0.47              |
| 6:17:376:LYS:HZ2   | 66:15:178:GLU:HG3   | 0.64                     | 0.47              |
| 6:17:659:TYR:O     | 6:17:663:VAL:HG23   | 2.14                     | 0.47              |
| 6:17:690:LEU:C     | 14:9:682:VAL:CG2    | 2.84                     | 0.47              |
| 6:17:692:LYS:CE    | 14:9:683:HIS:CD2    | 2.75                     | 0.47              |
| 6:17:845:TRP:CE2   | 14:9:644:LYS:CG     | 2.77                     | 0.47              |
| 8:3:356:A:H5'      | 8:3:374:A:H1'       | 1.96                     | 0.47              |
| 8:3:1063:A:H2'     | 8:3:1064:A:C8       | 2.49                     | 0.47              |
| 8:3:1385:U:H2'     | 8:3:1386:G:O4'      | 2.15                     | 0.47              |
| 8:3:2017:G:H5''    | 56:r:42:LYS:HB2     | 1.96                     | 0.47              |
| 10:5:20:C:H5''     | 16:AA:146:ALA:HB3   | 1.96                     | 0.47              |
| 10:5:192:A:H2'     | 10:5:193:G:C8       | 2.49                     | 0.47              |
| 10:5:1320:A:H62    | 10:5:1349:A:H5''    | 1.80                     | 0.47              |
| 15:A:197:PRO:HB3   | 20:E:178:PHE:HD1    | 1.79                     | 0.47              |
| 27:L:101:ARG:HH11  | 27:L:104:THR:HG22   | 1.79                     | 0.47              |
| 36:W:67:VAL:HB     | 36:W:104:LEU:HD23   | 1.96                     | 0.47              |
| 42:d:40:VAL:CG2    | 42:d:42:ASP:OD1     | 2.62                     | 0.47              |
| 42:d:49:PHE:CE2    | 42:d:146:ILE:HG23   | 2.50                     | 0.47              |
| 43:e:78:ALA:O      | 43:e:82:VAL:HG23    | 2.15                     | 0.47              |
| 61:w:20:ILE:HG22   | 61:w:65:TRP:HZ3     | 1.79                     | 0.47              |
| 61:w:53:THR:O      | 61:w:57:ILE:HD12    | 2.15                     | 0.47              |
| 64:13:230:TYR:OH   | 64:13:444:ASP:OD2   | 2.28                     | 0.47              |
| 64:13:323:GLY:HA3  | 64:13:679:TYR:CE2   | 2.49                     | 0.47              |
| 64:13:1062:ARG:NH1 | 67:18:73:VAL:CB     | 2.75                     | 0.47              |
| 65:14:853:TRP:CE2  | 65:14:861:ASN:ND2   | 2.82                     | 0.47              |
| 66:15:87:LEU:HD12  | 66:15:102:LEU:CD2   | 2.45                     | 0.47              |
| 66:15:1014:LYS:O   | 66:15:1016:ALA:N    | 2.48                     | 0.47              |
| 66:15:1208:PHE:CE2 | 66:15:1216:LYS:HE3  | 2.49                     | 0.47              |
| 3:10:113:LEU:HB2   | 3:10:124:ILE:HD11   | 1.95                     | 0.47              |
| 3:10:285:ASN:HD21  | 3:10:393:LEU:HD13   | 1.80                     | 0.47              |
| 6:17:710:PHE:O     | 14:9:649:VAL:N      | 2.43                     | 0.47              |
| 6:17:952:GLN:CD    | 61:w:74:LEU:HD22    | 2.39                     | 0.47              |
| 8:3:1353:G:OP1     | 8:3:1681:G:O2'      | 2.24                     | 0.47              |
| 8:3:1414:C:H2'     | 8:3:1415:A:C8       | 2.49                     | 0.47              |
| 8:3:1470:C:H2'     | 8:3:1471:A:H8       | 1.79                     | 0.47              |
| 8:3:1583:G:H2'     | 8:3:1584:U:C6       | 2.49                     | 0.47              |
| 8:3:1715:A:O2'     | 8:3:1769:A:H2'      | 2.15                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:3:1805:U:OP2     | 39:a:282:ARG:NH2    | 2.48                     | 0.47              |
| 10:5:253:G:H1      | 10:5:265:U:H3       | 1.62                     | 0.47              |
| 10:5:369:A:H4'     | 10:5:448:A:H62      | 1.80                     | 0.47              |
| 22:G:131:LYS:O     | 22:G:133:ILE:HG23   | 2.15                     | 0.47              |
| 27:L:79:HIS:HE1    | 33:R:65:ASP:OD2     | 1.97                     | 0.47              |
| 36:W:123:LEU:O     | 36:W:127:ILE:HG12   | 2.15                     | 0.47              |
| 41:c:40:VAL:HG12   | 41:c:101:LEU:HB2    | 1.96                     | 0.47              |
| 41:c:128:VAL:HG23  | 41:c:132:LEU:HD21   | 1.97                     | 0.47              |
| 41:c:209:GLY:O     | 41:c:212:LYS:HG3    | 2.15                     | 0.47              |
| 48:j:51:MET:HG3    | 48:j:52:VAL:HG13    | 1.96                     | 0.47              |
| 52:n:61:LYS:HE3    | 52:n:61:LYS:HB3     | 1.53                     | 0.47              |
| 55:q:14:VAL:HG23   | 55:q:97:PHE:HZ      | 1.80                     | 0.47              |
| 56:r:18:ARG:NH2    | 56:r:22:GLN:OE1     | 2.48                     | 0.47              |
| 64:13:658:ASN:ND2  | 64:13:955:GLU:OE1   | 2.47                     | 0.47              |
| 65:14:168:PRO:HG3  | 65:14:183:ALA:HA    | 1.96                     | 0.47              |
| 65:14:789:TYR:HB2  | 65:14:847:TYR:CE1   | 2.50                     | 0.47              |
| 66:15:937:LYS:HE2  | 66:15:941:GLU:OE1   | 2.15                     | 0.47              |
| 67:16:105:TRP:HH2  | 67:16:152:TYR:HB2   | 1.80                     | 0.47              |
| 6:17:397:LYS:HE3   | 66:15:65:ASP:OD1    | 2.14                     | 0.47              |
| 6:17:846:THR:HG22  | 6:17:928:PHE:CD1    | 2.50                     | 0.47              |
| 8:3:37:G:H1'       | 8:3:490:A:C4        | 2.50                     | 0.47              |
| 8:3:632:A:H2'      | 8:3:633:G:H8        | 1.78                     | 0.47              |
| 8:3:728:A:O2'      | 8:3:1381:A:N3       | 2.45                     | 0.47              |
| 8:3:1619:A:H8      | 8:3:1619:A:H5''     | 1.79                     | 0.47              |
| 8:3:2077:A:H2'     | 8:3:2078:A:C8       | 2.50                     | 0.47              |
| 8:3:2334:U:H3      | 8:3:2397:G:H1       | 1.63                     | 0.47              |
| 8:3:2343:A:H5''    | 8:3:2343:A:H8       | 1.79                     | 0.47              |
| 8:3:2580:A:OP2     | 40:b:151:ARG:N      | 2.48                     | 0.47              |
| 8:3:2706:U:H2'     | 8:3:2707:A:H8       | 1.80                     | 0.47              |
| 8:3:2838:G:H2'     | 8:3:2883:A:H61      | 1.79                     | 0.47              |
| 10:5:18:U:H2'      | 10:5:19:C:C6        | 2.49                     | 0.47              |
| 10:5:214:U:H2'     | 10:5:215:C:C6       | 2.50                     | 0.47              |
| 10:5:214:U:H2'     | 10:5:215:C:H6       | 1.80                     | 0.47              |
| 13:8:54:5MU:H2'    | 13:8:55:PSU:H6      | 1.80                     | 0.47              |
| 14:9:447:HIS:CE1   | 14:9:451:GLN:CD     | 2.93                     | 0.47              |
| 25:J:106:LYS:HE3   | 25:J:106:LYS:HB3    | 1.62                     | 0.47              |
| 42:d:140:GLU:OE2   | 18:x:27:SER:HB2     | 2.15                     | 0.47              |
| 64:13:305:LYS:HD2  | 64:13:573:PHE:CG    | 2.50                     | 0.47              |
| 65:14:386:ILE:HD13 | 65:14:949:TYR:CE1   | 2.50                     | 0.47              |
| 6:17:258:ASN:CG    | 65:14:1126:LEU:HD12 | 1.85                     | 0.47              |
| 6:17:955:LYS:HZ2   | 14:9:799:GLU:HB3    | 0.55                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:3:15:A:O2'        | 8:3:17:G:N7         | 2.48                     | 0.47              |
| 8:3:1803:U:H2'      | 8:3:1804:A:H8       | 1.80                     | 0.47              |
| 8:3:1819:G:N2       | 39:a:54:THR:HG21    | 2.29                     | 0.47              |
| 10:5:399:C:H5'      | 19:C:131:THR:HG23   | 1.97                     | 0.47              |
| 10:5:789:A:O2'      | 10:5:791:A:N7       | 2.46                     | 0.47              |
| 10:5:916:U:O2       | 16:AA:79:THR:OG1    | 2.29                     | 0.47              |
| 10:5:918:A:O2'      | 10:5:1374:C:OP2     | 2.29                     | 0.47              |
| 10:5:1214:A:H2'     | 10:5:1272:C:H41     | 1.80                     | 0.47              |
| 14:9:184:PHE:HB2    | 58:t:57:LYS:HZ3     | 1.79                     | 0.47              |
| 39:a:209:ASN:OD1    | 39:a:210:LEU:HG     | 2.15                     | 0.47              |
| 53:o:56:ARG:HG2     | 53:o:57:GLY:N       | 2.30                     | 0.47              |
| 64:13:204:TYR:O     | 64:13:501:GLY:HA3   | 2.15                     | 0.47              |
| 66:15:1212:VAL:HG21 | 66:15:1248:LEU:HD12 | 1.97                     | 0.47              |
| 1:0:32:LYS:O        | 1:0:36:LYS:HG2      | 2.15                     | 0.46              |
| 8:3:1848:U:C2       | 8:3:1849:G:C8       | 3.03                     | 0.46              |
| 8:3:2841:A:H2'      | 8:3:2842:G:H8       | 1.79                     | 0.46              |
| 9:4:27:A:H5''       | 52:n:36:LEU:CD1     | 2.45                     | 0.46              |
| 9:4:76:A:H62        | 9:4:88:G:H21        | 1.62                     | 0.46              |
| 10:5:711:G:H2'      | 10:5:712:A:C8       | 2.50                     | 0.46              |
| 10:5:998:G:O2'      | 10:5:1000:A:OP1     | 2.32                     | 0.46              |
| 19:C:60:MET:HB2     | 19:C:191:ILE:HG12   | 1.98                     | 0.46              |
| 19:C:64:TYR:HD1     | 19:C:110:ARG:NH1    | 2.13                     | 0.46              |
| 40:b:97:THR:HG22    | 40:b:100:ASN:OD1    | 2.15                     | 0.46              |
| 46:h:57:ALA:HA      | 46:h:63:PHE:CD2     | 2.51                     | 0.46              |
| 64:13:253:LYS:HE3   | 64:13:348:GLU:CD    | 2.40                     | 0.46              |
| 65:14:531:PHE:HZ    | 65:14:563:ILE:CG2   | 2.25                     | 0.46              |
| 66:15:2:SER:HB2     | 66:15:96:ILE:HD13   | 1.96                     | 0.46              |
| 66:15:60:TYR:HB3    | 66:15:72:LEU:HB2    | 1.97                     | 0.46              |
| 66:15:288:PHE:O     | 66:15:302:LYS:NZ    | 2.44                     | 0.46              |
| 67:18:195:LYS:CE    | 67:18:199:ASP:OD1   | 2.60                     | 0.46              |
| 6:17:430:PRO:HD3    | 66:15:549:LEU:HD23  | 1.96                     | 0.46              |
| 6:17:693:THR:HG1    | 14:9:682:VAL:HG23   | 0.31                     | 0.46              |
| 8:3:1889:U:H2'      | 8:3:1890:U:C6       | 2.50                     | 0.46              |
| 10:5:275:A:H5''     | 10:5:276:U:H3'      | 1.96                     | 0.46              |
| 10:5:458:G:H2'      | 10:5:459:C:C6       | 2.50                     | 0.46              |
| 10:5:1051:U:O2'     | 24:I:60:SER:OG      | 2.23                     | 0.46              |
| 15:A:37:TRP:HB2     | 15:A:204:THR:HG22   | 1.97                     | 0.46              |
| 15:A:68:ALA:O       | 15:A:72:VAL:HG12    | 2.15                     | 0.46              |
| 15:A:131:ASN:O      | 15:A:135:GLU:HG2    | 2.15                     | 0.46              |
| 20:E:93:GLU:OE2     | 32:Q:92:ARG:NH2     | 2.49                     | 0.46              |
| 23:H:30:ILE:HG23    | 23:H:37:PRO:HG3     | 1.96                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:K:57:LYS:CD     | 37:Y:45:A:C4'     | 2.80                     | 0.46              |
| 31:P:52:GLU:HG2    | 31:P:52:GLU:O     | 2.15                     | 0.46              |
| 36:W:141:LEU:HD23  | 36:W:173:GLU:HG3  | 1.97                     | 0.46              |
| 48:j:71:ARG:HH22   | 48:j:104:ARG:HH11 | 1.63                     | 0.46              |
| 64:13:899:ARG:NH1  | 64:13:1215:LEU:O  | 2.38                     | 0.46              |
| 64:13:1213:LEU:CD1 | 67:18:276:ASN:HB3 | 2.44                     | 0.46              |
| 65:14:152:LYS:NZ   | 65:14:505:ASP:OD2 | 2.48                     | 0.46              |
| 5:12:85:TRP:CE2    | 6:17:9:PHE:HA     | 2.48                     | 0.46              |
| 8:3:103:G:OP1      | 14:9:783:GLU:CD   | 2.58                     | 0.46              |
| 8:3:947:A:H62      | 50:l:12:PRO:HA    | 1.80                     | 0.46              |
| 8:3:1091:G:H4'     | 8:3:1121:A:C8     | 2.50                     | 0.46              |
| 8:3:1355:C:O3'     | 51:m:107:ARG:NH2  | 2.48                     | 0.46              |
| 8:3:1560:U:C2'     | 14:9:246:LEU:O    | 2.63                     | 0.46              |
| 8:3:1561:G:O2'     | 14:9:299:LYS:CE   | 2.62                     | 0.46              |
| 8:3:2094:A:H2'     | 8:3:2095:A:C8     | 2.49                     | 0.46              |
| 10:5:1463:A:H2'    | 10:5:1464:G:C8    | 2.50                     | 0.46              |
| 14:9:798:ARG:NH1   | 61:w:21:LYS:H     | 2.08                     | 0.46              |
| 16:AA:160:ILE:HG12 | 16:AA:176:SER:O   | 2.15                     | 0.46              |
| 23:H:32:VAL:HG22   | 23:H:67:VAL:HG11  | 1.98                     | 0.46              |
| 26:K:86:ASN:ND2    | 26:K:118:VAL:H    | 2.14                     | 0.46              |
| 29:N:29:LEU:O      | 29:N:33:ILE:HG12  | 2.15                     | 0.46              |
| 36:W:52:GLN:HB2    | 36:W:72:ALA:HB3   | 1.98                     | 0.46              |
| 44:f:33:LYS:HB3    | 44:f:35:LEU:HG    | 1.96                     | 0.46              |
| 46:h:50:MET:SD     | 46:h:50:MET:C     | 2.98                     | 0.46              |
| 62:y:28:SER:OG     | 62:y:37:LYS:NZ    | 2.45                     | 0.46              |
| 64:13:853:TRP:CH2  | 64:13:859:LYS:HD3 | 2.50                     | 0.46              |
| 64:13:1217:LYS:HD3 | 67:18:274:PRO:HB2 | 1.98                     | 0.46              |
| 65:14:290:LEU:HD23 | 65:14:295:MET:HB2 | 1.98                     | 0.46              |
| 66:15:900:GLN:HE22 | 66:15:934:GLU:HG2 | 1.68                     | 0.46              |
| 66:15:1105:VAL:CG2 | 67:16:255:ARG:CG  | 2.89                     | 0.46              |
| 67:16:62:ILE:HG22  | 67:16:68:SER:HB2  | 1.97                     | 0.46              |
| 6:17:426:LYS:HD3   | 66:15:181:ALA:O   | 2.00                     | 0.46              |
| 6:17:699:ILE:HG23  | 14:9:692:LYS:HD3  | 1.95                     | 0.46              |
| 6:17:703:ASN:CB    | 14:9:663:ASN:HB3  | 2.20                     | 0.46              |
| 8:3:874:U:H2'      | 8:3:875:G:H8      | 1.79                     | 0.46              |
| 8:3:1464:G:H1      | 8:3:1590:U:H3     | 1.63                     | 0.46              |
| 9:4:41:C:H2'       | 9:4:43:A:C8       | 2.50                     | 0.46              |
| 24:I:7:VAL:HG23    | 24:I:8:LYS:H      | 1.81                     | 0.46              |
| 26:K:127:ARG:NH2   | 26:K:134:LYS:HG3  | 2.31                     | 0.46              |
| 34:S:36:HIS:O      | 34:S:36:HIS:ND1   | 2.38                     | 0.46              |
| 39:a:83:VAL:HG22   | 39:a:121:ILE:HD11 | 1.97                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 44:f:68:LEU:HD22    | 44:f:108:LEU:HD21  | 1.98                     | 0.46              |
| 55:q:4:ILE:HG13     | 55:q:40:MET:HB3    | 1.97                     | 0.46              |
| 66:15:50:VAL:HG13   | 66:15:817:MET:CE   | 2.45                     | 0.46              |
| 66:15:1130:SER:O    | 66:15:1216:LYS:NZ  | 2.37                     | 0.46              |
| 66:15:1271:ARG:HH12 | 67:16:256:HIS:H    | 1.64                     | 0.46              |
| 6:17:383:ALA:HA     | 66:15:64:LYS:HZ3   | 1.79                     | 0.46              |
| 6:17:692:LYS:O      | 14:9:686:HIS:N     | 2.43                     | 0.46              |
| 8:3:388:U:H2'       | 8:3:389:C:C6       | 2.51                     | 0.46              |
| 8:3:610:G:H2'       | 8:3:611:A:C8       | 2.50                     | 0.46              |
| 8:3:1248:A:H2'      | 8:3:1249:A:C8      | 2.51                     | 0.46              |
| 8:3:1561:G:H1'      | 14:9:299:LYS:HZ3   | 1.79                     | 0.46              |
| 8:3:1597:U:H2'      | 8:3:1598:U:C6      | 2.51                     | 0.46              |
| 8:3:2146:A:H2'      | 8:3:2147:G:H8      | 1.81                     | 0.46              |
| 8:3:2540:G:N2       | 8:3:2671:G:O2'     | 2.48                     | 0.46              |
| 20:E:28:THR:HG21    | 20:E:72:PHE:HA     | 1.96                     | 0.46              |
| 20:E:140:GLN:HB2    | 20:E:141:PRO:HD2   | 1.98                     | 0.46              |
| 42:d:16:LEU:HD13    | 42:d:20:PHE:HE2    | 1.80                     | 0.46              |
| 42:d:60:ILE:HD13    | 42:d:140:GLU:HB2   | 1.98                     | 0.46              |
| 42:d:128:TYR:HB3    | 42:d:156:LEU:HD23  | 1.97                     | 0.46              |
| 53:o:115:LYS:HE3    | 53:o:115:LYS:HB2   | 1.75                     | 0.46              |
| 65:14:52:VAL:HG21   | 65:14:563:ILE:HD12 | 1.95                     | 0.46              |
| 65:14:923:GLY:C     | 65:14:925:GLY:H    | 2.23                     | 0.46              |
| 66:15:288:PHE:HE2   | 66:15:488:GLN:NE2  | 2.13                     | 0.46              |
| 6:17:691:THR:O      | 14:9:682:VAL:CG1   | 2.61                     | 0.46              |
| 8:3:102:A:H1'       | 14:9:782:ASP:CA    | 2.45                     | 0.46              |
| 8:3:103:G:OP1       | 14:9:783:GLU:OE2   | 2.34                     | 0.46              |
| 8:3:154:U:H2'       | 8:3:155:A:C8       | 2.50                     | 0.46              |
| 8:3:464:A:C6        | 8:3:465:A:C6       | 3.04                     | 0.46              |
| 8:3:1306:G:H2'      | 8:3:1307:G:C8      | 2.48                     | 0.46              |
| 8:3:2691:C:H5''     | 53:o:56:ARG:HH22   | 1.80                     | 0.46              |
| 9:4:7:G:H2'         | 9:4:8:C:C6         | 2.50                     | 0.46              |
| 10:5:737:U:OP1      | 29:N:35:GLN:NE2    | 2.48                     | 0.46              |
| 12:7:5:G:H2'        | 12:7:6:G:H8        | 1.81                     | 0.46              |
| 15:A:49:ARG:CG      | 15:A:50:LYS:H      | 2.26                     | 0.46              |
| 17:AB:40:U:O2       | 37:Y:41:U:C6       | 2.67                     | 0.46              |
| 20:E:130:VAL:N      | 20:E:131:PRO:HD2   | 2.31                     | 0.46              |
| 30:O:1:MET:HE2      | 30:O:1:MET:HA      | 1.98                     | 0.46              |
| 36:W:219:PRO:HB3    | 36:W:222:ILE:HD12  | 1.97                     | 0.46              |
| 40:b:63:ASN:OD1     | 40:b:64:LYS:N      | 2.47                     | 0.46              |
| 41:c:194:ALA:O      | 41:c:195:ASN:HB3   | 2.16                     | 0.46              |
| 52:n:31:MET:CE      | 52:n:44:TRP:CD1    | 2.99                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:o:30:GLU:OE1    | 53:o:92:ARG:HD3     | 2.15                     | 0.46              |
| 65:14:340:PHE:HD2  | 65:14:400:GLN:OE1   | 1.98                     | 0.46              |
| 66:15:98:TRP:CG    | 66:15:99:PRO:HD3    | 2.50                     | 0.46              |
| 66:15:879:TRP:CD2  | 66:15:932:LEU:HD11  | 2.51                     | 0.46              |
| 6:17:426:LYS:CG    | 66:15:184:GLN:CD    | 2.79                     | 0.46              |
| 6:17:700:LEU:CG    | 14:9:658:LEU:CA     | 2.90                     | 0.46              |
| 6:17:895:PHE:HB3   | 6:17:903:ASN:OD1    | 2.16                     | 0.46              |
| 8:3:196:G:O2'      | 8:3:712:A:N1        | 2.45                     | 0.46              |
| 8:3:614:C:H2'      | 8:3:615:G:H8        | 1.79                     | 0.46              |
| 8:3:909:U:H2'      | 8:3:910:G:C8        | 2.51                     | 0.46              |
| 8:3:1598:U:H2'     | 8:3:1599:C:C6       | 2.50                     | 0.46              |
| 8:3:1954:C:H2'     | 8:3:1955:G:H8       | 1.80                     | 0.46              |
| 10:5:483:U:H2'     | 10:5:484:A:H8       | 1.81                     | 0.46              |
| 10:5:1024:U:O2'    | 10:5:1025:U:OP1     | 2.34                     | 0.46              |
| 13:8:28:U:H2'      | 13:8:29:U:C6        | 2.50                     | 0.46              |
| 13:8:54:5MU:H2'    | 13:8:55:PSU:C6      | 2.51                     | 0.46              |
| 17:AB:44:A:C2'     | 37:Y:44:A:N3        | 2.49                     | 0.46              |
| 25:J:14:ILE:HG21   | 25:J:93:PHE:CZ      | 2.51                     | 0.46              |
| 44:f:30:LEU:HB3    | 44:f:36:ALA:HB3     | 1.97                     | 0.46              |
| 46:h:50:MET:HE1    | 46:h:52:PRO:CG      | 2.46                     | 0.46              |
| 61:w:16:VAL:HG12   | 61:w:58:LEU:HD21    | 1.98                     | 0.46              |
| 18:x:2:LYS:HG3     | 18:x:3:LYS:H        | 1.79                     | 0.46              |
| 65:14:309:GLN:NE2  | 65:14:318:SER:HB2   | 2.30                     | 0.46              |
| 65:14:1122:LYS:HB2 | 66:15:150:PHE:CE1   | 2.50                     | 0.46              |
| 66:15:355:ASP:CG   | 66:15:406:ASN:HD22  | 2.24                     | 0.46              |
| 6:17:262:SER:HB2   | 65:14:1098:THR:HG23 | 1.98                     | 0.46              |
| 6:17:424:VAL:HG11  | 66:15:180:PHE:HB2   | 1.96                     | 0.46              |
| 6:17:703:ASN:O     | 14:9:663:ASN:C      | 2.59                     | 0.46              |
| 8:3:1473:C:H2'     | 8:3:1474:C:H6       | 1.79                     | 0.46              |
| 8:3:2118:U:OP2     | 8:3:2152:C:N4       | 2.48                     | 0.46              |
| 8:3:2797:C:H3'     | 8:3:2798:A:O4'      | 2.15                     | 0.46              |
| 10:5:369:A:H2'     | 10:5:370:A:H8       | 1.81                     | 0.46              |
| 10:5:941:A:H2'     | 10:5:942:G:H8       | 1.77                     | 0.46              |
| 16:AA:91:LEU:HD21  | 16:AA:192:ILE:HD12  | 1.98                     | 0.46              |
| 17:AB:44:A:N3      | 37:Y:45:A:C6        | 2.84                     | 0.46              |
| 23:H:131:LYS:HE3   | 23:H:132:ARG:HH12   | 1.81                     | 0.46              |
| 32:Q:41:CYS:HA     | 32:Q:78:ASN:HA      | 1.97                     | 0.46              |
| 34:S:20:ASN:O      | 34:S:24:GLN:NE2     | 2.48                     | 0.46              |
| 46:h:57:ALA:HA     | 46:h:63:PHE:HE2     | 1.80                     | 0.46              |
| 48:j:54:LYS:HE3    | 48:j:54:LYS:HB3     | 1.82                     | 0.46              |
| 48:j:66:LYS:O      | 48:j:78:LYS:NZ      | 2.42                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 52:n:109:ALA:HB1   | 52:n:114:LEU:HD12   | 1.98                     | 0.46              |
| 64:13:912:LEU:HD22 | 64:13:1180:LEU:HD11 | 1.96                     | 0.46              |
| 66:15:686:ILE:HD13 | 66:15:1039:GLY:HA2  | 1.98                     | 0.46              |
| 6:17:390:ALA:H     | 66:15:71:ARG:NH1    | 2.09                     | 0.46              |
| 8:3:190:G:H2'      | 8:3:191:G:H8        | 1.79                     | 0.46              |
| 8:3:386:U:H2'      | 8:3:387:U:H6        | 1.81                     | 0.46              |
| 8:3:600:U:OP2      | 49:k:30:LYS:NZ      | 2.48                     | 0.46              |
| 8:3:603:G:H2'      | 8:3:2037:A:N7       | 2.31                     | 0.46              |
| 8:3:909:U:H2'      | 8:3:910:G:H8        | 1.81                     | 0.46              |
| 8:3:1334:U:H2'     | 8:3:1335:A:H8       | 1.81                     | 0.46              |
| 8:3:2781:C:H2'     | 8:3:2782:A:C8       | 2.50                     | 0.46              |
| 10:5:117:U:H2'     | 10:5:118:C:C6       | 2.51                     | 0.46              |
| 14:9:808:GLN:CA    | 61:w:79:THR:CB      | 2.83                     | 0.46              |
| 15:A:46:GLU:HB3    | 15:A:57:VAL:HG22    | 1.97                     | 0.46              |
| 22:G:61:GLU:HG2    | 22:G:65:LYS:HA      | 1.96                     | 0.46              |
| 23:H:121:TYR:CE1   | 23:H:127:PRO:HG3    | 2.51                     | 0.46              |
| 41:c:60:GLY:HA3    | 41:c:80:ARG:HD3     | 1.98                     | 0.46              |
| 45:g:55:LYS:HB2    | 45:g:58:ILE:HG22    | 1.98                     | 0.46              |
| 50:l:56:LYS:HB2    | 50:l:56:LYS:HE3     | 1.78                     | 0.46              |
| 59:u:79:GLY:HA2    | 59:u:100:HIS:CD2    | 2.51                     | 0.46              |
| 18:x:6:HIS:O       | 18:x:8:PRO:HD3      | 2.16                     | 0.46              |
| 64:13:195:ASP:CA   | 64:13:545:ARG:NH1   | 2.77                     | 0.46              |
| 64:13:1018:SER:CB  | 67:18:258:VAL:HG12  | 2.30                     | 0.46              |
| 66:15:1237:PRO:O   | 66:15:1239:HIS:N    | 2.49                     | 0.46              |
| 3:10:275:SER:OG    | 6:17:970:SER:HB3    | 1.96                     | 0.46              |
| 6:17:261:LYS:CB    | 65:14:1130:LYS:HE3  | 2.46                     | 0.46              |
| 8:3:153:U:H2'      | 8:3:154:U:C6        | 2.51                     | 0.46              |
| 8:3:1389:G:H2'     | 8:3:1390:C:H6       | 1.81                     | 0.46              |
| 8:3:1560:U:O5'     | 14:9:248:GLU:CB     | 2.64                     | 0.46              |
| 8:3:2108:C:N4      | 8:3:2109:A:H62      | 2.14                     | 0.46              |
| 9:4:82:U:H2'       | 9:4:83:U:H4'        | 1.96                     | 0.46              |
| 10:5:1142:G:N2     | 10:5:1145:A:OP2     | 2.45                     | 0.46              |
| 12:7:29:G:H5'      | 27:L:117:ALA:CB     | 2.46                     | 0.46              |
| 15:A:22:LYS:HZ2    | 15:A:251:ASP:HA     | 1.81                     | 0.46              |
| 17:AB:43:A:OP1     | 37:Y:43:A:P         | 2.05                     | 0.46              |
| 19:C:102:TYR:CD2   | 19:C:110:ARG:HB2    | 2.50                     | 0.46              |
| 19:C:144:LEU:HG    | 19:C:145:LYS:H      | 1.81                     | 0.46              |
| 23:H:47:ILE:HG13   | 23:H:50:MET:HE3     | 1.98                     | 0.46              |
| 26:K:114:THR:HG23  | 26:K:115:LEU:H      | 1.81                     | 0.46              |
| 30:O:19:ILE:HG22   | 30:O:36:ILE:HB      | 1.98                     | 0.46              |
| 42:d:165:GLU:OE1   | 42:d:165:GLU:CA     | 2.53                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 44:f:108:LEU:C      | 44:f:108:LEU:CD1    | 2.88                     | 0.46              |
| 45:g:11:VAL:HG12    | 45:g:58:ILE:HG13    | 1.98                     | 0.46              |
| 64:13:972:ASN:CB    | 67:18:256:HIS:CE1   | 2.99                     | 0.46              |
| 64:13:1051:ILE:HD12 | 64:13:1110:LEU:HD11 | 1.98                     | 0.46              |
| 65:14:1218:VAL:CG1  | 65:14:1242:LEU:HD22 | 2.46                     | 0.46              |
| 67:16:242:ALA:O     | 67:16:244:LYS:N     | 2.49                     | 0.46              |
| 6:17:171:ARG:HH12   | 6:17:318:GLU:CD     | 2.24                     | 0.45              |
| 6:17:376:LYS:HE3    | 66:15:178:GLU:CB    | 2.16                     | 0.45              |
| 6:17:702:GLU:N      | 14:9:662:LEU:CA     | 2.71                     | 0.45              |
| 6:17:710:PHE:HE1    | 14:9:649:VAL:CG2    | 2.07                     | 0.45              |
| 8:3:1493:A:N7       | 8:3:1579:G:H2'      | 2.31                     | 0.45              |
| 8:3:1830:G:OP1      | 39:a:58:GLN:NE2     | 2.49                     | 0.45              |
| 8:3:1957:G:N2       | 8:3:1961:A:C5       | 2.84                     | 0.45              |
| 8:3:2072:C:H2'      | 8:3:2073:C:H6       | 1.79                     | 0.45              |
| 8:3:2309:A:H2'      | 8:3:2310:C:H6       | 1.81                     | 0.45              |
| 8:3:2798:A:O3'      | 8:3:2896:G:N2       | 2.49                     | 0.45              |
| 10:5:892:G:N2       | 10:5:895:A:OP2      | 2.49                     | 0.45              |
| 23:H:98:LYS:C       | 23:H:98:LYS:HD3     | 2.41                     | 0.45              |
| 27:L:16:GLU:OE2     | 27:L:16:GLU:N       | 2.33                     | 0.45              |
| 30:O:39:LEU:HD12    | 30:O:40:ASN:N       | 2.31                     | 0.45              |
| 31:P:23:THR:O       | 31:P:23:THR:OG1     | 2.35                     | 0.45              |
| 40:b:123:ILE:HG23   | 40:b:128:PHE:O      | 2.15                     | 0.45              |
| 41:c:125:THR:HG22   | 41:c:125:THR:O      | 2.16                     | 0.45              |
| 52:n:9:ARG:HG3      | 52:n:9:ARG:NH1      | 2.31                     | 0.45              |
| 57:s:55:VAL:HG22    | 57:s:83:ILE:HD13    | 1.97                     | 0.45              |
| 64:13:1020:MET:SD   | 67:18:256:HIS:HB3   | 2.55                     | 0.45              |
| 65:14:579:VAL:HG11  | 65:14:644:VAL:HG21  | 1.97                     | 0.45              |
| 66:15:1106:SER:H    | 67:16:254:LYS:HB3   | 1.68                     | 0.45              |
| 6:17:386:VAL:HG12   | 66:15:176:ASN:HB2   | 1.71                     | 0.45              |
| 8:3:1473:C:H1'      | 8:3:1580:G:N2       | 2.30                     | 0.45              |
| 8:3:2687:A:H2'      | 8:3:2688:C:C6       | 2.51                     | 0.45              |
| 8:3:2706:U:H2'      | 8:3:2707:A:C8       | 2.51                     | 0.45              |
| 10:5:80:U:H2'       | 10:5:81:A:C8        | 2.50                     | 0.45              |
| 10:5:500:G:OP1      | 26:K:128:SER:HB3    | 2.16                     | 0.45              |
| 14:9:784:GLU:O      | 61:w:6:GLU:OE1      | 2.34                     | 0.45              |
| 23:H:17:ALA:HB2     | 23:H:80:ALA:HB1     | 1.98                     | 0.45              |
| 31:P:43:LYS:HG2     | 31:P:45:TYR:CE1     | 2.51                     | 0.45              |
| 36:W:220:ALA:O      | 36:W:222:ILE:N      | 2.48                     | 0.45              |
| 48:j:22:ILE:HD11    | 48:j:42:SER:HB3     | 1.97                     | 0.45              |
| 54:p:101:GLU:CD     | 54:p:104:LYS:HE3    | 2.42                     | 0.45              |
| 65:14:1281:VAL:HG11 | 65:14:1286:ILE:HB   | 1.98                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 66:15:363:ASP:CG    | 66:15:424:HIS:HD2  | 2.24                     | 0.45              |
| 66:15:1154:GLU:OE1  | 67:16:72:ALA:C     | 2.59                     | 0.45              |
| 67:18:3:ASN:HB2     | 67:18:154:GLU:OE2  | 2.17                     | 0.45              |
| 67:18:113:VAL:HG13  | 67:18:181:VAL:HG21 | 1.98                     | 0.45              |
| 6:17:386:VAL:HG13   | 66:15:174:ASP:CB   | 2.42                     | 0.45              |
| 6:17:431:VAL:HA     | 66:15:138:VAL:H    | 1.81                     | 0.45              |
| 6:17:831:PHE:CE2    | 6:17:913:VAL:HG21  | 2.52                     | 0.45              |
| 6:17:955:LYS:HD2    | 14:9:799:GLU:OE1   | 2.17                     | 0.45              |
| 8:3:10:U:H2'        | 8:3:11:U:H4'       | 1.98                     | 0.45              |
| 8:3:102:A:C5        | 14:9:786:MET:CE    | 2.87                     | 0.45              |
| 8:3:1447:A:O2'      | 8:3:1449:G:N7      | 2.40                     | 0.45              |
| 10:5:573:G:H4'      | 10:5:574:C:O5'     | 2.17                     | 0.45              |
| 12:7:18:G:O2'       | 12:7:57:G:N2       | 2.29                     | 0.45              |
| 14:9:798:ARG:CZ     | 61:w:18:LEU:O      | 2.65                     | 0.45              |
| 23:H:30:ILE:CG2     | 23:H:37:PRO:HG3    | 2.46                     | 0.45              |
| 23:H:125:ARG:HG2    | 23:H:126:ALA:N     | 2.31                     | 0.45              |
| 42:d:73:ALA:HA      | 42:d:79:LEU:HG     | 1.97                     | 0.45              |
| 48:j:61:VAL:HB      | 48:j:87:ILE:HD13   | 1.98                     | 0.45              |
| 49:k:20:LEU:HB3     | 49:k:32:SER:HB3    | 1.97                     | 0.45              |
| 49:k:112:ILE:HG22   | 49:k:128:VAL:HG12  | 1.99                     | 0.45              |
| 56:r:2:ILE:HG13     | 56:r:113:GLU:OE1   | 2.16                     | 0.45              |
| 63:z:11:CYS:SG      | 63:z:12:ASN:N      | 2.89                     | 0.45              |
| 64:13:1213:LEU:HD13 | 67:18:276:ASN:CB   | 2.47                     | 0.45              |
| 65:14:753:ILE:HG21  | 65:14:782:TRP:CE2  | 2.51                     | 0.45              |
| 65:14:1136:PHE:CD2  | 65:14:1140:ASN:ND2 | 2.84                     | 0.45              |
| 66:15:82:GLU:OE2    | 66:15:120:LYS:CE   | 2.60                     | 0.45              |
| 66:15:773:LYS:HE2   | 66:15:945:GLU:OE2  | 2.16                     | 0.45              |
| 3:10:430:PHE:CZ     | 3:10:434:LEU:HD11  | 2.51                     | 0.45              |
| 8:3:599:U:H5''      | 49:k:30:LYS:HE3    | 1.97                     | 0.45              |
| 8:3:922:C:H2'       | 8:3:923:A:C8       | 2.51                     | 0.45              |
| 8:3:1166:G:N2       | 8:3:1167:U:O4      | 2.41                     | 0.45              |
| 8:3:1323:A:H2'      | 8:3:1324:A:C8      | 2.51                     | 0.45              |
| 8:3:1801:U:H2'      | 8:3:1802:C:H6      | 1.81                     | 0.45              |
| 8:3:2701:A:H2'      | 8:3:2702:G:H8      | 1.81                     | 0.45              |
| 10:5:487:A:O2'      | 10:5:488:U:O3'     | 2.34                     | 0.45              |
| 10:5:1215:U:H4'     | 21:F:37:LEU:HD21   | 1.97                     | 0.45              |
| 19:C:72:ARG:HB3     | 19:C:204:VAL:HG21  | 1.98                     | 0.45              |
| 19:C:75:PHE:CD1     | 19:C:75:PHE:C      | 2.95                     | 0.45              |
| 19:C:101:VAL:O      | 19:C:104:MET:HB3   | 2.16                     | 0.45              |
| 24:I:31:ILE:HD11    | 24:I:96:ILE:HG21   | 1.98                     | 0.45              |
| 53:o:54:ARG:HD3     | 53:o:56:ARG:HB2    | 1.97                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 64:13:200:SER:HB2   | 64:13:292:LEU:HD23 | 1.98                     | 0.45              |
| 64:13:941:PHE:HB2   | 64:13:973:PHE:CE1  | 2.51                     | 0.45              |
| 66:15:87:LEU:HD12   | 66:15:102:LEU:HD22 | 1.97                     | 0.45              |
| 66:15:397:SER:HB3   | 66:15:408:ARG:CZ   | 2.46                     | 0.45              |
| 67:16:163:TYR:CD1   | 67:16:205:PHE:HZ   | 2.35                     | 0.45              |
| 5:12:85:TRP:CB      | 6:17:11:TRP:CE3    | 2.87                     | 0.45              |
| 8:3:42:U:H2'        | 8:3:43:A:H8        | 1.82                     | 0.45              |
| 8:3:45:U:H2'        | 8:3:46:A:O4'       | 2.16                     | 0.45              |
| 8:3:1201:A:H2'      | 8:3:1202:A:C8      | 2.52                     | 0.45              |
| 8:3:1603:A:O5'      | 39:a:63:LYS:NZ     | 2.49                     | 0.45              |
| 8:3:2010:A:H2'      | 8:3:2011:G:O4'     | 2.17                     | 0.45              |
| 8:3:2575:G:H2'      | 8:3:2576:A:C8      | 2.52                     | 0.45              |
| 8:3:2634:C:H2'      | 8:3:2635:G:C8      | 2.52                     | 0.45              |
| 10:5:510:U:H2'      | 10:5:511:A:C8      | 2.50                     | 0.45              |
| 14:9:795:GLN:CB     | 61:w:18:LEU:CD2    | 2.69                     | 0.45              |
| 16:AA:215:ASN:O     | 16:AA:216:LEU:C    | 2.59                     | 0.45              |
| 16:AA:219:LEU:H     | 16:AA:219:LEU:HD12 | 1.80                     | 0.45              |
| 36:W:47:ASN:OD1     | 36:W:48:TYR:CD2    | 2.68                     | 0.45              |
| 40:b:56:THR:HG22    | 40:b:78:THR:HG22   | 1.97                     | 0.45              |
| 42:d:13:ALA:O       | 42:d:17:GLN:HB2    | 2.17                     | 0.45              |
| 45:g:74:THR:HG22    | 45:g:110:CYS:HB2   | 1.97                     | 0.45              |
| 46:h:13:ASN:OD1     | 46:h:50:MET:CE     | 2.65                     | 0.45              |
| 65:14:1229:ASP:OD2  | 65:14:1240:LYS:NZ  | 2.49                     | 0.45              |
| 66:15:1097:LEU:HD11 | 66:15:1251:MET:HG3 | 1.99                     | 0.45              |
| 67:18:167:VAL:HG12  | 67:18:170:LEU:HG   | 1.97                     | 0.45              |
| 67:16:21:LYS:HZ1    | 67:16:76:GLU:CD    | 2.24                     | 0.45              |
| 3:10:253:PHE:HD2    | 6:17:15:ILE:CD1    | 2.09                     | 0.45              |
| 6:17:279:GLN:OE1    | 65:14:1122:LYS:HB2 | 2.10                     | 0.45              |
| 6:17:373:VAL:CB     | 66:15:172:PRO:CG   | 2.86                     | 0.45              |
| 8:3:196:G:N2        | 8:3:196:G:OP2      | 2.49                     | 0.45              |
| 8:3:666:G:N2        | 8:3:669:A:OP2      | 2.31                     | 0.45              |
| 8:3:780:G:O2'       | 8:3:783:G:H1'      | 2.17                     | 0.45              |
| 8:3:853:G:N1        | 8:3:1219:U:OP2     | 2.40                     | 0.45              |
| 8:3:1279:U:H5'      | 54:p:3:ILE:HB      | 1.98                     | 0.45              |
| 8:3:1893:C:H2'      | 8:3:1894:U:H6      | 1.81                     | 0.45              |
| 8:3:2299:U:O2'      | 8:3:2382:A:N3      | 2.49                     | 0.45              |
| 10:5:108:C:OP1      | 10:5:307:C:O2'     | 2.35                     | 0.45              |
| 10:5:1096:A:H2'     | 10:5:1097:G:H8     | 1.81                     | 0.45              |
| 10:5:1467:A:HO2'    | 37:Y:44:A:C1'      | 2.30                     | 0.45              |
| 14:9:275:LYS:HB3    | 57:s:22:GLY:HA2    | 1.89                     | 0.45              |
| 14:9:787:LYS:HB3    | 61:w:3:VAL:HA      | 1.36                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:AB:54:A:H1'     | 17:AB:55:A:C8      | 2.52                     | 0.45              |
| 27:L:7:ILE:H       | 27:L:7:ILE:HD12    | 1.82                     | 0.45              |
| 39:a:139:ALA:HB1   | 39:a:194:LYS:NZ    | 2.32                     | 0.45              |
| 41:c:136:THR:HG22  | 41:c:138:GLY:H     | 1.81                     | 0.45              |
| 61:w:16:VAL:HA     | 61:w:19:VAL:HG12   | 1.98                     | 0.45              |
| 64:13:81:TYR:CE1   | 64:13:111:GLU:HG3  | 2.52                     | 0.45              |
| 5:12:96:LEU:HD13   | 6:17:661:LEU:HA    | 1.04                     | 0.45              |
| 6:17:689:ALA:O     | 14:9:679:ASP:O     | 2.31                     | 0.45              |
| 8:3:98:C:P         | 61:w:40:LYS:NZ     | 2.90                     | 0.45              |
| 8:3:897:A:N3       | 9:4:77:G:O2'       | 2.47                     | 0.45              |
| 8:3:928:G:H2'      | 8:3:929:G:H8       | 1.81                     | 0.45              |
| 8:3:1471:A:H2'     | 8:3:1472:C:H6      | 1.81                     | 0.45              |
| 8:3:1561:G:N7      | 14:9:248:GLU:CD    | 2.75                     | 0.45              |
| 8:3:2204:C:H2'     | 8:3:2205:U:C6      | 2.51                     | 0.45              |
| 8:3:2845:U:H2'     | 8:3:2846:A:C8      | 2.51                     | 0.45              |
| 10:5:374:G:H2'     | 10:5:375:C:C6      | 2.51                     | 0.45              |
| 14:9:87:GLN:OE1    | 14:9:110:LEU:HB3   | 2.16                     | 0.45              |
| 15:A:176:LEU:HD12  | 15:A:176:LEU:HA    | 1.86                     | 0.45              |
| 20:E:153:LYS:HG3   | 20:E:153:LYS:O     | 2.16                     | 0.45              |
| 22:G:41:LYS:HA     | 22:G:44:ILE:HG22   | 1.98                     | 0.45              |
| 40:b:6:ILE:HG22    | 40:b:207:ILE:HB    | 1.98                     | 0.45              |
| 42:d:104:ILE:HG23  | 42:d:105:TYR:HD2   | 1.79                     | 0.45              |
| 64:13:1216:LEU:HB2 | 67:18:276:ASN:OXT  | 2.17                     | 0.45              |
| 65:14:152:LYS:NZ   | 65:14:505:ASP:CG   | 2.75                     | 0.45              |
| 6:17:78:GLY:N      | 65:14:1272:SER:CB  | 2.43                     | 0.45              |
| 6:17:279:GLN:HG3   | 65:14:1122:LYS:CB  | 2.29                     | 0.45              |
| 6:17:699:ILE:CB    | 14:9:689:ILE:HG12  | 2.37                     | 0.45              |
| 6:17:702:GLU:OE2   | 14:9:781:PHE:HE2   | 1.85                     | 0.45              |
| 8:3:11:U:C2        | 8:3:2898:A:C2      | 3.05                     | 0.45              |
| 8:3:713:C:H2'      | 8:3:714:G:C8       | 2.51                     | 0.45              |
| 8:3:1388:G:C8      | 8:3:1389:G:C8      | 3.05                     | 0.45              |
| 8:3:2376:C:H2'     | 8:3:2377:A:C8      | 2.52                     | 0.45              |
| 8:3:2665:A:O2'     | 43:e:163:LYS:NZ    | 2.50                     | 0.45              |
| 10:5:18:U:H2'      | 10:5:19:C:H6       | 1.82                     | 0.45              |
| 10:5:425:G:H4'     | 10:5:426:U:O5'     | 2.16                     | 0.45              |
| 10:5:1376:G:H2'    | 10:5:1377:C:O4'    | 2.17                     | 0.45              |
| 10:5:1384:A:H2'    | 10:5:1385:A:C8     | 2.52                     | 0.45              |
| 16:AA:160:ILE:HD13 | 16:AA:170:ILE:HG22 | 1.99                     | 0.45              |
| 30:O:6:LEU:HD11    | 30:O:68:THR:HB     | 1.98                     | 0.45              |
| 39:a:143:GLU:HA    | 39:a:170:ILE:HB    | 1.98                     | 0.45              |
| 40:b:22:GLU:HG2    | 48:j:72:LYS:HE3    | 1.98                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 40:b:30:TYR:OH      | 40:b:189:MET:HE1    | 2.17                     | 0.45              |
| 42:d:7:HIS:HA       | 42:d:10:LYS:HD2     | 1.98                     | 0.45              |
| 42:d:39:GLY:HA2     | 42:d:86:GLY:HA2     | 1.98                     | 0.45              |
| 44:f:97:ILE:HA      | 44:f:100:GLN:HE21   | 1.81                     | 0.45              |
| 66:15:161:THR:CG2   | 66:15:283:SER:OG    | 2.65                     | 0.45              |
| 6:17:261:LYS:HG3    | 65:14:1130:LYS:CD   | 2.41                     | 0.45              |
| 6:17:615:PHE:CE1    | 6:17:619:ILE:HD12   | 2.52                     | 0.45              |
| 8:3:103:G:OP1       | 14:9:783:GLU:HB2    | 2.16                     | 0.45              |
| 8:3:259:A:O2'       | 8:3:422:A:OP1       | 2.30                     | 0.45              |
| 8:3:1128:G:H2'      | 8:3:1129:U:C6       | 2.52                     | 0.45              |
| 8:3:1458:A:H2'      | 8:3:1459:A:C8       | 2.52                     | 0.45              |
| 8:3:1798:A:N1       | 8:3:1836:A:H4'      | 2.32                     | 0.45              |
| 8:3:2196:G:H2'      | 8:3:2197:U:H6       | 1.81                     | 0.45              |
| 10:5:295:G:H2'      | 10:5:296:A:C8       | 2.52                     | 0.45              |
| 10:5:707:G:H2'      | 10:5:708:A:H8       | 1.81                     | 0.45              |
| 24:I:20:ASP:OD2     | 36:W:217:ARG:NH1    | 2.42                     | 0.45              |
| 40:b:97:THR:HG23    | 40:b:99:GLN:H       | 1.82                     | 0.45              |
| 44:f:61:ASN:HA      | 44:f:64:LEU:HG      | 1.98                     | 0.45              |
| 46:h:101:ALA:HA     | 46:h:124:VAL:HG11   | 1.99                     | 0.45              |
| 47:i:4:THR:HA       | 55:q:12:TYR:CE1     | 2.52                     | 0.45              |
| 51:m:33:THR:OG1     | 51:m:34:THR:N       | 2.49                     | 0.45              |
| 64:13:283:ARG:HG3   | 64:13:290:ASP:OD1   | 2.14                     | 0.45              |
| 64:13:1161:LEU:HD21 | 64:13:1180:LEU:HD12 | 1.98                     | 0.45              |
| 65:14:197:ILE:O     | 65:14:483:ARG:NH2   | 2.48                     | 0.45              |
| 66:15:54:GLU:HG2    | 66:15:814:GLN:HE21  | 1.76                     | 0.45              |
| 3:10:238:PHE:CD1    | 6:17:563:VAL:CG2    | 2.96                     | 0.45              |
| 6:17:258:ASN:HB3    | 65:14:1102:PHE:HB3  | 1.97                     | 0.45              |
| 6:17:382:ASP:CB     | 66:15:64:LYS:NZ     | 2.61                     | 0.45              |
| 8:3:141:A:C2        | 8:3:1437:A:H1'      | 2.52                     | 0.45              |
| 8:3:450:C:H2'       | 8:3:451:A:C8        | 2.52                     | 0.45              |
| 8:3:755:C:H2'       | 8:3:756:A:C8        | 2.50                     | 0.45              |
| 8:3:1099:C:H3'      | 8:3:1100:U:C6       | 2.52                     | 0.45              |
| 8:3:1294:G:OP1      | 62:y:16:ARG:NH2     | 2.41                     | 0.45              |
| 8:3:1623:U:H2'      | 8:3:1624:A:C8       | 2.52                     | 0.45              |
| 8:3:1697:C:O2'      | 8:3:2694:A:H4'      | 2.17                     | 0.45              |
| 8:3:1931:C:H2'      | 8:3:1932:C:C6       | 2.52                     | 0.45              |
| 8:3:2141:A:N6       | 8:3:2164:G:O2'      | 2.50                     | 0.45              |
| 8:3:2420:A:H2'      | 8:3:2421:U:O4'      | 2.17                     | 0.45              |
| 8:3:2522:U:H2'      | 8:3:2523:C:C6       | 2.51                     | 0.45              |
| 10:5:381:C:H2'      | 10:5:382:U:C6       | 2.52                     | 0.45              |
| 10:5:1468:A:C2'     | 37:Y:43:A:N3        | 2.80                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:8:1:G:H2'       | 13:8:2:G:C8        | 2.52                     | 0.45              |
| 23:H:83:LEU:O      | 23:H:86:VAL:HG12   | 2.16                     | 0.45              |
| 32:Q:65:SER:OG     | 32:Q:69:LYS:HB2    | 2.17                     | 0.45              |
| 42:d:34:ILE:HD12   | 42:d:96:MET:HB2    | 1.99                     | 0.45              |
| 44:f:84:HIS:CE1    | 44:f:93:ILE:HD13   | 2.52                     | 0.45              |
| 49:k:13:ARG:HA     | 49:k:13:ARG:HD2    | 1.62                     | 0.45              |
| 53:o:103:TYR:CE2   | 53:o:104:MET:HE3   | 2.52                     | 0.45              |
| 56:r:114:ARG:O     | 56:r:118:ILE:HG13  | 2.17                     | 0.45              |
| 64:13:10:GLN:HB3   | 67:18:197:ASN:ND2  | 2.27                     | 0.45              |
| 64:13:197:THR:OG1  | 64:13:329:LYS:CE   | 2.64                     | 0.45              |
| 64:13:408:LYS:HD3  | 64:13:440:TYR:OH   | 2.17                     | 0.45              |
| 65:14:59:ASP:OD2   | 65:14:555:LYS:HD2  | 2.17                     | 0.45              |
| 66:15:314:PHE:CE2  | 66:15:323:ILE:CD1  | 3.00                     | 0.45              |
| 3:10:311:GLN:O     | 65:14:89:ASN:CG    | 2.58                     | 0.44              |
| 6:17:698:SER:CA    | 14:9:689:ILE:HG21  | 2.44                     | 0.44              |
| 6:17:710:PHE:O     | 14:9:649:VAL:HB    | 2.17                     | 0.44              |
| 8:3:159:G:H2'      | 8:3:160:A:H8       | 1.81                     | 0.44              |
| 8:3:333:A:N3       | 8:3:353:G:O2'      | 2.46                     | 0.44              |
| 8:3:2309:A:H2'     | 8:3:2310:C:C6      | 2.51                     | 0.44              |
| 8:3:2586:G:H1'     | 40:b:143:PHE:CZ    | 2.53                     | 0.44              |
| 10:5:1401:A:H2'    | 10:5:1402:U:H6     | 1.83                     | 0.44              |
| 15:A:84:PHE:N      | 15:A:84:PHE:CD1    | 2.85                     | 0.44              |
| 22:G:63:LYS:HG3    | 22:G:63:LYS:O      | 2.17                     | 0.44              |
| 26:K:29:ASN:ND2    | 26:K:32:ASN:HB3    | 2.29                     | 0.44              |
| 26:K:46:VAL:HG12   | 26:K:92:VAL:HG22   | 1.99                     | 0.44              |
| 29:N:21:SER:OG     | 29:N:22:ILE:N      | 2.50                     | 0.44              |
| 34:S:43:ASN:O      | 34:S:44:LEU:C      | 2.59                     | 0.44              |
| 36:W:26:SER:OG     | 36:W:27:HIS:N      | 2.50                     | 0.44              |
| 39:a:138:LEU:HD23  | 39:a:141:ILE:HD12  | 1.97                     | 0.44              |
| 39:a:167:TYR:HB3   | 39:a:202:VAL:HG13  | 1.98                     | 0.44              |
| 41:c:39:LEU:HD13   | 49:k:13:ARG:NH1    | 2.32                     | 0.44              |
| 50:l:10:ARG:HG2    | 50:l:10:ARG:HH11   | 1.83                     | 0.44              |
| 64:13:150:PHE:HE2  | 66:15:1169:ASP:OD2 | 2.00                     | 0.44              |
| 64:13:211:GLN:OE1  | 64:13:215:GLN:CD   | 2.60                     | 0.44              |
| 64:13:734:LEU:HD11 | 64:13:885:LYS:O    | 2.11                     | 0.44              |
| 64:13:1217:LYS:HE3 | 67:18:276:ASN:HA   | 1.98                     | 0.44              |
| 65:14:608:ASN:ND2  | 66:15:251:ASP:H    | 2.09                     | 0.44              |
| 65:14:855:LEU:HD23 | 65:14:859:LEU:HD21 | 1.98                     | 0.44              |
| 65:14:912:SER:O    | 65:14:914:VAL:HG23 | 2.17                     | 0.44              |
| 67:16:167:VAL:CG1  | 67:16:170:LEU:HD21 | 2.46                     | 0.44              |
| 3:10:227:ILE:CD1   | 6:17:112:VAL:N     | 2.64                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:12:96:LEU:HB3    | 6:17:664:ILE:CB    | 2.44                     | 0.44              |
| 6:17:256:THR:CG2   | 65:14:1100:THR:O   | 2.62                     | 0.44              |
| 6:17:386:VAL:CG2   | 66:15:174:ASP:C    | 2.73                     | 0.44              |
| 6:17:697:TYR:HD2   | 14:9:637:CYS:SG    | 2.40                     | 0.44              |
| 6:17:700:LEU:CG    | 14:9:658:LEU:HA    | 2.40                     | 0.44              |
| 8:3:410:G:N7       | 60:v:60:LYS:HD2    | 2.32                     | 0.44              |
| 8:3:1836:A:H3'     | 8:3:1837:C:H6      | 1.83                     | 0.44              |
| 8:3:2130:A:H2'     | 8:3:2131:G:C8      | 2.53                     | 0.44              |
| 8:3:2623:U:H2'     | 8:3:2624:C:C6      | 2.52                     | 0.44              |
| 10:5:476:U:H5'     | 10:5:477:U:OP1     | 2.18                     | 0.44              |
| 10:5:725:A:H2'     | 10:5:726:A:C8      | 2.52                     | 0.44              |
| 10:5:1115:G:H1'    | 10:5:1116:U:H5     | 1.82                     | 0.44              |
| 14:9:313:LYS:CE    | 38:Z:2:UNK:C       | 2.83                     | 0.44              |
| 35:T:2:PRO:HB3     | 35:T:21:VAL:HG11   | 1.99                     | 0.44              |
| 36:W:160:LEU:HD23  | 36:W:160:LEU:HA    | 1.80                     | 0.44              |
| 43:e:121:PRO:HG2   | 43:e:124:LEU:HD22  | 2.00                     | 0.44              |
| 46:h:11:LYS:HD3    | 46:h:54:VAL:HG22   | 1.99                     | 0.44              |
| 57:s:63:THR:H      | 57:s:75:SER:HB3    | 1.82                     | 0.44              |
| 65:14:887:ASN:HB2  | 65:14:1210:TYR:CE1 | 2.52                     | 0.44              |
| 66:15:12:ARG:CZ    | 66:15:801:SER:O    | 2.65                     | 0.44              |
| 66:15:1105:VAL:CG2 | 67:16:255:ARG:HG3  | 2.48                     | 0.44              |
| 66:15:1271:ARG:NH2 | 67:16:253:VAL:HG12 | 2.32                     | 0.44              |
| 5:12:92:ILE:HG23   | 6:17:660:GLY:CA    | 1.90                     | 0.44              |
| 6:17:261:LYS:HB3   | 65:14:1098:THR:O   | 2.17                     | 0.44              |
| 6:17:382:ASP:HB3   | 66:15:64:LYS:CE    | 2.47                     | 0.44              |
| 6:17:692:LYS:N     | 14:9:682:VAL:CB    | 2.80                     | 0.44              |
| 6:17:703:ASN:ND2   | 14:9:785:LEU:O     | 2.50                     | 0.44              |
| 7:2:9:PRO:HD3      | 7:2:16:ILE:HD11    | 1.98                     | 0.44              |
| 8:3:102:A:H61      | 14:9:785:LEU:HD23  | 1.81                     | 0.44              |
| 8:3:683:G:H2'      | 8:3:684:A:H8       | 1.82                     | 0.44              |
| 8:3:1270:C:H2'     | 8:3:1271:A:C8      | 2.51                     | 0.44              |
| 8:3:1605:A:H2'     | 8:3:1606:A:H8      | 1.82                     | 0.44              |
| 8:3:1755:A:H2'     | 8:3:1756:A:C8      | 2.52                     | 0.44              |
| 8:3:2394:A:O2'     | 59:u:70:ASP:OD1    | 2.34                     | 0.44              |
| 8:3:2638:G:H2'     | 8:3:2639:G:C8      | 2.52                     | 0.44              |
| 8:3:2793:U:H2'     | 8:3:2794:U:H6      | 1.83                     | 0.44              |
| 10:5:1142:G:O2'    | 10:5:1144:A:N6     | 2.43                     | 0.44              |
| 10:5:1473:U:C5     | 37:Y:41:U:H5'      | 2.12                     | 0.44              |
| 14:9:227:GLY:H     | 58:t:53:LYS:HE3    | 1.83                     | 0.44              |
| 14:9:787:LYS:CB    | 61:w:6:GLU:HG3     | 2.47                     | 0.44              |
| 15:A:202:CYS:SG    | 15:A:214:ILE:HG23  | 2.57                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 21:F:136:LYS:O     | 21:F:140:THR:HG22   | 2.17                     | 0.44              |
| 24:I:23:LEU:HD13   | 36:W:217:ARG:NH2    | 2.30                     | 0.44              |
| 26:K:86:ASN:O      | 26:K:88:GLN:HG2     | 2.17                     | 0.44              |
| 27:L:65:ILE:HG22   | 27:L:67:GLY:H       | 1.82                     | 0.44              |
| 43:e:27:VAL:HG12   | 43:e:82:VAL:HG21    | 1.98                     | 0.44              |
| 43:e:89:LYS:HB3    | 43:e:168:PHE:HB2    | 1.98                     | 0.44              |
| 44:f:58:TYR:HA     | 44:f:61:ASN:HD21    | 1.81                     | 0.44              |
| 48:j:19:VAL:HG13   | 48:j:41:VAL:HB      | 1.99                     | 0.44              |
| 50:l:43:ASP:HA     | 50:l:94:VAL:HA      | 1.99                     | 0.44              |
| 52:n:83:LYS:HB2    | 52:n:83:LYS:HE2     | 1.69                     | 0.44              |
| 54:p:27:ARG:HD3    | 54:p:37:THR:HG21    | 1.99                     | 0.44              |
| 57:s:30:VAL:HG12   | 57:s:80:LEU:HD13    | 1.99                     | 0.44              |
| 58:t:1:MET:HG2     | 58:t:2:GLN:N        | 2.25                     | 0.44              |
| 65:14:242:LYS:CE   | 65:14:396:GLU:OE2   | 2.65                     | 0.44              |
| 65:14:386:ILE:HG21 | 65:14:949:TYR:CZ    | 2.52                     | 0.44              |
| 65:14:610:ILE:CB   | 66:15:248:THR:OG1   | 2.53                     | 0.44              |
| 66:15:807:LYS:CE   | 66:15:811:ASN:CG    | 2.81                     | 0.44              |
| 66:15:977:LEU:CD1  | 66:15:1255:LEU:HD21 | 2.47                     | 0.44              |
| 67:16:125:ALA:HB1  | 67:16:127:ASP:OD1   | 2.16                     | 0.44              |
| 6:17:364:TYR:CE1   | 6:17:399:ARG:NH1    | 2.85                     | 0.44              |
| 8:3:867:G:H2'      | 8:3:868:C:C6        | 2.53                     | 0.44              |
| 8:3:1109:G:H2'     | 8:3:1110:C:O4'      | 2.17                     | 0.44              |
| 8:3:2896:G:H3'     | 8:3:2897:G:H5'      | 1.98                     | 0.44              |
| 10:5:260:C:H2'     | 10:5:261:G:O4'      | 2.18                     | 0.44              |
| 10:5:677:C:H2'     | 10:5:678:A:H8       | 1.83                     | 0.44              |
| 10:5:821:U:H2'     | 10:5:822:A:C8       | 2.52                     | 0.44              |
| 10:5:1032:G:H2'    | 10:5:1033:U:O4'     | 2.17                     | 0.44              |
| 14:9:352:ILE:H     | 14:9:352:ILE:HD12   | 1.83                     | 0.44              |
| 17:AB:40:U:C2      | 37:Y:41:U:H5        | 2.20                     | 0.44              |
| 17:AB:41:U:H3'     | 37:Y:42:C:C6        | 2.52                     | 0.44              |
| 21:F:17:PHE:HB3    | 21:F:58:LEU:HD22    | 2.00                     | 0.44              |
| 21:F:116:LEU:HB3   | 21:F:117:GLU:OE1    | 2.16                     | 0.44              |
| 23:H:65:ILE:HG22   | 23:H:67:VAL:HG23    | 1.98                     | 0.44              |
| 24:I:18:SER:OG     | 24:I:20:ASP:O       | 2.35                     | 0.44              |
| 26:K:46:VAL:C      | 26:K:68:VAL:HG23    | 2.43                     | 0.44              |
| 36:W:141:LEU:HD21  | 36:W:171:TYR:HB3    | 2.00                     | 0.44              |
| 57:s:28:VAL:HG22   | 57:s:82:VAL:HG22    | 1.98                     | 0.44              |
| 66:15:330:LEU:HD12 | 66:15:504:ILE:HD12  | 2.00                     | 0.44              |
| 66:15:712:SER:HB2  | 66:15:717:GLU:OE1   | 2.18                     | 0.44              |
| 67:18:57:THR:HG21  | 67:18:115:TRP:O     | 2.17                     | 0.44              |
| 6:17:181:TYR:CD1   | 6:17:289:LYS:HE2    | 2.52                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:3:102:A:C6      | 14:9:786:MET:CE    | 2.87                     | 0.44              |
| 8:3:1116:U:H2'    | 8:3:1117:U:C6      | 2.52                     | 0.44              |
| 8:3:1588:A:H2'    | 8:3:1589:A:H8      | 1.80                     | 0.44              |
| 8:3:1596:U:H2'    | 8:3:1597:U:C6      | 2.52                     | 0.44              |
| 8:3:1919:A:H2     | 10:5:1382:C:O2'    | 1.98                     | 0.44              |
| 8:3:2293:C:OP1    | 63:z:27:LYS:HG3    | 2.18                     | 0.44              |
| 8:3:2294:A:H4'    | 8:3:2295:A:O4'     | 2.18                     | 0.44              |
| 13:8:11:C:H2'     | 13:8:12:U:C6       | 2.53                     | 0.44              |
| 14:9:196:GLU:H    | 14:9:196:GLU:CD    | 2.25                     | 0.44              |
| 15:A:40:LYS:HB3   | 15:A:40:LYS:HE3    | 1.73                     | 0.44              |
| 19:C:27:LYS:HE2   | 19:C:27:LYS:HB2    | 1.78                     | 0.44              |
| 20:E:164:GLY:O    | 20:E:166:PHE:CD2   | 2.70                     | 0.44              |
| 30:O:50:ILE:HG13  | 30:O:51:ASP:N      | 2.33                     | 0.44              |
| 39:a:209:ASN:OD1  | 39:a:210:LEU:CD2   | 2.66                     | 0.44              |
| 46:h:58:TYR:CZ    | 46:h:60:ASP:HB3    | 2.52                     | 0.44              |
| 53:o:19:LYS:HE2   | 53:o:82:HIS:HA     | 2.00                     | 0.44              |
| 53:o:85:ASN:O     | 53:o:86:ILE:HD13   | 2.16                     | 0.44              |
| 66:15:1219:MET:CE | 66:15:1247:ARG:NH2 | 2.77                     | 0.44              |
| 6:17:955:LYS:NZ   | 14:9:799:GLU:HB3   | 0.94                     | 0.44              |
| 8:3:1036:A:H2'    | 8:3:1037:A:C8      | 2.52                     | 0.44              |
| 8:3:1560:U:H5''   | 14:9:249:ASP:CB    | 2.48                     | 0.44              |
| 8:3:1567:U:H2'    | 8:3:1568:C:O4'     | 2.18                     | 0.44              |
| 8:3:1809:A:H2'    | 8:3:1810:A:C8      | 2.53                     | 0.44              |
| 8:3:1879:A:H2'    | 8:3:1880:G:O4'     | 2.18                     | 0.44              |
| 8:3:2657:C:H2'    | 8:3:2658:U:H6      | 1.83                     | 0.44              |
| 8:3:2695:U:H2'    | 8:3:2696:G:O4'     | 2.18                     | 0.44              |
| 10:5:1138:U:H2'   | 10:5:1139:A:H8     | 1.81                     | 0.44              |
| 10:5:1153:G:N7    | 23:H:101:LYS:NZ    | 2.60                     | 0.44              |
| 10:5:1361:G:H2'   | 10:5:1362:G:H8     | 1.82                     | 0.44              |
| 14:9:234:ALA:O    | 57:s:14:GLU:OE1    | 2.35                     | 0.44              |
| 15:A:93:LYS:HE3   | 15:A:93:LYS:HB2    | 1.79                     | 0.44              |
| 19:C:49:GLY:O     | 19:C:53:GLN:HB2    | 2.18                     | 0.44              |
| 19:C:124:LEU:HD13 | 19:C:129:VAL:HG21  | 2.00                     | 0.44              |
| 20:E:49:ILE:HG23  | 20:E:83:LEU:HD23   | 1.99                     | 0.44              |
| 23:H:89:LEU:HD13  | 23:H:96:LEU:HD23   | 2.00                     | 0.44              |
| 34:S:68:LEU:O     | 34:S:72:ASN:ND2    | 2.48                     | 0.44              |
| 47:i:99:GLN:O     | 47:i:99:GLN:HG2    | 2.18                     | 0.44              |
| 49:k:75:GLN:OE1   | 49:k:76:GLU:N      | 2.51                     | 0.44              |
| 58:t:3:ARG:NH2    | 58:t:4:ILE:HD11    | 2.33                     | 0.44              |
| 63:z:9:LEU:HD21   | 63:z:34:LEU:HD12   | 2.00                     | 0.44              |
| 64:13:28:LEU:HD22 | 64:13:765:LEU:HD21 | 1.99                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 64:13:287:ASN:C    | 64:13:289:GLY:H     | 2.25                     | 0.44              |
| 64:13:984:GLN:CG   | 64:13:1133:THR:CA   | 2.87                     | 0.44              |
| 64:13:1217:LYS:CE  | 67:18:274:PRO:CB    | 2.96                     | 0.44              |
| 65:14:138:GLU:OE1  | 65:14:169:LYS:HE3   | 2.17                     | 0.44              |
| 66:15:179:PHE:HD2  | 66:15:633:PRO:HG2   | 1.82                     | 0.44              |
| 66:15:991:TRP:O    | 66:15:1246:SER:HA   | 2.17                     | 0.44              |
| 66:15:1104:SER:OG  | 67:16:256:HIS:C     | 2.61                     | 0.44              |
| 8:3:270:G:H1'      | 8:3:315:A:N6        | 2.32                     | 0.44              |
| 8:3:868:C:H2'      | 8:3:869:U:C6        | 2.53                     | 0.44              |
| 8:3:1441:A:H2'     | 8:3:1442:G:H8       | 1.83                     | 0.44              |
| 8:3:1705:U:H1'     | 40:b:135:HIS:CE1    | 2.53                     | 0.44              |
| 8:3:2745:G:H2'     | 8:3:2746:A:C8       | 2.53                     | 0.44              |
| 10:5:519:G:H4'     | 26:K:83:GLU:HG2     | 2.00                     | 0.44              |
| 10:5:537:A:H2'     | 10:5:538:G:C8       | 2.53                     | 0.44              |
| 20:E:40:LEU:HB2    | 20:E:57:TYR:HB2     | 1.99                     | 0.44              |
| 22:G:56:ASN:OD1    | 22:G:73:ASN:HB2     | 2.18                     | 0.44              |
| 23:H:129:PHE:CE1   | 23:H:131:LYS:HB2    | 2.52                     | 0.44              |
| 25:J:35:LEU:HB3    | 25:J:70:MET:HE1     | 2.00                     | 0.44              |
| 36:W:37:ASP:OD1    | 36:W:38:GLU:N       | 2.50                     | 0.44              |
| 40:b:189:MET:HE3   | 40:b:189:MET:HB2    | 1.81                     | 0.44              |
| 54:p:71:GLN:OE1    | 54:p:109:VAL:HG21   | 2.18                     | 0.44              |
| 65:14:1141:PHE:HB3 | 65:14:1181:PHE:HE2  | 1.81                     | 0.44              |
| 66:15:869:LEU:HD21 | 66:15:1263:PHE:HA   | 1.99                     | 0.44              |
| 66:15:1207:LYS:CE  | 66:15:1252:SER:OG   | 2.65                     | 0.44              |
| 3:10:313:GLU:OE2   | 65:14:88:ARG:CZ     | 2.64                     | 0.44              |
| 5:12:85:TRP:HB3    | 6:17:11:TRP:CE3     | 2.52                     | 0.44              |
| 6:17:261:LYS:HB2   | 65:14:1126:LEU:HD21 | 1.98                     | 0.44              |
| 6:17:386:VAL:N     | 66:15:176:ASN:ND2   | 2.63                     | 0.44              |
| 6:17:426:LYS:CG    | 66:15:184:GLN:CG    | 2.95                     | 0.44              |
| 8:3:196:G:O6       | 8:3:207:C:O2'       | 2.20                     | 0.44              |
| 8:3:227:A:O2'      | 8:3:456:G:N3        | 2.44                     | 0.44              |
| 8:3:312:U:H2'      | 8:3:313:G:H8        | 1.82                     | 0.44              |
| 8:3:1127:C:H2'     | 8:3:1128:G:O4'      | 2.17                     | 0.44              |
| 8:3:1956:G:C4      | 8:3:1957:G:C8       | 3.06                     | 0.44              |
| 10:5:821:U:O2      | 22:G:11:HIS:NE2     | 2.51                     | 0.44              |
| 14:9:808:GLN:CA    | 61:w:79:THR:HG23    | 2.19                     | 0.44              |
| 20:E:142:ARG:O     | 20:E:145:ARG:N      | 2.39                     | 0.44              |
| 23:H:95:GLU:OE2    | 23:H:95:GLU:N       | 2.46                     | 0.44              |
| 24:I:62:HIS:ND1    | 24:I:63:VAL:HG13    | 2.32                     | 0.44              |
| 34:S:48:TYR:CD2    | 34:S:69:LYS:HD2     | 2.52                     | 0.44              |
| 36:W:152:ILE:HD12  | 36:W:205:ILE:HD12   | 1.98                     | 0.44              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 42:d:29:PRO:CG    | 42:d:169:LEU:HB2    | 2.47                     | 0.44              |
| 42:d:117:LEU:HD23 | 42:d:117:LEU:C      | 2.43                     | 0.44              |
| 42:d:123:ASP:OD1  | 42:d:127:ASN:ND2    | 2.51                     | 0.44              |
| 49:k:120:LEU:HD23 | 49:k:120:LEU:H      | 1.83                     | 0.44              |
| 64:13:371:LEU:HB3 | 64:13:442:VAL:HB    | 2.00                     | 0.44              |
| 67:18:163:TYR:CD1 | 67:18:205:PHE:HZ    | 2.36                     | 0.44              |
| 6:17:373:VAL:HG13 | 66:15:171:LYS:O     | 2.16                     | 0.44              |
| 8:3:158:U:H2'     | 8:3:159:G:C8        | 2.53                     | 0.44              |
| 8:3:1343:C:H2'    | 8:3:1344:U:C6       | 2.53                     | 0.44              |
| 8:3:2224:A:H2'    | 8:3:2225:G:C8       | 2.53                     | 0.44              |
| 8:3:2358:U:H2'    | 8:3:2359:G:O4'      | 2.18                     | 0.44              |
| 8:3:2557:G:H2'    | 8:3:2558:G:H8       | 1.83                     | 0.44              |
| 8:3:2657:C:H2'    | 8:3:2658:U:C6       | 2.53                     | 0.44              |
| 8:3:2755:G:OP1    | 43:e:77:ASN:ND2     | 2.50                     | 0.44              |
| 8:3:2842:G:C4     | 8:3:2843:G:C8       | 3.06                     | 0.44              |
| 10:5:354:U:H2'    | 10:5:355:A:C8       | 2.48                     | 0.44              |
| 10:5:1385:A:H2'   | 10:5:1386:C:C6      | 2.52                     | 0.44              |
| 14:9:704:ILE:CG2  | 58:t:6:LYS:HE2      | 2.48                     | 0.44              |
| 15:A:282:LEU:HB3  | 15:A:283:ASN:H      | 1.51                     | 0.44              |
| 19:C:42:PHE:N     | 19:C:42:PHE:CD1     | 2.86                     | 0.44              |
| 19:C:103:ARG:HB2  | 19:C:167:VAL:HG21   | 1.99                     | 0.44              |
| 19:C:170:ASN:O    | 19:C:173:THR:OG1    | 2.33                     | 0.44              |
| 27:L:12:GLN:H     | 27:L:12:GLN:CD      | 2.25                     | 0.44              |
| 35:T:36:LEU:H     | 35:T:41:ARG:HH21    | 1.65                     | 0.44              |
| 39:a:72:LYS:HB3   | 39:a:74:THR:HG22    | 2.00                     | 0.44              |
| 41:c:136:THR:HA   | 41:c:142:VAL:HG11   | 2.00                     | 0.44              |
| 41:c:156:ASN:HA   | 41:c:177:ASN:OD1    | 2.18                     | 0.44              |
| 44:f:15:ARG:HG2   | 44:f:16:PHE:CD1     | 2.53                     | 0.44              |
| 48:j:77:LEU:HD13  | 53:o:77:LYS:HE2     | 2.00                     | 0.44              |
| 62:y:13:ARG:HD2   | 62:y:17:ARG:NH2     | 2.33                     | 0.44              |
| 64:13:341:PRO:HG3 | 64:13:443:LEU:HD22  | 1.99                     | 0.44              |
| 66:15:653:ASP:HB3 | 66:15:782:LYS:HD2   | 2.00                     | 0.44              |
| 2:1:10:ARG:NH1    | 8:3:254:G:OP2       | 2.42                     | 0.43              |
| 6:17:260:GLN:H    | 65:14:1126:LEU:HD22 | 1.81                     | 0.43              |
| 6:17:262:SER:HB2  | 65:14:1098:THR:CG2  | 2.48                     | 0.43              |
| 6:17:262:SER:HA   | 65:14:1096:ILE:HA   | 1.99                     | 0.43              |
| 6:17:399:ARG:NH2  | 6:17:417:GLU:OE2    | 2.51                     | 0.43              |
| 6:17:424:VAL:HG13 | 66:15:140:ASN:HD21  | 1.83                     | 0.43              |
| 6:17:692:LYS:HE3  | 14:9:683:HIS:HD2    | 1.77                     | 0.43              |
| 8:3:316:C:O2      | 8:3:316:C:O4'       | 2.36                     | 0.43              |
| 8:3:558:C:H5''    | 8:3:575:C:O2'       | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:789:A:H2'      | 8:3:790:U:C6       | 2.53                     | 0.43              |
| 8:3:1572:U:H2'     | 8:3:1573:A:H8      | 1.83                     | 0.43              |
| 8:3:1848:U:H2'     | 8:3:1849:G:H8      | 1.83                     | 0.43              |
| 8:3:2814:A:H4'     | 40:b:64:LYS:HD2    | 2.00                     | 0.43              |
| 9:4:85:A:H2'       | 9:4:86:G:C8        | 2.53                     | 0.43              |
| 10:5:331:C:H2'     | 10:5:332:A:C8      | 2.53                     | 0.43              |
| 10:5:590:G:H1      | 10:5:644:U:H3      | 1.65                     | 0.43              |
| 10:5:999:C:OP1     | 10:5:1023:G:N2     | 2.49                     | 0.43              |
| 10:5:1070:G:H2'    | 10:5:1071:A:C8     | 2.53                     | 0.43              |
| 22:G:114:ALA:HB3   | 22:G:125:ASP:HB3   | 2.00                     | 0.43              |
| 32:Q:64:LEU:HD21   | 32:Q:68:ALA:HA     | 2.00                     | 0.43              |
| 38:Z:2:UNK:HA      | 58:t:50:GLN:HB2    | 1.98                     | 0.43              |
| 42:d:74:ILE:O      | 42:d:79:LEU:N      | 2.51                     | 0.43              |
| 51:m:74:ASP:O      | 51:m:78:LEU:HB2    | 2.18                     | 0.43              |
| 66:15:664:PHE:CE1  | 66:15:668:LEU:HD12 | 2.53                     | 0.43              |
| 6:17:81:ASN:HB2    | 65:14:1293:GLN:CB  | 2.45                     | 0.43              |
| 6:17:277:SER:HB3   | 65:14:1124:LYS:HA  | 1.95                     | 0.43              |
| 8:3:145:A:O2'      | 57:s:42:LEU:HD11   | 2.18                     | 0.43              |
| 8:3:620:G:H1       | 49:k:34:ARG:NH1    | 2.13                     | 0.43              |
| 8:3:869:U:H2'      | 8:3:870:A:H8       | 1.83                     | 0.43              |
| 8:3:883:A:H2'      | 8:3:884:A:C8       | 2.53                     | 0.43              |
| 8:3:1098:G:H2'     | 8:3:1099:C:C6      | 2.53                     | 0.43              |
| 8:3:1254:U:H2'     | 8:3:1255:G:C8      | 2.53                     | 0.43              |
| 8:3:2174:G:H2'     | 8:3:2175:U:C6      | 2.53                     | 0.43              |
| 8:3:2541:C:H2'     | 8:3:2542:A:O4'     | 2.18                     | 0.43              |
| 14:9:184:PHE:HB3   | 58:t:57:LYS:CE     | 2.48                     | 0.43              |
| 15:A:285:THR:HG23  | 15:A:286:ARG:HD3   | 2.00                     | 0.43              |
| 19:C:64:TYR:HD1    | 19:C:110:ARG:HH12  | 1.66                     | 0.43              |
| 19:C:117:VAL:HG22  | 19:C:122:VAL:HG11  | 2.00                     | 0.43              |
| 20:E:71:ASP:N      | 20:E:71:ASP:OD1    | 2.47                     | 0.43              |
| 39:a:83:VAL:HG13   | 39:a:97:SER:HB3    | 1.99                     | 0.43              |
| 41:c:52:ILE:HG21   | 41:c:92:GLY:HA3    | 1.99                     | 0.43              |
| 41:c:135:LYS:HA    | 41:c:135:LYS:HD2   | 1.71                     | 0.43              |
| 47:i:80:HIS:ND1    | 47:i:81:SER:O      | 2.50                     | 0.43              |
| 50:l:109:ILE:HG22  | 50:l:114:MET:HG3   | 1.99                     | 0.43              |
| 64:13:968:LEU:HD22 | 64:13:973:PHE:CD2  | 2.53                     | 0.43              |
| 65:14:295:MET:HE3  | 65:14:296:PHE:HE2  | 1.83                     | 0.43              |
| 65:14:827:TYR:CE2  | 65:14:832:LEU:HD12 | 2.53                     | 0.43              |
| 6:17:430:PRO:N     | 66:15:549:LEU:CD2  | 2.82                     | 0.43              |
| 8:3:9:G:H2'        | 8:3:10:U:H6        | 1.80                     | 0.43              |
| 8:3:764:G:O2'      | 8:3:798:G:H4'      | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:1227:C:C2      | 8:3:1228:G:C8      | 3.07                     | 0.43              |
| 8:3:1560:U:H4'     | 14:9:250:GLU:H     | 1.82                     | 0.43              |
| 8:3:2243:G:H2'     | 8:3:2244:U:C6      | 2.54                     | 0.43              |
| 10:5:381:C:H2'     | 10:5:382:U:H6      | 1.84                     | 0.43              |
| 10:5:821:U:H2'     | 10:5:822:A:H8      | 1.83                     | 0.43              |
| 14:9:199:LYS:HZ2   | 58:t:59:SER:CB     | 2.31                     | 0.43              |
| 14:9:798:ARG:NE    | 61:w:18:LEU:CA     | 2.47                     | 0.43              |
| 16:AA:86:MET:HE2   | 16:AA:86:MET:HB3   | 1.85                     | 0.43              |
| 19:C:9:LYS:HB3     | 19:C:9:LYS:HE2     | 1.67                     | 0.43              |
| 33:R:76:PRO:O      | 33:R:76:PRO:HD2    | 2.18                     | 0.43              |
| 42:d:49:PHE:CD2    | 42:d:146:ILE:HG23  | 2.53                     | 0.43              |
| 42:d:70:ALA:HB3    | 42:d:79:LEU:HD11   | 2.00                     | 0.43              |
| 43:e:18:LEU:HD11   | 43:e:53:LEU:HD13   | 2.00                     | 0.43              |
| 43:e:42:LEU:HD12   | 43:e:42:LEU:HA     | 1.87                     | 0.43              |
| 45:g:28:ASP:O      | 45:g:32:MET:HE1    | 2.17                     | 0.43              |
| 50:l:104:PHE:HE2   | 50:l:125:LEU:HD11  | 1.84                     | 0.43              |
| 51:m:17:THR:O      | 51:m:21:GLN:HG3    | 2.17                     | 0.43              |
| 56:r:1:MET:CE      | 56:r:62:HIS:HB3    | 2.48                     | 0.43              |
| 64:13:1217:LYS:NZ  | 67:18:274:PRO:O    | 2.50                     | 0.43              |
| 65:14:158:THR:HG23 | 65:14:270:GLN:O    | 2.19                     | 0.43              |
| 3:10:235:ILE:CG1   | 6:17:564:GLY:N     | 2.81                     | 0.43              |
| 8:3:26:G:O2'       | 56:r:78:GLN:O      | 2.32                     | 0.43              |
| 8:3:159:G:H2'      | 8:3:160:A:C8       | 2.54                     | 0.43              |
| 8:3:858:A:H2'      | 8:3:859:G:C8       | 2.53                     | 0.43              |
| 8:3:1281:A:OP1     | 54:p:9:THR:HG22    | 2.18                     | 0.43              |
| 10:5:372:G:N2      | 10:5:383:U:O2      | 2.51                     | 0.43              |
| 10:5:623:G:H4'     | 30:O:16:THR:HG21   | 2.00                     | 0.43              |
| 30:O:6:LEU:HD22    | 30:O:17:TYR:HD2    | 1.84                     | 0.43              |
| 42:d:53:ALA:HA     | 42:d:56:GLU:OE1    | 2.19                     | 0.43              |
| 42:d:114:PHE:CD1   | 42:d:114:PHE:C     | 2.96                     | 0.43              |
| 46:h:63:PHE:HB2    | 46:h:65:PHE:CZ     | 2.53                     | 0.43              |
| 46:h:77:LYS:HD3    | 46:h:83:GLU:O      | 2.19                     | 0.43              |
| 61:w:20:ILE:HD12   | 61:w:21:LYS:H      | 1.80                     | 0.43              |
| 64:13:357:ASP:OD1  | 64:13:439:ASN:HB3  | 2.18                     | 0.43              |
| 64:13:908:VAL:HA   | 64:13:912:LEU:HD23 | 2.00                     | 0.43              |
| 64:13:1011:THR:HB  | 64:13:1020:MET:SD  | 2.58                     | 0.43              |
| 64:13:1213:LEU:HB2 | 67:18:276:ASN:CB   | 2.29                     | 0.43              |
| 65:14:49:LEU:HD21  | 65:14:530:LEU:HD23 | 2.01                     | 0.43              |
| 65:14:250:THR:O    | 65:14:280:PHE:HA   | 2.18                     | 0.43              |
| 65:14:863:LYS:NZ   | 65:14:1224:GLU:O   | 2.43                     | 0.43              |
| 66:15:1129:LYS:NZ  | 66:15:1201:ASP:OD2 | 2.40                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:1:51:ASP:O       | 2:1:55:ILE:HG12     | 2.18                     | 0.43              |
| 6:17:838:ARG:NH2   | 6:17:879:GLY:CA     | 2.82                     | 0.43              |
| 8:3:1093:U:H3      | 8:3:1115:G:H1       | 1.65                     | 0.43              |
| 8:3:1471:A:H2'     | 8:3:1472:C:C6       | 2.54                     | 0.43              |
| 8:3:1479:A:N6      | 8:3:1487:U:O4       | 2.52                     | 0.43              |
| 8:3:2141:A:OP2     | 8:3:2164:G:N2       | 2.41                     | 0.43              |
| 8:3:2623:U:H2'     | 8:3:2624:C:H6       | 1.83                     | 0.43              |
| 8:3:2687:A:H2'     | 8:3:2688:C:H6       | 1.83                     | 0.43              |
| 10:5:631:C:H2'     | 10:5:632:A:C8       | 2.53                     | 0.43              |
| 10:5:733:A:H2'     | 10:5:734:A:C8       | 2.54                     | 0.43              |
| 10:5:894:A:H2'     | 10:5:895:A:C8       | 2.53                     | 0.43              |
| 10:5:1205:C:N4     | 27:L:104:THR:OG1    | 2.51                     | 0.43              |
| 14:9:798:ARG:NE    | 61:w:21:LYS:HB3     | 2.29                     | 0.43              |
| 19:C:123:LEU:HD22  | 19:C:128:THR:HG22   | 2.00                     | 0.43              |
| 26:K:47:CYS:SG     | 26:K:48:THR:N       | 2.91                     | 0.43              |
| 35:T:4:ILE:HD11    | 35:T:21:VAL:HG21    | 1.99                     | 0.43              |
| 36:W:61:THR:HG22   | 36:W:62:GLN:N       | 2.26                     | 0.43              |
| 43:e:23:ASP:HA     | 43:e:38:LEU:HB2     | 1.99                     | 0.43              |
| 50:l:38:LYS:HE2    | 50:l:38:LYS:HB3     | 1.88                     | 0.43              |
| 50:l:67:ARG:HD3    | 50:l:105:GLU:OE2    | 2.18                     | 0.43              |
| 57:s:16:VAL:O      | 57:s:20:GLN:HG3     | 2.17                     | 0.43              |
| 64:13:10:GLN:HA    | 67:18:197:ASN:ND2   | 2.34                     | 0.43              |
| 64:13:80:GLN:NE2   | 64:13:122:GLN:HE22  | 2.17                     | 0.43              |
| 64:13:850:TYR:OH   | 64:13:970:PRO:O     | 2.29                     | 0.43              |
| 64:13:912:LEU:HD21 | 64:13:1180:LEU:HD11 | 1.99                     | 0.43              |
| 65:14:27:LEU:HD11  | 65:14:707:VAL:HG11  | 2.00                     | 0.43              |
| 6:17:14:LYS:HG2    | 6:17:615:PHE:CE1    | 2.53                     | 0.43              |
| 6:17:388:ALA:HB2   | 66:15:180:PHE:HZ    | 1.81                     | 0.43              |
| 6:17:690:LEU:CA    | 14:9:682:VAL:CG2    | 2.88                     | 0.43              |
| 6:17:803:GLY:HA3   | 6:17:916:PHE:CZ     | 2.53                     | 0.43              |
| 8:3:356:A:OP2      | 41:c:174:ASN:HB2    | 2.19                     | 0.43              |
| 8:3:767:C:H2'      | 8:3:768:G:O4'       | 2.19                     | 0.43              |
| 8:3:1389:G:H2'     | 8:3:1390:C:C6       | 2.54                     | 0.43              |
| 8:3:1755:A:H2'     | 8:3:1756:A:H8       | 1.83                     | 0.43              |
| 8:3:2537:G:H5''    | 8:3:2538:A:H5''     | 2.00                     | 0.43              |
| 8:3:2798:A:OP1     | 8:3:2798:A:H4'      | 2.18                     | 0.43              |
| 10:5:231:U:H2'     | 10:5:232:G:H8       | 1.84                     | 0.43              |
| 36:W:3:GLN:N       | 36:W:3:GLN:OE1      | 2.51                     | 0.43              |
| 40:b:47:TYR:CD1    | 40:b:85:ARG:NE      | 2.85                     | 0.43              |
| 44:f:69:LYS:O      | 44:f:72:ILE:HG13    | 2.18                     | 0.43              |
| 50:l:36:ALA:HB2    | 50:l:103:MET:HE2    | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:13:80:GLN:HE22  | 64:13:122:GLN:HE22 | 1.66                     | 0.43              |
| 65:14:401:ILE:CD1  | 65:14:615:LEU:HD21 | 2.49                     | 0.43              |
| 66:15:182:ASN:HB3  | 66:15:574:MET:HE3  | 2.00                     | 0.43              |
| 6:17:79:SER:HB3    | 65:14:1269:ALA:O   | 2.14                     | 0.43              |
| 6:17:373:VAL:CG1   | 66:15:172:PRO:CG   | 2.92                     | 0.43              |
| 6:17:387:VAL:CG1   | 66:15:67:ASN:HB2   | 2.34                     | 0.43              |
| 6:17:697:TYR:CZ    | 14:9:636:PHE:C     | 2.84                     | 0.43              |
| 6:17:706:ILE:C     | 14:9:655:SER:OG    | 2.62                     | 0.43              |
| 8:3:117:C:H2'      | 8:3:118:G:O4'      | 2.18                     | 0.43              |
| 8:3:470:U:O2       | 8:3:471:A:N6       | 2.43                     | 0.43              |
| 8:3:488:G:C8       | 41:c:59:ARG:HD2    | 2.53                     | 0.43              |
| 8:3:524:G:N2       | 8:3:527:A:OP2      | 2.33                     | 0.43              |
| 8:3:527:A:N1       | 56:r:7:GLN:NE2     | 2.66                     | 0.43              |
| 8:3:675:U:H2'      | 8:3:676:U:C6       | 2.53                     | 0.43              |
| 8:3:1509:U:H3      | 8:3:1530:G:H1      | 1.67                     | 0.43              |
| 8:3:2001:C:H5''    | 70:3:3214:PUT:H21  | 2.01                     | 0.43              |
| 8:3:2704:U:H2'     | 8:3:2705:G:C8      | 2.53                     | 0.43              |
| 9:4:81:U:H2'       | 9:4:82:U:O4'       | 2.19                     | 0.43              |
| 9:4:85:A:H2'       | 9:4:86:G:H8        | 1.84                     | 0.43              |
| 10:5:259:A:H2'     | 10:5:260:C:H6      | 1.84                     | 0.43              |
| 10:5:369:A:H61     | 10:5:387:G:H1'     | 1.84                     | 0.43              |
| 10:5:561:A:H2      | 26:K:12:ARG:NH1    | 2.17                     | 0.43              |
| 10:5:1212:C:H3'    | 10:5:1213:A:H5'    | 2.00                     | 0.43              |
| 10:5:1332:U:H3     | 10:5:1338:A:H61    | 1.66                     | 0.43              |
| 14:9:105:GLY:HA2   | 14:9:530:GLN:H     | 1.83                     | 0.43              |
| 15:A:30:VAL:HG13   | 15:A:53:ASN:HB3    | 2.01                     | 0.43              |
| 15:A:171:ARG:HG2   | 15:A:172:LEU:N     | 2.33                     | 0.43              |
| 21:F:67:ASN:O      | 21:F:137:LYS:NZ    | 2.40                     | 0.43              |
| 28:M:19:ARG:HG3    | 28:M:19:ARG:NH1    | 2.33                     | 0.43              |
| 41:c:191:LEU:HD23  | 41:c:191:LEU:HA    | 1.86                     | 0.43              |
| 42:d:171:ARG:HA    | 42:d:171:ARG:NH1   | 2.34                     | 0.43              |
| 45:g:99:VAL:O      | 45:g:103:LYS:HG3   | 2.18                     | 0.43              |
| 46:h:70:THR:CG2    | 46:h:71:PRO:HD2    | 2.49                     | 0.43              |
| 53:o:42:LYS:HG2    | 53:o:43:VAL:H      | 1.83                     | 0.43              |
| 55:q:60:GLU:HB2    | 55:q:91:LYS:HD3    | 1.99                     | 0.43              |
| 65:14:101:THR:HG22 | 65:14:703:GLN:HE21 | 1.83                     | 0.43              |
| 65:14:638:LYS:NZ   | 65:14:663:LYS:O    | 2.41                     | 0.43              |
| 66:15:1094:PHE:CZ  | 66:15:1096:GLY:HA2 | 2.54                     | 0.43              |
| 67:16:238:ALA:O    | 67:16:240:ALA:N    | 2.47                     | 0.43              |
| 6:17:385:ASP:CB    | 66:15:175:PRO:CB   | 2.77                     | 0.43              |
| 6:17:429:ASP:C     | 66:15:549:LEU:HD13 | 2.44                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:17:705:ASP:CA    | 14:9:665:HIS:CE1    | 3.00                     | 0.43              |
| 8:3:42:U:H2'       | 8:3:43:A:C8         | 2.54                     | 0.43              |
| 8:3:317:U:H2'      | 8:3:318:U:C6        | 2.53                     | 0.43              |
| 8:3:450:C:H2'      | 8:3:451:A:H8        | 1.83                     | 0.43              |
| 8:3:479:A:OP1      | 41:c:47:GLN:N       | 2.49                     | 0.43              |
| 8:3:739:G:O2'      | 8:3:761:G:N2        | 2.50                     | 0.43              |
| 8:3:1144:C:P       | 45:g:77:LYS:HG2     | 2.58                     | 0.43              |
| 8:3:1434:U:H2'     | 8:3:1435:A:H8       | 1.84                     | 0.43              |
| 8:3:2038:A:O2'     | 8:3:2462:G:N2       | 2.50                     | 0.43              |
| 8:3:2482:U:H3'     | 8:3:2483:C:C5       | 2.53                     | 0.43              |
| 8:3:2523:C:H2'     | 8:3:2524:U:H6       | 1.83                     | 0.43              |
| 8:3:2644:U:H2'     | 8:3:2645:U:C6       | 2.53                     | 0.43              |
| 9:4:11:A:C2'       | 9:4:12:U:H5''       | 2.48                     | 0.43              |
| 10:5:57:U:H2'      | 10:5:58:G:C8        | 2.53                     | 0.43              |
| 10:5:1002:A:H2'    | 10:5:1003:A:O4'     | 2.19                     | 0.43              |
| 10:5:1402:U:H2'    | 10:5:1403:A:H8      | 1.84                     | 0.43              |
| 10:5:1467:A:O2'    | 37:Y:44:A:H1'       | 2.17                     | 0.43              |
| 40:b:13:MET:HE3    | 40:b:13:MET:HB2     | 1.74                     | 0.43              |
| 42:d:31:LEU:HD23   | 42:d:96:MET:SD      | 2.59                     | 0.43              |
| 42:d:60:ILE:HD11   | 42:d:138:PHE:HB3    | 2.00                     | 0.43              |
| 44:f:58:TYR:HA     | 44:f:61:ASN:ND2     | 2.34                     | 0.43              |
| 46:h:106:GLN:OE1   | 46:h:106:GLN:N      | 2.51                     | 0.43              |
| 52:n:13:LYS:HB2    | 52:n:13:LYS:HE3     | 1.67                     | 0.43              |
| 59:u:101:LYS:O     | 59:u:102:LEU:C      | 2.61                     | 0.43              |
| 63:z:31:LYS:HE2    | 63:z:31:LYS:HB3     | 1.91                     | 0.43              |
| 64:13:392:LEU:O    | 64:13:395:ILE:HG12  | 2.19                     | 0.43              |
| 65:14:878:LEU:HD13 | 65:14:1244:LEU:HD11 | 2.00                     | 0.43              |
| 66:15:342:VAL:HG22 | 66:15:359:MET:HE2   | 2.01                     | 0.43              |
| 6:17:429:ASP:O     | 66:15:549:LEU:CB    | 2.58                     | 0.43              |
| 8:3:852:C:H2'      | 8:3:853:G:O4'       | 2.18                     | 0.43              |
| 8:3:1102:A:H2'     | 8:3:1102:A:N3       | 2.33                     | 0.43              |
| 8:3:2353:G:N3      | 8:3:2389:A:H2'      | 2.34                     | 0.43              |
| 8:3:2764:U:H4'     | 8:3:2765:A:OP1      | 2.17                     | 0.43              |
| 15:A:119:ASN:HD21  | 15:A:122:THR:HG23   | 1.83                     | 0.43              |
| 32:Q:48:GLN:HG3    | 32:Q:50:ARG:O       | 2.18                     | 0.43              |
| 44:f:88:PRO:HG2    | 44:f:89:TYR:CD1     | 2.54                     | 0.43              |
| 46:h:120:ALA:CA    | 46:h:123:MET:SD     | 3.05                     | 0.43              |
| 54:p:6:GLY:O       | 54:p:8:GLN:OE1      | 2.37                     | 0.43              |
| 56:r:12:ILE:O      | 56:r:101:SER:OG     | 2.30                     | 0.43              |
| 59:u:57:THR:HG23   | 59:u:57:THR:O       | 2.18                     | 0.43              |
| 64:13:713:SER:HA   | 64:13:729:ILE:HD11  | 2.01                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 65:14:139:TYR:CZ   | 65:14:154:LEU:HD23  | 2.54                     | 0.43              |
| 65:14:888:LYS:NZ   | 65:14:1198:TYR:O    | 2.52                     | 0.43              |
| 65:14:1028:ARG:HA  | 65:14:1032:GLN:HB2  | 2.01                     | 0.43              |
| 67:18:42:ALA:N     | 67:18:201:ILE:HD11  | 2.33                     | 0.43              |
| 8:3:80:U:H2'       | 8:3:81:C:C6         | 2.54                     | 0.43              |
| 8:3:670:G:H2'      | 8:3:671:C:C6        | 2.54                     | 0.43              |
| 8:3:1524:C:C2      | 8:3:1525:G:C8       | 3.07                     | 0.43              |
| 8:3:2106:G:N2      | 8:3:2199:C:O2       | 2.52                     | 0.43              |
| 8:3:2239:U:H5''    | 60:v:29:TRP:HD1     | 1.83                     | 0.43              |
| 8:3:2845:U:H2'     | 8:3:2846:A:H8       | 1.84                     | 0.43              |
| 10:5:212:G:H2'     | 10:5:213:U:C6       | 2.54                     | 0.43              |
| 10:5:927:C:C5      | 21:F:1:MET:HG3      | 2.54                     | 0.43              |
| 10:5:991:A:H2'     | 10:5:992:U:H6       | 1.84                     | 0.43              |
| 10:5:1078:G:H5'    | 10:5:1078:G:C8      | 2.51                     | 0.43              |
| 10:5:1368:U:O2'    | 10:5:1476:C:O2'     | 2.33                     | 0.43              |
| 14:9:163:PRO:HG3   | 58:t:60:THR:HA      | 1.29                     | 0.43              |
| 14:9:791:LEU:CD1   | 61:w:50:LEU:HD11    | 2.48                     | 0.43              |
| 15:A:64:SER:HB2    | 15:A:214:ILE:O      | 2.19                     | 0.43              |
| 15:A:293:ARG:NH2   | 35:T:50:GLN:HG2     | 2.32                     | 0.43              |
| 20:E:139:THR:OG1   | 20:E:140:GLN:N      | 2.51                     | 0.43              |
| 33:R:16:LEU:O      | 33:R:20:ILE:HG13    | 2.19                     | 0.43              |
| 40:b:106:GLU:HA    | 40:b:217:VAL:HA     | 2.01                     | 0.43              |
| 54:p:6:GLY:O       | 54:p:7:LYS:HB3      | 2.19                     | 0.43              |
| 65:14:295:MET:HE1  | 65:14:308:ILE:HD11  | 2.00                     | 0.43              |
| 66:15:965:LEU:HD12 | 66:15:1269:LEU:HD11 | 2.01                     | 0.43              |
| 6:17:706:ILE:CB    | 14:9:659:ASN:H      | 2.31                     | 0.42              |
| 8:3:1101:U:H3      | 8:3:1103:G:H3'      | 1.83                     | 0.42              |
| 8:3:1183:A:H2'     | 8:3:1184:U:C6       | 2.54                     | 0.42              |
| 8:3:1321:C:H2'     | 8:3:1322:A:O4'      | 2.18                     | 0.42              |
| 8:3:1543:U:H2'     | 8:3:1544:G:C8       | 2.54                     | 0.42              |
| 8:3:1585:A:N3      | 8:3:1585:A:H2'      | 2.34                     | 0.42              |
| 8:3:2072:C:H2'     | 8:3:2073:C:C6       | 2.54                     | 0.42              |
| 8:3:2583:U:C4'     | 40:b:148:GLN:HE21   | 2.32                     | 0.42              |
| 10:5:379:A:C5      | 10:5:380:G:H1'      | 2.54                     | 0.42              |
| 12:7:7:A:H3'       | 12:7:8:4SU:H5''     | 2.00                     | 0.42              |
| 15:A:46:GLU:O      | 15:A:47:PRO:C       | 2.61                     | 0.42              |
| 16:AA:69:ARG:HD2   | 16:AA:168:ALA:HB1   | 2.00                     | 0.42              |
| 23:H:34:ARG:HG2    | 23:H:34:ARG:NH1     | 2.34                     | 0.42              |
| 27:L:2:ALA:N       | 27:L:8:ASP:HA       | 2.34                     | 0.42              |
| 47:i:59:ILE:HB     | 47:i:127:VAL:HG23   | 2.01                     | 0.42              |
| 65:14:201:ASN:HA   | 65:14:483:ARG:NH2   | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:15:51:ASN:ND2   | 66:15:651:TYR:CE2  | 2.87                     | 0.42              |
| 66:15:714:PRO:HG2  | 66:15:761:ILE:CG2  | 2.48                     | 0.42              |
| 5:12:87:THR:C      | 6:17:14:LYS:HB3    | 2.43                     | 0.42              |
| 5:12:96:LEU:HD22   | 6:17:661:LEU:HD12  | 1.99                     | 0.42              |
| 6:17:424:VAL:CG2   | 66:15:171:LYS:HD2  | 2.49                     | 0.42              |
| 8:3:849:C:H1'      | 8:3:1255:G:H21     | 1.83                     | 0.42              |
| 8:3:1071:G:C6      | 8:3:1155:G:C6      | 3.07                     | 0.42              |
| 8:3:1317:C:H2'     | 8:3:1318:U:H6      | 1.84                     | 0.42              |
| 8:3:1566:A:H3'     | 8:3:1567:U:C6      | 2.54                     | 0.42              |
| 8:3:2068:G:H2'     | 8:3:2509:C:O2'     | 2.19                     | 0.42              |
| 8:3:2068:G:OP1     | 41:c:69:LYS:NZ     | 2.29                     | 0.42              |
| 8:3:2522:U:H2'     | 8:3:2523:C:H6      | 1.84                     | 0.42              |
| 10:5:196:G:H2'     | 10:5:197:A:H5''    | 2.01                     | 0.42              |
| 10:5:483:U:H2'     | 10:5:484:A:C8      | 2.54                     | 0.42              |
| 10:5:1026:A:N3     | 10:5:1026:A:H2'    | 2.33                     | 0.42              |
| 15:A:61:GLN:NE2    | 15:A:217:ALA:HA    | 2.34                     | 0.42              |
| 16:AA:110:GLU:HB2  | 16:AA:113:ASN:OD1  | 2.19                     | 0.42              |
| 19:C:34:ILE:HG13   | 19:C:39:GLY:HA2    | 2.01                     | 0.42              |
| 19:C:90:PHE:HA     | 19:C:93:LEU:CD2    | 2.49                     | 0.42              |
| 19:C:123:LEU:HB2   | 19:C:143:ARG:O     | 2.19                     | 0.42              |
| 23:H:54:LEU:HD12   | 23:H:54:LEU:HA     | 1.90                     | 0.42              |
| 41:c:133:PHE:CE2   | 41:c:161:VAL:HG22  | 2.54                     | 0.42              |
| 44:f:51:LEU:HA     | 44:f:54:GLN:HB2    | 2.00                     | 0.42              |
| 49:k:89:LYS:O      | 49:k:89:LYS:HG2    | 2.18                     | 0.42              |
| 59:u:99:LYS:O      | 59:u:100:HIS:C     | 2.61                     | 0.42              |
| 60:v:54:THR:O      | 60:v:58:LEU:HG     | 2.19                     | 0.42              |
| 64:13:765:LEU:HD12 | 64:13:781:LEU:HD11 | 2.01                     | 0.42              |
| 64:13:899:ARG:HH11 | 64:13:1215:LEU:C   | 2.23                     | 0.42              |
| 65:14:166:LEU:HD21 | 65:14:515:PHE:HZ   | 1.78                     | 0.42              |
| 66:15:330:LEU:HD21 | 66:15:488:GLN:CB   | 2.46                     | 0.42              |
| 66:15:1129:LYS:HD3 | 66:15:1204:TYR:CE2 | 2.54                     | 0.42              |
| 67:18:30:GLU:CD    | 67:18:44:TYR:HE2   | 2.27                     | 0.42              |
| 6:17:890:TYR:CE2   | 6:17:894:ASN:ND2   | 2.87                     | 0.42              |
| 8:3:397:G:H2'      | 8:3:398:C:C6       | 2.53                     | 0.42              |
| 8:3:606:G:N2       | 8:3:2038:A:OP1     | 2.51                     | 0.42              |
| 8:3:848:U:H2'      | 8:3:849:C:H6       | 1.85                     | 0.42              |
| 8:3:1635:G:OP1     | 57:s:61:LYS:HE3    | 2.19                     | 0.42              |
| 8:3:1670:U:O2'     | 8:3:1767:A:H1'     | 2.18                     | 0.42              |
| 10:5:196:G:HO2'    | 10:5:197:A:P       | 2.37                     | 0.42              |
| 10:5:348:C:H4'     | 10:5:350:G:OP1     | 2.20                     | 0.42              |
| 14:9:787:LYS:CE    | 61:w:4:ALA:H       | 2.33                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:9:791:LEU:HD22   | 61:w:7:LEU:HG       | 2.01                     | 0.42              |
| 19:C:16:PHE:CD1     | 19:C:190:GLY:HA2    | 2.53                     | 0.42              |
| 19:C:112:SER:O      | 19:C:116:LEU:HG     | 2.19                     | 0.42              |
| 20:E:8:LEU:HD11     | 20:E:57:TYR:CZ      | 2.53                     | 0.42              |
| 22:G:123:MET:HE3    | 22:G:123:MET:HB2    | 1.92                     | 0.42              |
| 24:I:94:LYS:HE3     | 24:I:94:LYS:HB3     | 1.83                     | 0.42              |
| 36:W:18:TRP:CZ3     | 36:W:215:LEU:HD21   | 2.54                     | 0.42              |
| 43:e:18:LEU:HD12    | 43:e:20:PHE:CE1     | 2.54                     | 0.42              |
| 44:f:4:ILE:HA       | 44:f:17:ASP:O       | 2.18                     | 0.42              |
| 66:15:314:PHE:CE2   | 66:15:323:ILE:HD12  | 2.55                     | 0.42              |
| 66:15:996:ASP:HB2   | 66:15:1057:LEU:HD13 | 1.99                     | 0.42              |
| 66:15:1271:ARG:NH2  | 67:16:253:VAL:CG1   | 2.82                     | 0.42              |
| 67:18:238:ALA:O     | 67:18:240:ALA:N     | 2.49                     | 0.42              |
| 5:12:85:TRP:CB      | 6:17:11:TRP:HE3     | 2.30                     | 0.42              |
| 5:12:96:LEU:HD13    | 6:17:661:LEU:C      | 2.09                     | 0.42              |
| 6:17:264:GLU:CB     | 65:14:1094:ASN:O    | 2.60                     | 0.42              |
| 6:17:600:ASN:CB     | 14:9:634:GLU:O      | 2.67                     | 0.42              |
| 8:3:995:A:N6        | 50:l:83:MET:HE1     | 2.34                     | 0.42              |
| 8:3:1431:A:HO2'     | 8:3:1497:A:HO2'     | 1.48                     | 0.42              |
| 8:3:1522:U:H5''     | 8:3:1523:C:H5       | 1.84                     | 0.42              |
| 8:3:1638:C:H2'      | 8:3:1639:C:H6       | 1.83                     | 0.42              |
| 8:3:2521:A:H2'      | 8:3:2522:U:C6       | 2.54                     | 0.42              |
| 8:3:2793:U:H2'      | 8:3:2794:U:C6       | 2.54                     | 0.42              |
| 10:5:595:G:N2       | 22:G:98:TYR:OH      | 2.51                     | 0.42              |
| 10:5:625:U:H2'      | 10:5:626:G:H8       | 1.84                     | 0.42              |
| 14:9:451:GLN:O      | 62:y:56:ALA:CA      | 2.67                     | 0.42              |
| 14:9:714:ILE:HD13   | 14:9:714:ILE:HG21   | 1.80                     | 0.42              |
| 16:AA:131:ILE:HD12  | 16:AA:134:GLY:HA2   | 2.02                     | 0.42              |
| 24:I:44:GLY:HA2     | 24:I:45:PRO:HD3     | 1.89                     | 0.42              |
| 35:T:36:LEU:HD13    | 35:T:40:MET:HG2     | 2.01                     | 0.42              |
| 41:c:14:GLU:HG3     | 41:c:16:GLU:H       | 1.84                     | 0.42              |
| 44:f:131:PHE:HA     | 44:f:140:VAL:O      | 2.18                     | 0.42              |
| 45:g:97:ASP:O       | 45:g:100:VAL:HG23   | 2.19                     | 0.42              |
| 52:n:38:HIS:HB3     | 52:n:57:SER:HB2     | 2.01                     | 0.42              |
| 64:13:1192:LEU:HD22 | 67:18:88:GLN:CG     | 2.21                     | 0.42              |
| 65:14:699:PRO:HD3   | 65:14:706:LEU:HD12  | 2.01                     | 0.42              |
| 66:15:940:PHE:CE1   | 66:15:944:LEU:HD11  | 2.54                     | 0.42              |
| 6:17:386:VAL:CA     | 66:15:175:PRO:N     | 2.81                     | 0.42              |
| 6:17:396:ARG:HD2    | 6:17:399:ARG:NH2    | 2.33                     | 0.42              |
| 6:17:426:LYS:HD3    | 66:15:184:GLN:N     | 2.26                     | 0.42              |
| 8:3:516:A:OP2       | 58:t:44:ARG:HD2     | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:3:698:A:H2'    | 8:3:699:U:C6      | 2.55                     | 0.42              |
| 8:3:887:A:H2'    | 8:3:888:A:C8      | 2.55                     | 0.42              |
| 8:3:995:A:H2'    | 8:3:996:A:C8      | 2.54                     | 0.42              |
| 8:3:1096:U:C5    | 46:h:11:LYS:HG3   | 2.55                     | 0.42              |
| 8:3:1104:A:H4'   | 8:3:1105:A:H2'    | 2.02                     | 0.42              |
| 8:3:1854:A:H3'   | 8:3:1855:A:H8     | 1.85                     | 0.42              |
| 8:3:2310:C:H2'   | 8:3:2311:G:C8     | 2.55                     | 0.42              |
| 8:3:2510:G:H5''  | 8:3:2511:A:H5''   | 2.01                     | 0.42              |
| 10:5:660:A:H2'   | 10:5:661:G:O4'    | 2.20                     | 0.42              |
| 12:7:29:G:H5''   | 27:L:118:ASN:H    | 1.84                     | 0.42              |
| 13:8:43:U:H2'    | 13:8:44:U:C6      | 2.55                     | 0.42              |
| 16:AA:86:MET:HE1 | 17:AB:49:U:C5     | 2.54                     | 0.42              |
| 17:AB:53:A:H2'   | 17:AB:54:A:C8     | 2.54                     | 0.42              |
| 22:G:101:PHE:CD1 | 22:G:101:PHE:C    | 2.98                     | 0.42              |
| 24:I:32:VAL:CG1  | 24:I:36:LYS:HD2   | 2.47                     | 0.42              |
| 25:J:43:MET:HE1  | 25:J:62:LYS:CD    | 2.49                     | 0.42              |
| 43:e:92:LEU:C    | 43:e:92:LEU:HD23  | 2.45                     | 0.42              |
| 46:h:63:PHE:O    | 46:h:65:PHE:CE2   | 2.73                     | 0.42              |
| 54:p:111:LYS:NZ  | 55:q:45:ILE:HG23  | 2.34                     | 0.42              |
| 58:t:47:LYS:H    | 58:t:47:LYS:HD3   | 1.84                     | 0.42              |
| 59:u:55:ARG:HA   | 59:u:55:ARG:HD3   | 1.76                     | 0.42              |
| 64:13:988:GLN:C  | 64:13:990:ALA:H   | 2.27                     | 0.42              |
| 64:13:1002:GLN:C | 64:13:1004:SER:H  | 2.27                     | 0.42              |
| 67:16:243:LYS:C  | 67:16:245:SER:N   | 2.77                     | 0.42              |
| 6:17:387:VAL:N   | 66:15:174:ASP:OD1 | 2.51                     | 0.42              |
| 6:17:703:ASN:C   | 14:9:664:MET:N    | 2.77                     | 0.42              |
| 6:17:703:ASN:CG  | 14:9:663:ASN:OD1  | 2.63                     | 0.42              |
| 6:17:710:PHE:CE2 | 14:9:654:LEU:HD22 | 2.48                     | 0.42              |
| 8:3:60:G:H2'     | 8:3:61:U:C6       | 2.54                     | 0.42              |
| 8:3:102:A:C1'    | 14:9:782:ASP:C    | 2.91                     | 0.42              |
| 8:3:830:A:H2'    | 8:3:831:U:C6      | 2.55                     | 0.42              |
| 8:3:1033:A:OP1   | 54:p:91:ARG:HD2   | 2.20                     | 0.42              |
| 8:3:1054:U:OP1   | 8:3:1070:U:O2'    | 2.23                     | 0.42              |
| 8:3:1306:G:H4'   | 51:m:31:ILE:HD12  | 2.01                     | 0.42              |
| 8:3:1561:G:C4'   | 14:9:299:LYS:CE   | 2.90                     | 0.42              |
| 8:3:2197:U:H2'   | 8:3:2198:G:C8     | 2.54                     | 0.42              |
| 8:3:2599:C:H2'   | 8:3:2600:G:H8     | 1.84                     | 0.42              |
| 10:5:190:A:H2'   | 10:5:191:A:C8     | 2.54                     | 0.42              |
| 10:5:1201:C:P    | 27:L:90:ARG:HH12  | 2.42                     | 0.42              |
| 14:9:340:ALA:HB2 | 14:9:346:ILE:HD11 | 2.02                     | 0.42              |
| 22:G:47:ILE:HG13 | 22:G:48:LEU:N     | 2.33                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:H:21:LEU:HD13  | 23:H:63:PHE:HB3   | 2.01                     | 0.42              |
| 42:d:5:LYS:HD3    | 42:d:97:TRP:CG    | 2.54                     | 0.42              |
| 42:d:5:LYS:HB3    | 42:d:5:LYS:HE3    | 1.91                     | 0.42              |
| 42:d:24:SER:OG    | 42:d:26:MET:SD    | 2.76                     | 0.42              |
| 58:t:25:LEU:HD12  | 58:t:37:GLU:HB3   | 2.01                     | 0.42              |
| 64:13:85:VAL:HG12 | 64:13:95:LYS:HE2  | 2.01                     | 0.42              |
| 65:14:33:LYS:HB3  | 65:14:729:TYR:CZ  | 2.54                     | 0.42              |
| 65:14:313:ALA:HB1 | 65:14:455:PRO:CG  | 2.45                     | 0.42              |
| 66:15:533:LYS:NZ  | 66:15:550:GLU:OE1 | 2.43                     | 0.42              |
| 66:15:1106:SER:OG | 67:16:256:HIS:HE1 | 2.02                     | 0.42              |
| 2:1:20:LYS:HD2    | 2:1:44:GLN:OE1    | 2.20                     | 0.42              |
| 5:12:86:VAL:O     | 6:17:11:TRP:O     | 2.38                     | 0.42              |
| 6:17:390:ALA:CA   | 66:15:71:ARG:HH12 | 2.32                     | 0.42              |
| 6:17:426:LYS:CG   | 66:15:184:GLN:CB  | 2.90                     | 0.42              |
| 6:17:584:ILE:HG12 | 6:17:838:ARG:NH2  | 2.35                     | 0.42              |
| 8:3:125:G:OP1     | 8:3:1404:C:O2'    | 2.31                     | 0.42              |
| 8:3:235:U:H2'     | 8:3:236:G:O4'     | 2.20                     | 0.42              |
| 8:3:628:A:H2'     | 8:3:629:G:H8      | 1.84                     | 0.42              |
| 8:3:1120:A:H2'    | 8:3:1121:A:C4     | 2.54                     | 0.42              |
| 8:3:1125:U:O2     | 8:3:1137:C:H1'    | 2.20                     | 0.42              |
| 8:3:1613:A:H2'    | 8:3:1614:G:O4'    | 2.19                     | 0.42              |
| 8:3:1828:A:H2'    | 8:3:1829:U:C6     | 2.55                     | 0.42              |
| 8:3:2300:A:H2'    | 8:3:2301:C:C6     | 2.55                     | 0.42              |
| 8:3:2691:C:OP1    | 53:o:56:ARG:NH1   | 2.50                     | 0.42              |
| 10:5:335:C:H2'    | 10:5:336:U:C6     | 2.55                     | 0.42              |
| 10:5:474:G:O2'    | 10:5:475:U:H5'    | 2.20                     | 0.42              |
| 10:5:579:G:N1     | 10:5:756:A:OP2    | 2.33                     | 0.42              |
| 10:5:1141:U:O2'   | 10:5:1142:G:H8    | 2.03                     | 0.42              |
| 13:8:44:U:H2'     | 13:8:45:G:O4'     | 2.20                     | 0.42              |
| 19:C:53:GLN:NE2   | 19:C:198:GLU:OE1  | 2.51                     | 0.42              |
| 20:E:36:GLN:OE1   | 20:E:36:GLN:N     | 2.31                     | 0.42              |
| 20:E:112:ARG:HG2  | 20:E:112:ARG:HH11 | 1.84                     | 0.42              |
| 23:H:42:PRO:O     | 23:H:44:LYS:HG2   | 2.20                     | 0.42              |
| 25:J:90:ILE:HD13  | 25:J:90:ILE:HA    | 1.91                     | 0.42              |
| 26:K:114:THR:HG23 | 26:K:115:LEU:N    | 2.35                     | 0.42              |
| 39:a:148:HIS:CD2  | 39:a:203:VAL:HG22 | 2.54                     | 0.42              |
| 40:b:14:SER:OG    | 40:b:15:GLN:N     | 2.52                     | 0.42              |
| 44:f:3:VAL:CG1    | 44:f:21:VAL:HG12  | 2.49                     | 0.42              |
| 47:i:4:THR:HA     | 55:q:12:TYR:HE1   | 1.85                     | 0.42              |
| 47:i:89:LYS:HB2   | 47:i:89:LYS:HE2   | 1.88                     | 0.42              |
| 54:p:65:ASN:O     | 54:p:69:ARG:HG3   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 54:p:73:MET:HG3    | 54:p:74:THR:N       | 2.35                     | 0.42              |
| 59:u:45:ILE:HD13   | 59:u:75:ALA:HB2     | 2.00                     | 0.42              |
| 65:14:507:ASP:OD1  | 65:14:507:ASP:N     | 2.51                     | 0.42              |
| 65:14:587:GLU:HG3  | 65:14:665:PHE:CD1   | 2.54                     | 0.42              |
| 66:15:510:PHE:CD2  | 66:15:511:LEU:HG    | 2.54                     | 0.42              |
| 66:15:1100:ASN:HB2 | 66:15:1117:PHE:CE1  | 2.55                     | 0.42              |
| 6:17:600:ASN:N     | 14:9:641:ARG:HD2    | 2.31                     | 0.42              |
| 6:17:698:SER:H     | 14:9:633:VAL:HG22   | 1.85                     | 0.42              |
| 6:17:845:TRP:HH2   | 14:9:644:LYS:HA     | 1.85                     | 0.42              |
| 8:3:86:A:C2        | 8:3:104:A:C5        | 3.08                     | 0.42              |
| 8:3:354:C:HO2'     | 8:3:356:A:H8        | 1.67                     | 0.42              |
| 8:3:449:C:H2'      | 8:3:450:C:C6        | 2.54                     | 0.42              |
| 8:3:528:U:H2'      | 8:3:529:G:C8        | 2.54                     | 0.42              |
| 8:3:1093:U:H3      | 8:3:1115:G:N2       | 2.18                     | 0.42              |
| 8:3:1495:A:H2'     | 8:3:1496:A:C8       | 2.55                     | 0.42              |
| 8:3:1562:A:H5'     | 14:9:299:LYS:HA     | 2.01                     | 0.42              |
| 8:3:1798:A:H2      | 8:3:1836:A:H4'      | 1.80                     | 0.42              |
| 8:3:2807:G:N3      | 8:3:2808:A:C8       | 2.87                     | 0.42              |
| 9:4:37:A:H2'       | 9:4:38:U:C6         | 2.55                     | 0.42              |
| 10:5:140:U:H2'     | 10:5:141:A:C8       | 2.55                     | 0.42              |
| 10:5:147:A:H2'     | 10:5:148:A:C8       | 2.55                     | 0.42              |
| 10:5:207:C:H2'     | 10:5:208:A:O4'      | 2.20                     | 0.42              |
| 10:5:403:A:H2'     | 10:5:404:A:H8       | 1.82                     | 0.42              |
| 10:5:712:A:H2'     | 10:5:713:A:C8       | 2.55                     | 0.42              |
| 10:5:909:A:O2'     | 10:5:911:G:H5''     | 2.20                     | 0.42              |
| 10:5:1273:A:H2'    | 10:5:1273:A:N3      | 2.34                     | 0.42              |
| 18:AC:92:ARG:HB3   | 24:I:106:PHE:CD1    | 2.54                     | 0.42              |
| 24:I:46:LEU:HG     | 24:I:79:LEU:HB3     | 2.02                     | 0.42              |
| 40:b:186:GLU:H     | 40:b:186:GLU:CD     | 2.28                     | 0.42              |
| 42:d:24:SER:HB3    | 42:d:27:GLN:HG3     | 2.02                     | 0.42              |
| 43:e:18:LEU:HA     | 43:e:26:ALA:O       | 2.20                     | 0.42              |
| 48:j:51:MET:HG3    | 48:j:52:VAL:N       | 2.35                     | 0.42              |
| 50:l:41:TRP:NE1    | 50:l:96:VAL:HG22    | 2.35                     | 0.42              |
| 64:13:385:SER:HB2  | 64:13:420:LYS:HB2   | 2.01                     | 0.42              |
| 65:14:863:LYS:CE   | 65:14:1224:GLU:HA   | 2.46                     | 0.42              |
| 65:14:877:PHE:CE1  | 65:14:1217:GLN:HG3  | 2.55                     | 0.42              |
| 66:15:990:SER:HB3  | 66:15:1248:LEU:HD23 | 2.02                     | 0.42              |
| 67:16:8:ASN:O      | 67:16:29:LYS:HD3    | 2.20                     | 0.42              |
| 67:16:21:LYS:NZ    | 67:16:76:GLU:CD     | 2.77                     | 0.42              |
| 67:16:105:TRP:CZ3  | 67:16:152:TYR:HD2   | 2.19                     | 0.42              |
| 6:17:709:ASP:N     | 14:9:670:PRO:CB     | 2.79                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:17:712:ILE:H     | 14:9:674:GLU:HA    | 1.85                     | 0.42              |
| 8:3:610:G:H5''     | 8:3:2510:G:C2      | 2.55                     | 0.42              |
| 8:3:1097:G:H3'     | 8:3:1098:G:H8      | 1.84                     | 0.42              |
| 8:3:2022:A:C2      | 62:y:3:VAL:HB      | 2.55                     | 0.42              |
| 8:3:2088:U:H2'     | 8:3:2089:A:H8      | 1.85                     | 0.42              |
| 8:3:2267:G:C8      | 8:3:2435:C:C4      | 3.08                     | 0.42              |
| 8:3:2357:G:O6      | 8:3:2377:A:N6      | 2.53                     | 0.42              |
| 14:9:808:GLN:OE1   | 57:s:96:GLU:HG2    | 2.19                     | 0.42              |
| 15:A:22:LYS:NZ     | 15:A:251:ASP:HA    | 2.34                     | 0.42              |
| 17:AB:41:U:O2'     | 37:Y:41:U:O2       | 2.28                     | 0.42              |
| 20:E:47:TYR:OH     | 32:Q:94:ARG:O      | 2.24                     | 0.42              |
| 39:a:220:ARG:HD2   | 39:a:224:ILE:O     | 2.20                     | 0.42              |
| 40:b:51:LEU:HA     | 40:b:83:GLU:HA     | 2.00                     | 0.42              |
| 41:c:39:LEU:HD13   | 49:k:13:ARG:HH12   | 1.84                     | 0.42              |
| 43:e:110:LEU:HG    | 43:e:155:ARG:HG3   | 2.02                     | 0.42              |
| 47:i:20:ILE:HG22   | 47:i:142:THR:HG23  | 2.02                     | 0.42              |
| 56:r:24:ILE:HG21   | 56:r:36:LEU:HD13   | 2.02                     | 0.42              |
| 62:y:9:SER:HB2     | 62:y:11:HIS:CD2    | 2.55                     | 0.42              |
| 64:13:356:VAL:CG2  | 64:13:362:VAL:HG21 | 2.46                     | 0.42              |
| 64:13:412:GLN:HG3  | 64:13:438:ASN:OD1  | 2.20                     | 0.42              |
| 64:13:1217:LYS:HE2 | 67:18:274:PRO:HB2  | 2.01                     | 0.42              |
| 65:14:325:GLU:OE1  | 65:14:451:SER:HB3  | 2.18                     | 0.42              |
| 66:15:178:GLU:CD   | 66:15:632:LYS:HD3  | 2.44                     | 0.42              |
| 67:18:202:SER:OG   | 67:18:204:HIS:CE1  | 2.69                     | 0.42              |
| 67:18:249:GLY:O    | 67:18:251:PHE:N    | 2.52                     | 0.42              |
| 67:16:128:ASN:O    | 67:16:136:LYS:NZ   | 2.52                     | 0.42              |
| 6:17:693:THR:HA    | 14:9:685:THR:HB    | 2.01                     | 0.42              |
| 6:17:696:ASN:O     | 14:9:658:LEU:CD2   | 2.68                     | 0.42              |
| 6:17:707:GLN:C     | 14:9:670:PRO:HB3   | 2.45                     | 0.42              |
| 6:17:767:MET:HE1   | 6:17:805:PHE:CE1   | 2.55                     | 0.42              |
| 8:3:11:U:C4        | 8:3:2637:A:C4      | 3.08                     | 0.42              |
| 8:3:741:A:H4'      | 39:a:7:ILE:HD13    | 2.02                     | 0.42              |
| 8:3:1007:C:O2      | 8:3:1019:A:H2      | 2.03                     | 0.42              |
| 8:3:1009:A:H5'     | 8:3:1219:U:H1'     | 2.01                     | 0.42              |
| 8:3:1092:A:N7      | 8:3:1121:A:H2'     | 2.35                     | 0.42              |
| 8:3:1121:A:O2'     | 8:3:1122:G:N7      | 2.49                     | 0.42              |
| 8:3:1125:U:H2'     | 8:3:1126:G:H8      | 1.82                     | 0.42              |
| 8:3:1639:C:H2'     | 8:3:1640:G:O4'     | 2.19                     | 0.42              |
| 8:3:2161:G:H2'     | 8:3:2162:U:C6      | 2.55                     | 0.42              |
| 8:3:2310:C:H2'     | 8:3:2311:G:H8      | 1.85                     | 0.42              |
| 8:3:2313:U:H3      | 42:d:151:GLY:H     | 1.68                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:3:2794:U:H2'    | 8:3:2795:C:H6      | 1.84                     | 0.42              |
| 8:3:2893:C:H2'    | 8:3:2894:G:O4'     | 2.20                     | 0.42              |
| 10:5:1388:A:H2    | 10:5:1462:G:H22    | 1.68                     | 0.42              |
| 16:AA:138:HIS:O   | 16:AA:202:GLN:NE2  | 2.53                     | 0.42              |
| 30:O:80:LYS:N     | 30:O:80:LYS:HD3    | 2.35                     | 0.42              |
| 36:W:127:ILE:HD13 | 36:W:127:ILE:N     | 2.35                     | 0.42              |
| 39:a:182:LEU:HD23 | 39:a:182:LEU:HA    | 1.85                     | 0.42              |
| 40:b:26:ILE:HD13  | 40:b:192:LEU:HG    | 2.02                     | 0.42              |
| 40:b:139:TYR:HB3  | 40:b:140:PRO:HD3   | 2.02                     | 0.42              |
| 44:f:68:LEU:CG    | 44:f:108:LEU:HD21  | 2.50                     | 0.42              |
| 45:g:93:LEU:HA    | 45:g:96:VAL:HG22   | 2.02                     | 0.42              |
| 45:g:122:ASP:HA   | 45:g:125:LYS:HG3   | 2.01                     | 0.42              |
| 48:j:71:ARG:HH22  | 48:j:104:ARG:NH1   | 2.18                     | 0.42              |
| 48:j:112:ASN:HA   | 48:j:115:LEU:HD12  | 2.00                     | 0.42              |
| 64:13:850:TYR:CZ  | 64:13:974:PHE:HB2  | 2.55                     | 0.42              |
| 64:13:1062:ARG:NE | 67:18:73:VAL:CG2   | 2.78                     | 0.42              |
| 66:15:289:ASP:OD2 | 66:15:538:LYS:HD2  | 2.19                     | 0.42              |
| 66:15:363:ASP:CG  | 66:15:424:HIS:CD2  | 2.97                     | 0.42              |
| 6:17:80:GLY:N     | 65:14:1271:ILE:CD1 | 2.82                     | 0.41              |
| 6:17:100:TYR:CE1  | 6:17:177:ILE:HG23  | 2.55                     | 0.41              |
| 6:17:511:ARG:NH1  | 6:17:902:ILE:HD12  | 2.36                     | 0.41              |
| 6:17:526:ILE:HG23 | 6:17:886:LEU:HD22  | 2.02                     | 0.41              |
| 6:17:593:PHE:CZ   | 6:17:597:ILE:HD11  | 2.54                     | 0.41              |
| 8:3:98:C:OP1      | 61:w:40:LYS:NZ     | 2.53                     | 0.41              |
| 8:3:609:U:H2'     | 8:3:610:G:C8       | 2.55                     | 0.41              |
| 8:3:1208:A:H2'    | 8:3:1209:U:H4'     | 2.01                     | 0.41              |
| 8:3:1836:A:H3'    | 8:3:1837:C:C6      | 2.55                     | 0.41              |
| 8:3:2228:U:H2'    | 8:3:2229:C:C6      | 2.54                     | 0.41              |
| 8:3:2797:C:H4'    | 8:3:2895:A:H2      | 1.84                     | 0.41              |
| 9:4:46:C:OP1      | 52:n:96:SER:HB3    | 2.19                     | 0.41              |
| 9:4:49:G:OP2      | 52:n:66:ASN:ND2    | 2.53                     | 0.41              |
| 10:5:1023:G:O2'   | 10:5:1024:U:H5''   | 2.20                     | 0.41              |
| 10:5:1241:G:H21   | 10:5:1243:A:H8     | 1.67                     | 0.41              |
| 13:8:61:C:O2'     | 13:8:62:C:H5'      | 2.20                     | 0.41              |
| 15:A:84:PHE:N     | 15:A:84:PHE:HD1    | 2.17                     | 0.41              |
| 15:A:119:ASN:CG   | 15:A:119:ASN:O     | 2.63                     | 0.41              |
| 16:AA:187:THR:O   | 16:AA:191:MET:HG3  | 2.19                     | 0.41              |
| 23:H:93:ASN:OD1   | 23:H:93:ASN:O      | 2.38                     | 0.41              |
| 23:H:93:ASN:CG    | 23:H:96:LEU:HD13   | 2.45                     | 0.41              |
| 25:J:86:LYS:HB2   | 25:J:86:LYS:HE3    | 1.77                     | 0.41              |
| 28:M:10:GLN:HG3   | 28:M:23:ARG:HG3    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:W:172:ILE:O     | 36:W:173:GLU:HG2    | 2.20                     | 0.41              |
| 36:W:186:ASP:HB3   | 36:W:205:ILE:HG22   | 2.01                     | 0.41              |
| 49:k:127:GLU:OE1   | 49:k:149:LEU:HD13   | 2.20                     | 0.41              |
| 61:w:39:ASP:O      | 61:w:41:PRO:HD3     | 2.19                     | 0.41              |
| 64:13:55:GLU:OE1   | 64:13:74:LYS:NZ     | 2.47                     | 0.41              |
| 64:13:1151:PHE:HD2 | 64:13:1171:ILE:HD11 | 1.83                     | 0.41              |
| 65:14:610:ILE:H    | 66:15:248:THR:CB    | 2.30                     | 0.41              |
| 6:17:43:GLY:CA     | 6:17:46:PHE:CE2     | 3.01                     | 0.41              |
| 6:17:256:THR:OG1   | 65:14:1100:THR:C    | 2.63                     | 0.41              |
| 6:17:275:ASN:CB    | 65:14:1126:LEU:N    | 2.76                     | 0.41              |
| 6:17:432:LYS:HE2   | 66:15:556:GLN:OE1   | 2.19                     | 0.41              |
| 6:17:696:ASN:CA    | 14:9:685:THR:C      | 2.62                     | 0.41              |
| 7:2:1:MET:HE3      | 8:3:2750:A:H5''     | 2.02                     | 0.41              |
| 8:3:87:G:O2'       | 8:3:104:A:N1        | 2.37                     | 0.41              |
| 8:3:158:U:H2'      | 8:3:159:G:H8        | 1.85                     | 0.41              |
| 8:3:279:U:H2'      | 8:3:280:A:C8        | 2.55                     | 0.41              |
| 8:3:381:A:H2'      | 8:3:382:U:C6        | 2.55                     | 0.41              |
| 8:3:788:G:H2'      | 8:3:789:A:C8        | 2.48                     | 0.41              |
| 8:3:963:U:H2'      | 8:3:964:A:C8        | 2.54                     | 0.41              |
| 8:3:1098:G:H2'     | 8:3:1099:C:H6       | 1.85                     | 0.41              |
| 8:3:1119:A:C8      | 45:g:53:VAL:CG2     | 3.01                     | 0.41              |
| 8:3:1227:C:H2'     | 8:3:1228:G:H8       | 1.85                     | 0.41              |
| 8:3:1341:U:H2'     | 8:3:1644:A:C2       | 2.55                     | 0.41              |
| 8:3:1838:A:H2'     | 8:3:1839:C:C6       | 2.54                     | 0.41              |
| 8:3:2460:C:H2'     | 8:3:2461:A:C8       | 2.56                     | 0.41              |
| 9:4:47:C:N4        | 9:4:48:A:H62        | 2.18                     | 0.41              |
| 9:4:56:A:C5        | 9:4:57:G:C8         | 3.08                     | 0.41              |
| 10:5:145:G:O2'     | 10:5:147:A:N6       | 2.41                     | 0.41              |
| 10:5:1053:U:H2'    | 10:5:1054:C:C6      | 2.56                     | 0.41              |
| 12:7:10:G:H2'      | 12:7:11:C:C6        | 2.55                     | 0.41              |
| 16:AA:154:ALA:HB3  | 16:AA:177:ASP:HB2   | 2.01                     | 0.41              |
| 21:F:91:PRO:O      | 21:F:95:LYS:HB2     | 2.19                     | 0.41              |
| 39:a:151:GLU:HG2   | 39:a:157:GLY:C      | 2.45                     | 0.41              |
| 43:e:20:PHE:CD1    | 43:e:25:ILE:HG12    | 2.55                     | 0.41              |
| 50:l:42:ILE:HD11   | 50:l:47:ILE:HD11    | 2.02                     | 0.41              |
| 56:r:22:GLN:HE21   | 56:r:22:GLN:HB3     | 1.63                     | 0.41              |
| 60:v:48:ILE:H      | 60:v:48:ILE:HG12    | 1.65                     | 0.41              |
| 64:13:928:VAL:HG21 | 64:13:1034:THR:HG23 | 2.01                     | 0.41              |
| 65:14:345:THR:HG23 | 65:14:380:LYS:HZ2   | 1.84                     | 0.41              |
| 65:14:806:VAL:HG23 | 65:14:944:PHE:CE2   | 2.55                     | 0.41              |
| 66:15:107:ASP:HB3  | 66:15:803:ILE:CD1   | 2.50                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 66:15:842:THR:O     | 66:15:848:LYS:HD2  | 2.20                     | 0.41              |
| 5:12:96:LEU:CB      | 6:17:664:ILE:HB    | 2.48                     | 0.41              |
| 6:17:596:ASN:O      | 14:9:641:ARG:HD3   | 2.20                     | 0.41              |
| 6:17:600:ASN:OD1    | 14:9:678:PHE:HZ    | 2.03                     | 0.41              |
| 6:17:693:THR:OG1    | 14:9:682:VAL:HG22  | 0.71                     | 0.41              |
| 6:17:711:PHE:HE1    | 14:9:642:ASN:ND2   | 2.01                     | 0.41              |
| 8:3:31:U:C2         | 8:3:32:G:C8        | 3.08                     | 0.41              |
| 8:3:337:U:H2'       | 8:3:338:G:H8       | 1.85                     | 0.41              |
| 8:3:933:A:O2'       | 13:8:56:C:N3       | 2.52                     | 0.41              |
| 8:3:1003:U:H2'      | 8:3:1004:U:C6      | 2.55                     | 0.41              |
| 8:3:1560:U:H5'      | 14:9:249:ASP:OD1   | 2.06                     | 0.41              |
| 8:3:2109:A:N6       | 8:3:2196:G:O6      | 2.52                     | 0.41              |
| 10:5:1074:U:O2'     | 10:5:1093:A:OP2    | 2.35                     | 0.41              |
| 10:5:1199:U:O2'     | 10:5:1296:C:OP1    | 2.37                     | 0.41              |
| 18:AC:100:LEU:O     | 24:I:94:LYS:HE3    | 2.20                     | 0.41              |
| 19:C:111:ARG:HG2    | 19:C:111:ARG:HH11  | 1.85                     | 0.41              |
| 20:E:90:LEU:HD23    | 32:Q:50:ARG:NH2    | 2.36                     | 0.41              |
| 28:M:31:ARG:H       | 28:M:31:ARG:HG2    | 1.70                     | 0.41              |
| 35:T:35:HIS:C       | 35:T:36:LEU:HD23   | 2.45                     | 0.41              |
| 36:W:89:THR:HG23    | 36:W:102:LEU:HD23  | 2.02                     | 0.41              |
| 44:f:41:LYS:HE2     | 44:f:46:ASP:HB3    | 2.01                     | 0.41              |
| 45:g:32:MET:SD      | 45:g:106:MET:HE1   | 2.60                     | 0.41              |
| 46:h:118:GLU:O      | 46:h:122:LYS:HG2   | 2.20                     | 0.41              |
| 49:k:47:THR:OG1     | 49:k:48:ARG:N      | 2.50                     | 0.41              |
| 50:l:47:ILE:HA      | 50:l:47:ILE:HD13   | 1.76                     | 0.41              |
| 52:n:65:GLY:HA2     | 52:n:101:ARG:HH11  | 1.85                     | 0.41              |
| 54:p:82:LEU:HD23    | 54:p:87:ILE:HB     | 2.02                     | 0.41              |
| 56:r:55:ILE:O       | 56:r:59:THR:HG23   | 2.21                     | 0.41              |
| 18:x:40:GLY:HA2     | 18:x:46:TYR:CE2    | 2.55                     | 0.41              |
| 64:13:10:GLN:CA     | 67:18:197:ASN:ND2  | 2.78                     | 0.41              |
| 64:13:90:SER:OG     | 64:13:95:LYS:HA    | 2.19                     | 0.41              |
| 66:15:1149:THR:HG21 | 66:15:1154:GLU:HB2 | 2.02                     | 0.41              |
| 2:1:10:ARG:HG2      | 49:k:64:LYS:HA     | 2.02                     | 0.41              |
| 5:12:85:TRP:CD1     | 6:17:9:PHE:CA      | 2.67                     | 0.41              |
| 6:17:385:ASP:HB3    | 66:15:175:PRO:HG3  | 0.97                     | 0.41              |
| 8:3:9:G:O4'         | 47:i:138:GLN:NE2   | 2.53                     | 0.41              |
| 8:3:764:G:OP1       | 39:a:10:SER:OG     | 2.38                     | 0.41              |
| 8:3:935:U:H3'       | 8:3:936:G:C8       | 2.55                     | 0.41              |
| 8:3:988:G:O6        | 8:3:1002:A:N6      | 2.54                     | 0.41              |
| 8:3:1089:A:O2'      | 45:g:29:TYR:O      | 2.38                     | 0.41              |
| 8:3:1095:U:N3       | 8:3:1097:G:O4'     | 2.53                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:3:1125:U:C2     | 8:3:1137:C:H1'     | 2.56                     | 0.41              |
| 8:3:1433:U:H2'    | 8:3:1434:U:H6      | 1.85                     | 0.41              |
| 8:3:1573:A:H2'    | 8:3:1574:G:O4'     | 2.20                     | 0.41              |
| 8:3:1673:U:O2'    | 8:3:2707:A:H4'     | 2.21                     | 0.41              |
| 8:3:1915:C:O2'    | 12:7:12:U:H5''     | 2.19                     | 0.41              |
| 8:3:1950:U:O4'    | 8:3:1952:G:H5'     | 2.20                     | 0.41              |
| 8:3:2200:U:H2'    | 8:3:2201:G:H5'     | 2.02                     | 0.41              |
| 8:3:2247:G:H5'    | 39:a:259:GLY:HA3   | 2.03                     | 0.41              |
| 8:3:2458:A:O2'    | 12:7:76:A:N1       | 2.47                     | 0.41              |
| 10:5:421:G:H5''   | 10:5:422:A:OP2     | 2.21                     | 0.41              |
| 10:5:1157:G:H4'   | 10:5:1158:A:H5'    | 2.03                     | 0.41              |
| 10:5:1197:G:OP2   | 10:5:1296:C:N4     | 2.50                     | 0.41              |
| 10:5:1201:C:OP2   | 27:L:90:ARG:NH1    | 2.53                     | 0.41              |
| 13:8:28:U:H2'     | 13:8:29:U:H6       | 1.84                     | 0.41              |
| 15:A:113:LEU:O    | 15:A:116:THR:OG1   | 2.38                     | 0.41              |
| 15:A:192:ASN:HD21 | 15:A:210:LEU:HA    | 1.85                     | 0.41              |
| 21:F:30:MET:HE1   | 21:F:35:LYS:HE3    | 2.02                     | 0.41              |
| 23:H:89:LEU:HD23  | 23:H:89:LEU:HA     | 1.82                     | 0.41              |
| 27:L:80:LEU:HD21  | 27:L:87:ARG:HG2    | 2.01                     | 0.41              |
| 42:d:119:LEU:N    | 42:d:119:LEU:HD13  | 2.35                     | 0.41              |
| 43:e:92:LEU:CD2   | 43:e:97:TYR:CB     | 2.96                     | 0.41              |
| 44:f:6:LYS:HE3    | 44:f:37:ALA:HB2    | 2.01                     | 0.41              |
| 46:h:72:VAL:HG12  | 46:h:108:LYS:HD3   | 2.02                     | 0.41              |
| 50:l:109:ILE:HG12 | 50:l:110:PRO:HD2   | 2.01                     | 0.41              |
| 51:m:56:ASN:O     | 51:m:60:ARG:HG2    | 2.21                     | 0.41              |
| 52:n:93:THR:C     | 52:n:95:GLY:H      | 2.29                     | 0.41              |
| 53:o:95:LYS:HA    | 53:o:95:LYS:HD2    | 1.75                     | 0.41              |
| 55:q:77:LYS:HA    | 55:q:77:LYS:HD3    | 1.82                     | 0.41              |
| 57:s:25:LYS:CE    | 57:s:90:ALA:HB2    | 2.41                     | 0.41              |
| 18:x:46:TYR:CD1   | 18:x:46:TYR:N      | 2.88                     | 0.41              |
| 64:13:398:GLN:HA  | 64:13:414:LYS:NZ   | 2.32                     | 0.41              |
| 66:15:871:LYS:HB2 | 66:15:897:VAL:HG11 | 2.03                     | 0.41              |
| 66:15:881:ARG:NH2 | 66:15:1274:LEU:HB3 | 2.32                     | 0.41              |
| 67:16:250:SER:O   | 67:16:252:GLY:N    | 2.51                     | 0.41              |
| 6:17:390:ALA:CA   | 66:15:71:ARG:NH1   | 2.81                     | 0.41              |
| 6:17:440:PHE:CE1  | 6:17:456:PHE:CD1   | 3.09                     | 0.41              |
| 8:3:402:A:H8      | 8:3:402:A:OP2      | 2.03                     | 0.41              |
| 8:3:776:U:H2'     | 8:3:777:C:C6       | 2.55                     | 0.41              |
| 8:3:1073:A:H2'    | 8:3:1074:A:C8      | 2.55                     | 0.41              |
| 8:3:1081:A:C2     | 45:g:61:ARG:HD2    | 2.55                     | 0.41              |
| 8:3:1671:C:H2'    | 8:3:1672:C:C6      | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:3:1780:A:N7      | 8:3:1836:A:H1'     | 2.36                     | 0.41              |
| 8:3:2892:U:H2'     | 8:3:2893:C:C6      | 2.56                     | 0.41              |
| 10:5:527:G:H22     | 26:K:61:ALA:HB2    | 1.85                     | 0.41              |
| 10:5:825:A:N3      | 15:A:39:PRO:HG2    | 2.35                     | 0.41              |
| 10:5:1027:A:H2'    | 10:5:1028:C:O4'    | 2.19                     | 0.41              |
| 14:9:87:GLN:HE22   | 14:9:110:LEU:HD23  | 1.85                     | 0.41              |
| 14:9:223:LEU:HA    | 14:9:328:ARG:HH21  | 1.86                     | 0.41              |
| 14:9:760:MET:HE2   | 14:9:760:MET:HB3   | 1.91                     | 0.41              |
| 16:AA:206:ARG:O    | 16:AA:210:ILE:HG12 | 2.21                     | 0.41              |
| 24:I:59:ARG:CZ     | 24:I:69:GLU:HB3    | 2.50                     | 0.41              |
| 25:J:21:ASN:O      | 25:J:21:ASN:ND2    | 2.30                     | 0.41              |
| 26:K:78:THR:HG21   | 26:K:95:LEU:HD22   | 2.02                     | 0.41              |
| 27:L:79:HIS:CE1    | 27:L:83:ILE:HD11   | 2.55                     | 0.41              |
| 35:T:13:LEU:CD1    | 35:T:17:LYS:HE2    | 2.50                     | 0.41              |
| 46:h:99:ALA:HA     | 46:h:102:LYS:HG2   | 2.03                     | 0.41              |
| 53:o:2:LYS:HA      | 53:o:2:LYS:HD3     | 1.88                     | 0.41              |
| 58:t:47:LYS:HE2    | 58:t:47:LYS:HB2    | 1.73                     | 0.41              |
| 64:13:149:PRO:HB3  | 66:15:1168:VAL:CA  | 2.35                     | 0.41              |
| 67:18:105:TRP:CZ3  | 67:18:152:TYR:HD2  | 2.18                     | 0.41              |
| 1:0:7:PRO:HG2      | 8:3:1337:G:H4'     | 2.03                     | 0.41              |
| 8:3:859:G:H2'      | 8:3:860:C:C6       | 2.56                     | 0.41              |
| 8:3:863:U:O2'      | 8:3:866:G:O6       | 2.39                     | 0.41              |
| 8:3:1130:A:H3'     | 8:3:1131:A:H8      | 1.85                     | 0.41              |
| 8:3:1487:U:H2'     | 8:3:1488:U:C6      | 2.56                     | 0.41              |
| 8:3:2303:U:O2'     | 8:3:2304:U:H5'     | 2.19                     | 0.41              |
| 10:5:196:G:H5'     | 34:S:49:SER:HA     | 2.02                     | 0.41              |
| 14:9:163:PRO:HB2   | 58:t:63:VAL:H      | 1.84                     | 0.41              |
| 16:AA:66:PHE:CE2   | 16:AA:96:ASN:HB3   | 2.56                     | 0.41              |
| 16:AA:161:ILE:HG22 | 16:AA:161:ILE:O    | 2.20                     | 0.41              |
| 18:AC:66:PHE:CZ    | 33:R:68:GLY:HA2    | 2.54                     | 0.41              |
| 34:S:68:LEU:HD23   | 34:S:68:LEU:HA     | 1.87                     | 0.41              |
| 40:b:56:THR:HA     | 40:b:78:THR:HA     | 2.01                     | 0.41              |
| 42:d:118:SER:O     | 42:d:119:LEU:HB2   | 2.20                     | 0.41              |
| 42:d:175:LEU:HG    | 42:d:177:LEU:HD21  | 2.03                     | 0.41              |
| 46:h:72:VAL:O      | 46:h:73:SER:OG     | 2.32                     | 0.41              |
| 55:q:33:ILE:HD12   | 55:q:33:ILE:HA     | 1.94                     | 0.41              |
| 58:t:55:ALA:HA     | 58:t:58:GLN:HB2    | 2.02                     | 0.41              |
| 64:13:646:LEU:HD23 | 64:13:690:ASN:OD1  | 2.20                     | 0.41              |
| 65:14:1036:GLN:OE1 | 66:15:155:LYS:NZ   | 2.54                     | 0.41              |
| 66:15:834:ASN:ND2  | 66:15:950:ASP:HA   | 2.34                     | 0.41              |
| 66:15:940:PHE:CZ   | 66:15:944:LEU:HD11 | 2.55                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 67:16:195:LYS:CE    | 67:16:199:ASP:OD1  | 2.68                     | 0.41              |
| 3:10:301:ILE:HB     | 3:10:302:PRO:HD3   | 2.01                     | 0.41              |
| 6:17:278:ALA:CB     | 66:15:170:SER:O    | 2.68                     | 0.41              |
| 6:17:699:ILE:HG21   | 14:9:689:ILE:O     | 2.20                     | 0.41              |
| 6:17:706:ILE:C      | 14:9:655:SER:CB    | 2.94                     | 0.41              |
| 6:17:845:TRP:CH2    | 14:9:644:LYS:HA    | 2.55                     | 0.41              |
| 8:3:66:A:H2'        | 8:3:67:C:C6        | 2.55                     | 0.41              |
| 8:3:304:U:C2        | 8:3:401:G:N2       | 2.88                     | 0.41              |
| 8:3:749:U:H1'       | 8:3:752:C:H5       | 1.86                     | 0.41              |
| 8:3:899:A:H2'       | 8:3:900:G:H8       | 1.86                     | 0.41              |
| 8:3:1806:G:C2       | 39:a:160:ILE:HG23  | 2.55                     | 0.41              |
| 8:3:1994:U:H2'      | 8:3:1995:G:H8      | 1.86                     | 0.41              |
| 8:3:2011:G:C4       | 8:3:2012:A:C8      | 3.09                     | 0.41              |
| 8:3:2098:U:H1'      | 60:v:34:GLN:NE2    | 2.36                     | 0.41              |
| 8:3:2316:G:N3       | 8:3:2316:G:H2'     | 2.35                     | 0.41              |
| 8:3:2406:U:H2'      | 8:3:2407:G:C8      | 2.56                     | 0.41              |
| 8:3:2681:G:H2'      | 8:3:2682:A:H8      | 1.85                     | 0.41              |
| 8:3:2794:U:H2'      | 8:3:2795:C:C6      | 2.56                     | 0.41              |
| 10:5:507:A:H5''     | 19:C:51:ALA:HB2    | 2.01                     | 0.41              |
| 10:5:823:C:H1'      | 22:G:24:ASN:HD22   | 1.85                     | 0.41              |
| 10:5:953:A:N6       | 33:R:77:THR:O      | 2.54                     | 0.41              |
| 10:5:1071:A:H5''    | 16:AA:76:ILE:HD12  | 2.02                     | 0.41              |
| 10:5:1163:A:O3'     | 28:M:58:LYS:NZ     | 2.53                     | 0.41              |
| 12:7:27:G:H2'       | 12:7:28:G:H8       | 1.86                     | 0.41              |
| 14:9:787:LYS:HD3    | 61:w:4:ALA:N       | 2.28                     | 0.41              |
| 19:C:60:MET:HG2     | 19:C:71:PHE:CE2    | 2.55                     | 0.41              |
| 22:G:18:LEU:HD13    | 22:G:41:LYS:HD2    | 2.02                     | 0.41              |
| 27:L:120:LYS:HG2    | 33:R:87:ARG:HE     | 1.86                     | 0.41              |
| 28:M:39:VAL:HG13    | 28:M:43:CYS:HB2    | 2.02                     | 0.41              |
| 30:O:50:ILE:HG23    | 30:O:52:GLU:HG3    | 2.02                     | 0.41              |
| 35:T:19:LYS:HE2     | 35:T:23:LEU:HD21   | 2.02                     | 0.41              |
| 43:e:107:ASN:HB3    | 43:e:117:LYS:HG3   | 2.02                     | 0.41              |
| 46:h:79:ALA:O       | 46:h:100:LYS:NZ    | 2.52                     | 0.41              |
| 47:i:122:ILE:HD12   | 47:i:122:ILE:HA    | 1.82                     | 0.41              |
| 50:l:76:LYS:HB3     | 50:l:91:GLU:HG3    | 2.02                     | 0.41              |
| 57:s:66:ARG:HA      | 57:s:66:ARG:HD2    | 1.55                     | 0.41              |
| 65:14:139:TYR:HB2   | 65:14:497:LEU:HD21 | 2.02                     | 0.41              |
| 65:14:1136:PHE:CE2  | 65:14:1140:ASN:ND2 | 2.89                     | 0.41              |
| 66:15:1155:LEU:HD11 | 66:15:1190:LYS:HG3 | 2.03                     | 0.41              |
| 2:1:28:HIS:HE1      | 8:3:2430:C:C5      | 2.39                     | 0.41              |
| 3:10:90:SER:HB3     | 3:10:91:PRO:HD3    | 2.02                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:12:84:VAL:C       | 6:17:8:SER:N        | 2.79                     | 0.41              |
| 6:17:277:SER:HB2    | 65:14:1123:ASN:C    | 2.46                     | 0.41              |
| 8:3:337:U:H2'       | 8:3:338:G:C8        | 2.56                     | 0.41              |
| 8:3:874:U:H2'       | 8:3:875:G:C8        | 2.56                     | 0.41              |
| 8:3:1048:A:OP1      | 54:p:69:ARG:NH2     | 2.50                     | 0.41              |
| 8:3:1059:G:OP2      | 8:3:1060:G:O2'      | 2.38                     | 0.41              |
| 8:3:1559:A:H2'      | 14:9:247:LYS:CB     | 2.46                     | 0.41              |
| 8:3:1560:U:H2'      | 8:3:1561:G:O4'      | 2.21                     | 0.41              |
| 8:3:1616:G:H2'      | 8:3:1617:U:H5'      | 2.02                     | 0.41              |
| 8:3:2325:U:H2'      | 8:3:2326:G:C8       | 2.55                     | 0.41              |
| 9:4:6:U:H2'         | 9:4:7:G:H8          | 1.86                     | 0.41              |
| 10:5:1026:A:H3'     | 10:5:1027:A:H8      | 1.86                     | 0.41              |
| 10:5:1045:C:H42     | 17:AB:46:G:N2       | 2.19                     | 0.41              |
| 10:5:1473:U:O2'     | 17:AB:41:U:OP1      | 2.35                     | 0.41              |
| 20:E:21:VAL:HG21    | 20:E:58:TYR:CG      | 2.56                     | 0.41              |
| 20:E:42:LEU:HD13    | 20:E:56:HIS:CE1     | 2.55                     | 0.41              |
| 26:K:16:LYS:HE3     | 26:K:16:LYS:HB3     | 1.91                     | 0.41              |
| 32:Q:76:THR:HG22    | 32:Q:78:ASN:OD1     | 2.21                     | 0.41              |
| 32:Q:78:ASN:OD1     | 32:Q:78:ASN:N       | 2.54                     | 0.41              |
| 39:a:12:SER:O       | 39:a:12:SER:OG      | 2.29                     | 0.41              |
| 41:c:7:ILE:HG22     | 41:c:127:LEU:O      | 2.20                     | 0.41              |
| 47:i:39:ILE:HG12    | 47:i:125:VAL:HG22   | 2.02                     | 0.41              |
| 49:k:115:ILE:HD13   | 49:k:115:ILE:HA     | 1.94                     | 0.41              |
| 61:w:33:LEU:HB2     | 61:w:38:LEU:HD12    | 2.03                     | 0.41              |
| 63:z:35:ASN:OD1     | 63:z:35:ASN:N       | 2.54                     | 0.41              |
| 64:13:6:ASN:HD22    | 67:18:198:LEU:HD22  | 1.28                     | 0.41              |
| 64:13:1213:LEU:HD13 | 67:18:276:ASN:HB2   | 2.03                     | 0.41              |
| 65:14:316:LYS:CD    | 65:14:454:GLN:NE2   | 2.84                     | 0.41              |
| 65:14:1118:THR:HG1  | 65:14:1136:PHE:HD2  | 1.68                     | 0.41              |
| 66:15:1256:PRO:CG   | 66:15:1260:LEU:HD23 | 2.51                     | 0.41              |
| 6:17:703:ASN:HD21   | 14:9:789:ASN:HB2    | 1.54                     | 0.41              |
| 8:3:34:C:H2'        | 8:3:35:U:C6         | 2.56                     | 0.41              |
| 8:3:454:G:H2'       | 8:3:455:G:H8        | 1.85                     | 0.41              |
| 8:3:573:A:H2'       | 8:3:574:G:O4'       | 2.21                     | 0.41              |
| 8:3:1077:G:H2'      | 8:3:1078:C:C6       | 2.56                     | 0.41              |
| 8:3:1139:C:H2'      | 8:3:1140:U:C6       | 2.55                     | 0.41              |
| 8:3:1559:A:C2'      | 14:9:247:LYS:CD     | 2.94                     | 0.41              |
| 8:3:1605:A:H2'      | 8:3:1606:A:C8       | 2.56                     | 0.41              |
| 8:3:1640:G:H5''     | 8:3:1641:A:O5'      | 2.21                     | 0.41              |
| 8:3:1816:A:H2'      | 8:3:1817:A:C8       | 2.56                     | 0.41              |
| 8:3:1871:U:OP1      | 8:3:2418:G:O2'      | 2.38                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:3:1906:G:H21    | 8:3:1909:C:N4      | 2.18                     | 0.41              |
| 8:3:2027:G:H5'    | 62:y:9:SER:HB3     | 2.01                     | 0.41              |
| 8:3:2380:U:H2'    | 8:3:2381:G:H8      | 1.86                     | 0.41              |
| 8:3:2688:C:H2'    | 8:3:2689:C:C6      | 2.56                     | 0.41              |
| 8:3:2701:A:H2'    | 8:3:2702:G:C8      | 2.56                     | 0.41              |
| 8:3:2841:A:H2'    | 8:3:2842:G:C8      | 2.56                     | 0.41              |
| 10:5:170:A:O2'    | 10:5:220:U:OP1     | 2.25                     | 0.41              |
| 10:5:525:G7M:O2'  | 10:5:533:A:N1      | 2.46                     | 0.41              |
| 10:5:1343:G:H5''  | 23:H:116:LYS:HB3   | 2.02                     | 0.41              |
| 10:5:1482:A:H2'   | 10:5:1483:C:C6     | 2.56                     | 0.41              |
| 12:7:28:G:H2'     | 12:7:29:G:H8       | 1.86                     | 0.41              |
| 12:7:34:G:C6      | 17:AB:42:C:C4      | 3.09                     | 0.41              |
| 14:9:227:GLY:N    | 58:t:53:LYS:CE     | 2.76                     | 0.41              |
| 14:9:788:ALA:CA   | 61:w:6:GLU:HG3     | 2.46                     | 0.41              |
| 15:A:292:THR:O    | 15:A:293:ARG:HB3   | 2.21                     | 0.41              |
| 19:C:131:THR:HA   | 19:C:132:PRO:HD3   | 1.88                     | 0.41              |
| 19:C:184:ARG:HD2  | 19:C:192:ASN:CG    | 2.46                     | 0.41              |
| 20:E:132:VAL:O    | 20:E:132:VAL:CG1   | 2.69                     | 0.41              |
| 23:H:121:TYR:HB2  | 23:H:125:ARG:HD3   | 2.02                     | 0.41              |
| 23:H:129:PHE:HE1  | 23:H:131:LYS:HB2   | 1.85                     | 0.41              |
| 26:K:86:ASN:HD21  | 26:K:118:VAL:H     | 1.68                     | 0.41              |
| 32:Q:73:ARG:NH1   | 32:Q:79:CYS:HA     | 2.36                     | 0.41              |
| 34:S:11:LEU:O     | 34:S:15:ILE:HG13   | 2.21                     | 0.41              |
| 36:W:70:TYR:HA    | 36:W:107:ASN:O     | 2.20                     | 0.41              |
| 42:d:43:ALA:HA    | 42:d:47:SER:HA     | 2.02                     | 0.41              |
| 42:d:65:PRO:HB2   | 42:d:87:CYS:HB2    | 2.02                     | 0.41              |
| 42:d:177:LEU:HB2  | 42:d:180:GLY:C     | 2.46                     | 0.41              |
| 47:i:18:TRP:HB3   | 47:i:140:PRO:HB3   | 2.02                     | 0.41              |
| 49:k:78:VAL:HG13  | 49:k:112:ILE:HA    | 2.02                     | 0.41              |
| 49:k:82:LEU:HA    | 49:k:85:ILE:HG22   | 2.03                     | 0.41              |
| 50:l:98:LYS:O     | 50:l:101:THR:HG23  | 2.21                     | 0.41              |
| 51:m:57:PHE:O     | 51:m:61:ARG:HG3    | 2.20                     | 0.41              |
| 54:p:10:ARG:HA    | 54:p:10:ARG:HD2    | 1.81                     | 0.41              |
| 54:p:43:LYS:HE2   | 55:q:73:HIS:HB3    | 2.03                     | 0.41              |
| 55:q:44:LYS:O     | 55:q:50:LEU:HD11   | 2.21                     | 0.41              |
| 63:z:21:THR:HG22  | 63:z:22:PHE:H      | 1.86                     | 0.41              |
| 64:13:153:ASP:O   | 64:13:157:LYS:HE3  | 2.21                     | 0.41              |
| 64:13:195:ASP:CA  | 64:13:545:ARG:HH12 | 2.30                     | 0.41              |
| 64:13:197:THR:CG2 | 64:13:507:LEU:HD22 | 2.51                     | 0.41              |
| 64:13:757:PRO:HD3 | 64:13:764:LEU:HD12 | 2.03                     | 0.41              |
| 64:13:899:ARG:HG2 | 64:13:1194:LEU:CD1 | 2.48                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:13:972:ASN:HB3   | 67:18:256:HIS:CE1   | 2.56                     | 0.41              |
| 64:13:1041:TYR:HE2  | 64:13:1066:GLN:OE1  | 2.02                     | 0.41              |
| 65:14:196:PHE:CE1   | 65:14:202:PRO:HG3   | 2.56                     | 0.41              |
| 65:14:862:TYR:CZ    | 65:14:866:LEU:HD11  | 2.56                     | 0.41              |
| 65:14:1281:VAL:CG1  | 65:14:1286:ILE:HB   | 2.51                     | 0.41              |
| 66:15:289:ASP:OD1   | 66:15:528:ARG:NH1   | 2.41                     | 0.41              |
| 66:15:957:ARG:HB3   | 66:15:1273:VAL:HG13 | 2.03                     | 0.41              |
| 66:15:1031:VAL:HG21 | 66:15:1058:LEU:CD1  | 2.49                     | 0.41              |
| 66:15:1162:LEU:HD12 | 66:15:1193:LEU:HD22 | 2.03                     | 0.41              |
| 66:15:1271:ARG:NH2  | 67:16:256:HIS:CD2   | 2.72                     | 0.41              |
| 67:18:117:PRO:HG2   | 67:18:152:TYR:CD1   | 2.56                     | 0.41              |
| 67:16:131:ALA:O     | 67:16:136:LYS:HE3   | 2.21                     | 0.41              |
| 6:17:711:PHE:CE1    | 14:9:648:LEU:HB3    | 2.55                     | 0.41              |
| 6:17:796:ALA:HA     | 6:17:923:LEU:CD2    | 2.51                     | 0.41              |
| 8:3:1351:G:H21      | 8:3:1650:A:H62      | 1.68                     | 0.41              |
| 8:3:1521:A:N3       | 8:3:1611:C:O2'      | 2.44                     | 0.41              |
| 8:3:1620:A:H2'      | 8:3:1621:U:C6       | 2.55                     | 0.41              |
| 8:3:1647:A:H61      | 8:3:1651:C:H2'      | 1.86                     | 0.41              |
| 8:3:1878:A:H3'      | 8:3:1879:A:H8       | 1.85                     | 0.41              |
| 8:3:2406:U:H2'      | 8:3:2407:G:H8       | 1.85                     | 0.41              |
| 10:5:330:C:O2'      | 10:5:1409:A:O2'     | 2.35                     | 0.41              |
| 10:5:459:C:H2'      | 10:5:460:A:O4'      | 2.20                     | 0.41              |
| 10:5:609:G:H8       | 10:5:609:G:O5'      | 2.04                     | 0.41              |
| 10:5:766:G:H4'      | 10:5:1488:A:H4'     | 2.03                     | 0.41              |
| 10:5:870:A:H2'      | 10:5:871:U:C6       | 2.56                     | 0.41              |
| 10:5:971:A:P        | 10:5:1332:U:HO2'    | 2.44                     | 0.41              |
| 10:5:1108:A:O3'     | 23:H:108:ARG:HG2    | 2.20                     | 0.41              |
| 13:8:16:U:H6        | 13:8:16:U:H2'       | 1.70                     | 0.41              |
| 20:E:50:LYS:HD2     | 20:E:50:LYS:HA      | 1.69                     | 0.41              |
| 20:E:184:GLU:H      | 20:E:184:GLU:CD     | 2.29                     | 0.41              |
| 26:K:18:LYS:HE2     | 26:K:18:LYS:HB2     | 1.70                     | 0.41              |
| 31:P:24:VAL:HG21    | 31:P:63:ILE:HD11    | 2.03                     | 0.41              |
| 32:Q:81:MET:HE3     | 32:Q:81:MET:HB2     | 1.94                     | 0.41              |
| 39:a:240:HIS:CE1    | 39:a:249:VAL:HG13   | 2.56                     | 0.41              |
| 44:f:82:LYS:HE2     | 44:f:125:GLU:OE2    | 2.21                     | 0.41              |
| 45:g:43:LYS:HE3     | 45:g:43:LYS:HB3     | 1.86                     | 0.41              |
| 49:k:31:THR:HG22    | 49:k:33:GLY:H       | 1.85                     | 0.41              |
| 52:n:106:ALA:O      | 52:n:110:ARG:HG3    | 2.21                     | 0.41              |
| 54:p:83:LYS:HE3     | 54:p:83:LYS:HB3     | 1.77                     | 0.41              |
| 64:13:639:TYR:CE2   | 64:13:701:LEU:HD11  | 2.56                     | 0.41              |
| 65:14:32:GLN:HG2    | 65:14:685:LYS:HA    | 2.03                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 65:14:338:ASN:O     | 65:14:445:ILE:HD11  | 2.21                     | 0.41              |
| 65:14:1032:GLN:HE22 | 66:15:540:ASN:CG    | 2.26                     | 0.41              |
| 66:15:958:PHE:CB    | 66:15:1273:VAL:HG11 | 2.51                     | 0.41              |
| 66:15:991:TRP:CH2   | 66:15:1260:LEU:HD11 | 2.56                     | 0.41              |
| 67:18:63:ASN:HB2    | 67:18:68:SER:O      | 2.21                     | 0.41              |
| 67:16:243:LYS:O     | 67:16:245:SER:N     | 2.52                     | 0.41              |
| 6:17:385:ASP:HA     | 66:15:65:ASP:CB     | 2.50                     | 0.40              |
| 6:17:387:VAL:HG13   | 66:15:68:ILE:HG12   | 1.95                     | 0.40              |
| 8:3:50:G:H22        | 8:3:180:A:C5'       | 2.30                     | 0.40              |
| 8:3:192:U:H2'       | 8:3:193:G:O4'       | 2.21                     | 0.40              |
| 8:3:412:A:C2        | 8:3:413:G:H1'       | 2.55                     | 0.40              |
| 8:3:1420:A:N6       | 14:9:241:ARG:NH1    | 2.67                     | 0.40              |
| 8:3:1441:A:H2'      | 8:3:1442:G:C8       | 2.56                     | 0.40              |
| 8:3:1512:A:H2'      | 8:3:1513:A:C8       | 2.56                     | 0.40              |
| 8:3:2025:C:H2'      | 8:3:2026:A:H8       | 1.86                     | 0.40              |
| 8:3:2255:A:H2'      | 8:3:2256:C:H6       | 1.86                     | 0.40              |
| 10:5:527:G:O6       | 26:K:59:ASN:HA      | 2.20                     | 0.40              |
| 10:5:870:A:H2'      | 10:5:871:U:H6       | 1.86                     | 0.40              |
| 12:7:35:A:N6        | 17:AB:41:U:N3       | 2.54                     | 0.40              |
| 14:9:184:PHE:HB3    | 58:t:57:LYS:HE2     | 2.01                     | 0.40              |
| 15:A:260:GLN:H      | 15:A:260:GLN:HG3    | 1.75                     | 0.40              |
| 22:G:18:LEU:HD21    | 22:G:45:LEU:HG      | 2.03                     | 0.40              |
| 22:G:27:LYS:HD3     | 22:G:27:LYS:HA      | 1.91                     | 0.40              |
| 44:f:82:LYS:NZ      | 44:f:146:ASN:HB3    | 2.36                     | 0.40              |
| 45:g:51:ILE:HA      | 45:g:82:VAL:O       | 2.20                     | 0.40              |
| 49:k:139:VAL:HG11   | 49:k:146:VAL:HG23   | 2.02                     | 0.40              |
| 64:13:161:TRP:HH2   | 64:13:291:PHE:CZ    | 2.39                     | 0.40              |
| 64:13:216:ILE:CD1   | 64:13:234:PHE:CE2   | 3.04                     | 0.40              |
| 64:13:884:GLU:OE1   | 64:13:898:TYR:OH    | 2.37                     | 0.40              |
| 64:13:1159:LEU:HD22 | 64:13:1176:VAL:HG22 | 2.02                     | 0.40              |
| 65:14:217:ASP:HB2   | 65:14:221:ASN:ND2   | 2.36                     | 0.40              |
| 65:14:228:ILE:HD11  | 65:14:392:VAL:HG13  | 2.03                     | 0.40              |
| 65:14:878:LEU:HD13  | 65:14:1244:LEU:HD21 | 2.03                     | 0.40              |
| 66:15:44:THR:HG23   | 66:15:655:LEU:HD22  | 2.03                     | 0.40              |
| 66:15:839:TRP:CD1   | 66:15:843:ASN:HD22  | 2.38                     | 0.40              |
| 66:15:1240:SER:O    | 66:15:1243:THR:OG1  | 2.26                     | 0.40              |
| 67:18:5:ASP:OD1     | 67:18:35:ARG:NH1    | 2.54                     | 0.40              |
| 67:18:58:ASP:CG     | 67:18:116:ASN:HD22  | 2.29                     | 0.40              |
| 67:18:140:ASP:OD1   | 67:18:177:HIS:CE1   | 2.65                     | 0.40              |
| 6:17:251:ASP:HA     | 65:14:1104:ALA:C    | 2.08                     | 0.40              |
| 8:3:569:U:H5'       | 54:p:41:ALA:HB1     | 2.02                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:3:1116:U:H5'     | 46:h:122:LYS:HE2    | 2.02                     | 0.40              |
| 8:3:1473:C:H2'     | 8:3:1474:C:C6       | 2.56                     | 0.40              |
| 8:3:1595:C:H2'     | 8:3:1596:U:C6       | 2.57                     | 0.40              |
| 8:3:1702:A:N3      | 8:3:1704:C:N4       | 2.70                     | 0.40              |
| 8:3:2100:G:H4'     | 44:f:24:GLY:HA3     | 2.02                     | 0.40              |
| 8:3:2644:U:H2'     | 8:3:2645:U:H6       | 1.87                     | 0.40              |
| 8:3:2858:A:H2'     | 8:3:2859:U:C6       | 2.56                     | 0.40              |
| 10:5:68:C:O2'      | 10:5:157:A:H1'      | 2.21                     | 0.40              |
| 10:5:707:G:H2'     | 10:5:708:A:C8       | 2.56                     | 0.40              |
| 10:5:1146:A:H2'    | 10:5:1147:U:C6      | 2.56                     | 0.40              |
| 13:8:47:3AU:O2'    | 13:8:48:C:O5'       | 2.39                     | 0.40              |
| 14:9:431:ARG:H     | 14:9:479:GLY:H      | 1.69                     | 0.40              |
| 15:A:60:LEU:HD23   | 15:A:60:LEU:HA      | 1.93                     | 0.40              |
| 15:A:223:GLN:HG2   | 15:A:224:SER:H      | 1.85                     | 0.40              |
| 16:AA:177:ASP:C    | 16:AA:178:ILE:HG12  | 2.45                     | 0.40              |
| 19:C:90:PHE:HA     | 19:C:93:LEU:HD23    | 2.02                     | 0.40              |
| 24:I:99:PRO:O      | 24:I:100:VAL:C      | 2.64                     | 0.40              |
| 32:Q:42:ARG:HG2    | 32:Q:42:ARG:HH11    | 1.86                     | 0.40              |
| 34:S:9:LYS:HE2     | 34:S:13:GLN:NE2     | 2.37                     | 0.40              |
| 36:W:95:ILE:HD12   | 36:W:95:ILE:HA      | 1.97                     | 0.40              |
| 40:b:9:VAL:HG13    | 40:b:30:TYR:HB3     | 2.04                     | 0.40              |
| 48:j:75:THR:HA     | 53:o:78:ASN:O       | 2.21                     | 0.40              |
| 54:p:40:GLN:HG3    | 54:p:44:TYR:CE2     | 2.57                     | 0.40              |
| 56:r:29:THR:HG23   | 56:r:55:ILE:CD1     | 2.50                     | 0.40              |
| 56:r:36:LEU:HD21   | 56:r:47:ILE:HB      | 2.02                     | 0.40              |
| 64:13:196:PRO:HG2  | 64:13:554:LEU:CD1   | 2.50                     | 0.40              |
| 64:13:986:ILE:HB   | 64:13:1130:PRO:HG3  | 2.03                     | 0.40              |
| 65:14:753:ILE:HG23 | 65:14:782:TRP:CE2   | 2.55                     | 0.40              |
| 66:15:973:TYR:HB2  | 66:15:1265:LEU:HD21 | 2.03                     | 0.40              |
| 67:18:15:GLN:OE1   | 67:18:90:GLN:CD     | 2.64                     | 0.40              |
| 6:17:373:VAL:C     | 66:15:172:PRO:O     | 2.64                     | 0.40              |
| 6:17:692:LYS:H     | 14:9:683:HIS:CE1    | 2.35                     | 0.40              |
| 6:17:702:GLU:N     | 14:9:661:GLU:C      | 2.76                     | 0.40              |
| 6:17:789:TYR:CD1   | 6:17:789:TYR:C      | 2.99                     | 0.40              |
| 8:3:515:A:O2'      | 8:3:517:G:H5'       | 2.21                     | 0.40              |
| 8:3:614:C:H2'      | 8:3:615:G:C8        | 2.55                     | 0.40              |
| 8:3:1559:A:O2'     | 14:9:249:ASP:CG     | 2.65                     | 0.40              |
| 8:3:1815:U:O2'     | 8:3:1816:A:O4'      | 2.39                     | 0.40              |
| 8:3:2294:A:H61     | 63:z:21:THR:HG21    | 1.85                     | 0.40              |
| 8:3:2565:G:O2'     | 13:8:74:C:H6        | 2.04                     | 0.40              |
| 8:3:2585:A:H2'     | 8:3:2622:A:N6       | 2.36                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:3:2770:U:H2'    | 8:3:2771:G:O4'     | 2.22                     | 0.40              |
| 9:4:76:A:H5''     | 50:l:20:LYS:HD2    | 2.03                     | 0.40              |
| 10:5:457:A:H2'    | 10:5:458:G:C8      | 2.57                     | 0.40              |
| 10:5:621:C:H2'    | 10:5:622:A:C8      | 2.56                     | 0.40              |
| 10:5:885:U:H2'    | 10:5:886:A:H8      | 1.87                     | 0.40              |
| 10:5:1488:A:H2'   | 10:5:1489:C:C6     | 2.57                     | 0.40              |
| 15:A:32:MET:HE1   | 15:A:205:ASN:ND2   | 2.37                     | 0.40              |
| 15:A:90:ASP:O     | 15:A:91:TYR:C      | 2.65                     | 0.40              |
| 15:A:136:LYS:HB2  | 15:A:136:LYS:HE3   | 1.85                     | 0.40              |
| 21:F:86:VAL:HG11  | 21:F:154:ARG:HG2   | 2.02                     | 0.40              |
| 21:F:142:LYS:HD3  | 21:F:142:LYS:HA    | 1.86                     | 0.40              |
| 32:Q:56:ASP:OD1   | 32:Q:56:ASP:N      | 2.54                     | 0.40              |
| 42:d:175:LEU:HD12 | 42:d:176:PRO:CD    | 2.49                     | 0.40              |
| 50:l:1:MET:HE2    | 50:l:1:MET:HB3     | 1.90                     | 0.40              |
| 58:t:10:VAL:HG21  | 58:t:74:LEU:HB3    | 2.03                     | 0.40              |
| 64:13:1217:LYS:CE | 67:18:275:LEU:O    | 2.61                     | 0.40              |
| 65:14:202:PRO:HB2 | 65:14:289:LEU:HD11 | 2.03                     | 0.40              |
| 66:15:877:ARG:HD3 | 66:15:1270:ILE:CG2 | 2.47                     | 0.40              |
| 6:17:206:LEU:CD2  | 6:17:480:LYS:HA    | 2.52                     | 0.40              |
| 8:3:24:U:H2'      | 8:3:25:G:H8        | 1.87                     | 0.40              |
| 8:3:165:U:O4      | 8:3:2226:U:H4'     | 2.20                     | 0.40              |
| 8:3:246:G:O2'     | 8:3:258:G:O6       | 2.35                     | 0.40              |
| 8:3:322:A:H2'     | 8:3:323:A:H8       | 1.85                     | 0.40              |
| 8:3:392:A:N3      | 8:3:392:A:H2'      | 2.37                     | 0.40              |
| 8:3:683:G:H2'     | 8:3:684:A:C8       | 2.56                     | 0.40              |
| 8:3:784:A:H4'     | 8:3:1301:G:N3      | 2.37                     | 0.40              |
| 8:3:964:A:H2'     | 8:3:965:U:H6       | 1.87                     | 0.40              |
| 8:3:1100:U:H2'    | 8:3:1101:U:C6      | 2.57                     | 0.40              |
| 8:3:1230:U:H2'    | 8:3:1231:G:C8      | 2.57                     | 0.40              |
| 8:3:1231:G:H2'    | 8:3:1232:U:C6      | 2.57                     | 0.40              |
| 8:3:1309:G:H2'    | 8:3:1310:U:C6      | 2.56                     | 0.40              |
| 9:4:65:G:H2'      | 9:4:66:A:H8        | 1.85                     | 0.40              |
| 10:5:416:U:O4     | 10:5:418:U:O2'     | 2.30                     | 0.40              |
| 10:5:768:G:H2'    | 10:5:769:U:C6      | 2.55                     | 0.40              |
| 10:5:995:U:O2'    | 10:5:996:U:OP1     | 2.38                     | 0.40              |
| 10:5:1062:C:H2'   | 10:5:1063:G:C8     | 2.56                     | 0.40              |
| 12:7:76:A:O2'     | 38:Z:36:ASP:O      | 2.31                     | 0.40              |
| 13:8:4:U:H2'      | 13:8:5:C:H6        | 1.83                     | 0.40              |
| 15:A:242:MET:HE2  | 15:A:242:MET:HB3   | 1.85                     | 0.40              |
| 25:J:13:ILE:HD13  | 25:J:78:PHE:CE2    | 2.57                     | 0.40              |
| 26:K:47:CYS:HA    | 26:K:68:VAL:HA     | 2.03                     | 0.40              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 30:O:19:ILE:HD13  | 30:O:19:ILE:HA      | 1.92                     | 0.40              |
| 39:a:189:THR:HB   | 39:a:279:ILE:HB     | 2.04                     | 0.40              |
| 44:f:82:LYS:H     | 44:f:82:LYS:HG2     | 1.70                     | 0.40              |
| 53:o:24:GLU:HA    | 53:o:55:ARG:NH1     | 2.36                     | 0.40              |
| 53:o:108:SER:HA   | 53:o:112:ALA:HB2    | 2.04                     | 0.40              |
| 56:r:88:ARG:HD2   | 56:r:88:ARG:HA      | 1.89                     | 0.40              |
| 57:s:48:TYR:HD2   | 57:s:91:ILE:HD13    | 1.87                     | 0.40              |
| 64:13:190:TRP:HB2 | 64:13:584:TRP:CD1   | 2.57                     | 0.40              |
| 64:13:333:PHE:HE1 | 64:13:514:LEU:HD21  | 1.86                     | 0.40              |
| 64:13:1044:LYS:CE | 64:13:1111:ASP:OD1  | 2.69                     | 0.40              |
| 65:14:619:LEU:O   | 65:14:953:ASN:ND2   | 2.50                     | 0.40              |
| 2:1:11:PHE:HB3    | 2:1:19:ILE:HG22     | 2.04                     | 0.40              |
| 6:17:262:SER:CA   | 65:14:1098:THR:N    | 2.62                     | 0.40              |
| 6:17:262:SER:HA   | 65:14:1096:ILE:HG23 | 1.69                     | 0.40              |
| 6:17:597:ILE:HG21 | 6:17:682:LEU:HD11   | 2.04                     | 0.40              |
| 6:17:598:LYS:HG2  | 14:9:678:PHE:CB     | 2.52                     | 0.40              |
| 8:3:322:A:H2'     | 8:3:323:A:C8        | 2.56                     | 0.40              |
| 8:3:387:U:H2'     | 8:3:388:U:C6        | 2.57                     | 0.40              |
| 8:3:1123:A:H62    | 46:h:130:GLN:HE22   | 1.69                     | 0.40              |
| 8:3:1457:A:H2'    | 8:3:1458:A:H8       | 1.83                     | 0.40              |
| 8:3:1700:G:O2'    | 48:j:6:THR:OG1      | 2.34                     | 0.40              |
| 8:3:2300:A:H2'    | 8:3:2301:C:H6       | 1.87                     | 0.40              |
| 8:3:2655:U:H2'    | 8:3:2656:G:C8       | 2.56                     | 0.40              |
| 10:5:69:G:H2'     | 10:5:70:A:O4'       | 2.21                     | 0.40              |
| 10:5:681:U:O2'    | 25:J:34:VAL:O       | 2.34                     | 0.40              |
| 10:5:1072:G:H2'   | 10:5:1073:A:H8      | 1.86                     | 0.40              |
| 13:8:36:U:H2'     | 13:8:37:T6A:C8      | 2.56                     | 0.40              |
| 15:A:22:LYS:HD3   | 15:A:22:LYS:HA      | 1.87                     | 0.40              |
| 15:A:83:LEU:HD21  | 15:A:108:ILE:HD12   | 2.04                     | 0.40              |
| 16:AA:67:GLU:H    | 16:AA:67:GLU:HG3    | 1.68                     | 0.40              |
| 18:AC:77:THR:O    | 18:AC:79:LYS:N      | 2.53                     | 0.40              |
| 21:F:19:ASN:OD1   | 21:F:22:VAL:N       | 2.51                     | 0.40              |
| 25:J:98:LEU:HD12  | 25:J:98:LEU:H       | 1.86                     | 0.40              |
| 29:N:3:ILE:H      | 29:N:3:ILE:HG12     | 1.67                     | 0.40              |
| 32:Q:64:LEU:HD22  | 32:Q:99:VAL:HG11    | 2.04                     | 0.40              |
| 41:c:4:LEU:HD12   | 41:c:4:LEU:HA       | 1.76                     | 0.40              |
| 47:i:21:VAL:HG21  | 47:i:146:SER:H      | 1.86                     | 0.40              |
| 61:w:38:LEU:HA    | 61:w:38:LEU:HD23    | 1.84                     | 0.40              |
| 63:z:7:THR:OG1    | 63:z:49:GLU:OE2     | 2.25                     | 0.40              |
| 64:13:235:PHE:CE2 | 64:13:354:ILE:HD11  | 2.54                     | 0.40              |
| 64:13:258:GLY:HA3 | 64:13:281:LYS:HD2   | 2.03                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 64:13:610:LYS:HE2  | 64:13:614:GLU:OE1   | 2.22                     | 0.40              |
| 64:13:1151:PHE:HE2 | 64:13:1171:ILE:HD12 | 1.86                     | 0.40              |
| 66:15:465:ILE:HA   | 66:15:466:PRO:HD3   | 1.83                     | 0.40              |
| 66:15:689:GLU:OE2  | 66:15:1040:SER:CB   | 2.70                     | 0.40              |
| 66:15:1071:PHE:HE2 | 66:15:1247:ARG:HG2  | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | 0     | 45/48 (94%)    | 45 (100%) | 0        | 0        | 100         | 100 |
| 2   | 1     | 57/59 (97%)    | 57 (100%) | 0        | 0        | 100         | 100 |
| 3   | 10    | 452/477 (95%)  | 444 (98%) | 6 (1%)   | 2 (0%)   | 30          | 67  |
| 4   | 11    | 74/76 (97%)    | 70 (95%)  | 2 (3%)   | 2 (3%)   | 4           | 25  |
| 5   | 12    | 102/125 (82%)  | 98 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 6   | 17    | 962/971 (99%)  | 902 (94%) | 44 (5%)  | 16 (2%)  | 7           | 36  |
| 7   | 2     | 35/37 (95%)    | 35 (100%) | 0        | 0        | 100         | 100 |
| 14  | 9     | 806/808 (100%) | 769 (95%) | 32 (4%)  | 5 (1%)   | 21          | 59  |
| 15  | A     | 262/294 (89%)  | 236 (90%) | 24 (9%)  | 2 (1%)   | 16          | 54  |
| 16  | AA    | 153/219 (70%)  | 145 (95%) | 7 (5%)   | 1 (1%)   | 18          | 56  |
| 18  | AC    | 41/97 (42%)    | 27 (66%)  | 14 (34%) | 0        | 100         | 100 |
| 18  | x     | 44/97 (45%)    | 36 (82%)  | 7 (16%)  | 1 (2%)   | 5           | 28  |
| 19  | C     | 202/205 (98%)  | 169 (84%) | 32 (16%) | 1 (0%)   | 24          | 63  |
| 20  | E     | 182/215 (85%)  | 157 (86%) | 22 (12%) | 3 (2%)   | 7           | 38  |
| 21  | F     | 153/155 (99%)  | 140 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 22  | G     | 139/142 (98%)  | 131 (94%) | 8 (6%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 23  | H     | 127/132 (96%) | 114 (90%) | 12 (9%)  | 1 (1%)   | 16          | 54  |
| 24  | I     | 102/108 (94%) | 88 (86%)  | 13 (13%) | 1 (1%)   | 12          | 49  |
| 25  | J     | 112/121 (93%) | 105 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 26  | K     | 133/139 (96%) | 120 (90%) | 12 (9%)  | 1 (1%)   | 16          | 54  |
| 27  | L     | 119/124 (96%) | 110 (92%) | 8 (7%)   | 1 (1%)   | 16          | 54  |
| 28  | M     | 58/61 (95%)   | 56 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 29  | N     | 83/86 (96%)   | 79 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 30  | O     | 85/94 (90%)   | 78 (92%)  | 5 (6%)   | 2 (2%)   | 4           | 27  |
| 31  | P     | 83/85 (98%)   | 71 (86%)  | 11 (13%) | 1 (1%)   | 10          | 44  |
| 32  | Q     | 69/104 (66%)  | 65 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 33  | R     | 84/87 (97%)   | 80 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 34  | S     | 77/87 (88%)   | 74 (96%)  | 2 (3%)   | 1 (1%)   | 9           | 42  |
| 35  | T     | 57/60 (95%)   | 54 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 36  | W     | 222/273 (81%) | 197 (89%) | 22 (10%) | 3 (1%)   | 9           | 40  |
| 38  | Z     | 3/36 (8%)     | 3 (100%)  | 0        | 0        | 100         | 100 |
| 39  | a     | 283/287 (99%) | 268 (95%) | 14 (5%)  | 1 (0%)   | 30          | 67  |
| 40  | b     | 227/287 (79%) | 219 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 41  | c     | 209/212 (99%) | 198 (95%) | 11 (5%)  | 0        | 100         | 100 |
| 42  | d     | 177/180 (98%) | 169 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 43  | e     | 174/184 (95%) | 161 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 44  | f     | 147/149 (99%) | 131 (89%) | 15 (10%) | 1 (1%)   | 18          | 56  |
| 45  | g     | 123/161 (76%) | 115 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 46  | h     | 126/137 (92%) | 120 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 47  | i     | 142/146 (97%) | 133 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 48  | j     | 120/122 (98%) | 115 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 49  | k     | 148/151 (98%) | 138 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 50  | l     | 134/139 (96%) | 132 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 51  | m     | 117/124 (94%) | 112 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 52  | n     | 114/116 (98%) | 109 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 53  | o     | 116/119 (98%) | 107 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 54  | p     | 116/127 (91%) | 114 (98%) | 2 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 55  | q     | 97/100 (97%)      | 92 (95%)    | 5 (5%)   | 0        | 100         | 100 |
| 56  | r     | 140/159 (88%)     | 136 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 57  | s     | 93/194 (48%)      | 89 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 58  | t     | 109/111 (98%)     | 102 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| 59  | u     | 86/104 (83%)      | 82 (95%)    | 4 (5%)   | 0        | 100         | 100 |
| 60  | v     | 62/65 (95%)       | 62 (100%)   | 0        | 0        | 100         | 100 |
| 61  | w     | 108/111 (97%)     | 102 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 62  | y     | 54/57 (95%)       | 53 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 63  | z     | 48/53 (91%)       | 47 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 64  | 13    | 1214/1217 (100%)  | 1119 (92%)  | 62 (5%)  | 33 (3%)  | 4           | 25  |
| 65  | 14    | 1295/1298 (100%)  | 1184 (91%)  | 75 (6%)  | 36 (3%)  | 4           | 24  |
| 66  | 15    | 1271/1274 (100%)  | 1147 (90%)  | 83 (6%)  | 41 (3%)  | 3           | 21  |
| 67  | 16    | 273/276 (99%)     | 241 (88%)   | 22 (8%)  | 10 (4%)  | 2           | 20  |
| 67  | 18    | 273/276 (99%)     | 243 (89%)   | 20 (7%)  | 10 (4%)  | 2           | 20  |
| All | All   | 12719/13558 (94%) | 11795 (93%) | 748 (6%) | 176 (1%) | 11          | 40  |

All (176) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | 17    | 398  | LEU  |
| 6   | 17    | 715  | ASN  |
| 6   | 17    | 950  | LYS  |
| 14  | 9     | 742  | GLN  |
| 16  | AA    | 216  | LEU  |
| 20  | E     | 143  | LEU  |
| 31  | P     | 54   | LEU  |
| 64  | 13    | 998  | GLN  |
| 64  | 13    | 999  | GLN  |
| 65  | 14    | 651  | THR  |
| 66  | 15    | 241  | ASN  |
| 66  | 15    | 371  | VAL  |
| 66  | 15    | 1226 | SER  |
| 4   | 11    | 27   | SER  |
| 6   | 17    | 43   | GLY  |
| 6   | 17    | 265  | GLY  |
| 6   | 17    | 376  | LYS  |
| 6   | 17    | 400  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | 17    | 705  | ASP  |
| 6   | 17    | 714  | LYS  |
| 14  | 9     | 123  | LYS  |
| 14  | 9     | 375  | ALA  |
| 15  | A     | 219  | ASN  |
| 19  | C     | 81   | GLN  |
| 34  | S     | 37   | LYS  |
| 64  | 13    | 380  | GLN  |
| 64  | 13    | 382  | GLN  |
| 64  | 13    | 426  | ALA  |
| 64  | 13    | 428  | LEU  |
| 64  | 13    | 432  | ASN  |
| 64  | 13    | 479  | GLN  |
| 64  | 13    | 519  | THR  |
| 64  | 13    | 829  | GLN  |
| 64  | 13    | 833  | THR  |
| 64  | 13    | 987  | GLN  |
| 64  | 13    | 992  | LEU  |
| 64  | 13    | 997  | LYS  |
| 64  | 13    | 1001 | GLN  |
| 65  | 14    | 430  | THR  |
| 65  | 14    | 654  | THR  |
| 65  | 14    | 659  | THR  |
| 65  | 14    | 1167 | LYS  |
| 66  | 15    | 278  | GLN  |
| 66  | 15    | 373  | ARG  |
| 66  | 15    | 380  | ASP  |
| 66  | 15    | 422  | GLY  |
| 66  | 15    | 478  | GLN  |
| 66  | 15    | 482  | GLN  |
| 66  | 15    | 484  | THR  |
| 66  | 15    | 728  | ASP  |
| 66  | 15    | 730  | LYS  |
| 66  | 15    | 923  | GLY  |
| 66  | 15    | 1020 | ASN  |
| 66  | 15    | 1080 | ARG  |
| 66  | 15    | 1229 | THR  |
| 66  | 15    | 1231 | THR  |
| 67  | 18    | 244  | LYS  |
| 67  | 18    | 246  | TYR  |
| 67  | 16    | 239  | ALA  |
| 67  | 16    | 241  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 67  | 16    | 244  | LYS  |
| 67  | 16    | 246  | TYR  |
| 3   | 10    | 104  | THR  |
| 6   | 17    | 949  | HIS  |
| 15  | A     | 54   | ASP  |
| 24  | I     | 100  | VAL  |
| 30  | O     | 47   | LYS  |
| 30  | O     | 49   | LYS  |
| 36  | W     | 221  | HIS  |
| 44  | f     | 12   | LEU  |
| 64  | 13    | 288  | LYS  |
| 64  | 13    | 476  | ASN  |
| 64  | 13    | 481  | GLN  |
| 64  | 13    | 539  | ASN  |
| 64  | 13    | 835  | ASN  |
| 64  | 13    | 994  | LEU  |
| 65  | 14    | 364  | LEU  |
| 65  | 14    | 431  | GLU  |
| 65  | 14    | 432  | THR  |
| 65  | 14    | 433  | THR  |
| 65  | 14    | 650  | SER  |
| 65  | 14    | 657  | SER  |
| 65  | 14    | 910  | LEU  |
| 65  | 14    | 916  | LEU  |
| 65  | 14    | 920  | GLN  |
| 65  | 14    | 982  | ALA  |
| 66  | 15    | 276  | THR  |
| 66  | 15    | 449  | SER  |
| 66  | 15    | 469  | ARG  |
| 66  | 15    | 476  | THR  |
| 66  | 15    | 479  | GLN  |
| 66  | 15    | 480  | VAL  |
| 66  | 15    | 481  | GLN  |
| 66  | 15    | 483  | THR  |
| 66  | 15    | 726  | ALA  |
| 66  | 15    | 741  | LEU  |
| 66  | 15    | 751  | LYS  |
| 66  | 15    | 755  | THR  |
| 66  | 15    | 924  | MET  |
| 66  | 15    | 1015 | THR  |
| 67  | 18    | 220  | ASN  |
| 67  | 18    | 229  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 67  | 18    | 239  | ALA  |
| 67  | 18    | 241  | ALA  |
| 67  | 18    | 245  | SER  |
| 67  | 18    | 247  | SER  |
| 67  | 18    | 250  | SER  |
| 67  | 16    | 220  | ASN  |
| 67  | 16    | 229  | ASN  |
| 67  | 16    | 240  | ALA  |
| 67  | 16    | 243  | LYS  |
| 67  | 16    | 247  | SER  |
| 4   | 11    | 44   | LYS  |
| 6   | 17    | 504  | PRO  |
| 6   | 17    | 702  | GLU  |
| 6   | 17    | 707  | GLN  |
| 14  | 9     | 701  | THR  |
| 39  | a     | 128  | ILE  |
| 64  | 13    | 273  | ASN  |
| 64  | 13    | 989  | VAL  |
| 64  | 13    | 991  | SER  |
| 64  | 13    | 1000 | MET  |
| 64  | 13    | 1002 | GLN  |
| 65  | 14    | 426  | THR  |
| 65  | 14    | 775  | ASN  |
| 65  | 14    | 907  | LEU  |
| 65  | 14    | 918  | GLN  |
| 65  | 14    | 985  | SER  |
| 65  | 14    | 988  | VAL  |
| 65  | 14    | 1046 | GLN  |
| 65  | 14    | 1048 | LEU  |
| 66  | 15    | 485  | SER  |
| 66  | 15    | 724  | ASP  |
| 67  | 18    | 243  | LYS  |
| 67  | 16    | 245  | SER  |
| 3   | 10    | 311  | GLN  |
| 6   | 17    | 81   | ASN  |
| 20  | E     | 163  | MET  |
| 20  | E     | 169  | VAL  |
| 36  | W     | 46   | VAL  |
| 36  | W     | 216  | ASN  |
| 64  | 13    | 430  | THR  |
| 64  | 13    | 486  | ASN  |
| 64  | 13    | 523  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 64  | 13    | 529  | LEU  |
| 65  | 14    | 373  | THR  |
| 65  | 14    | 436  | ASN  |
| 65  | 14    | 773  | GLY  |
| 65  | 14    | 914  | VAL  |
| 65  | 14    | 983  | GLN  |
| 65  | 14    | 997  | GLY  |
| 65  | 14    | 1000 | THR  |
| 65  | 14    | 1164 | GLN  |
| 66  | 15    | 584  | LYS  |
| 66  | 15    | 605  | ARG  |
| 66  | 15    | 610  | ASP  |
| 66  | 15    | 1018 | ALA  |
| 6   | 17    | 378  | ASN  |
| 23  | H     | 27   | HIS  |
| 26  | K     | 128  | SER  |
| 27  | L     | 98   | ARG  |
| 18  | x     | 18   | SER  |
| 64  | 13    | 831  | SER  |
| 65  | 14    | 361  | THR  |
| 65  | 14    | 372  | GLY  |
| 65  | 14    | 924  | GLN  |
| 65  | 14    | 979  | THR  |
| 66  | 15    | 376  | ILE  |
| 14  | 9     | 431  | ARG  |
| 64  | 13    | 1077 | GLY  |
| 65  | 14    | 980  | GLY  |
| 64  | 13    | 995  | VAL  |
| 66  | 15    | 1232 | ILE  |
| 6   | 17    | 259  | GLY  |
| 66  | 15    | 729  | GLY  |
| 66  | 15    | 756  | VAL  |

### 5.3.2 Protein sidechains [i](#)

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   | 0     | 40/41 (98%)    | 40 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 51/51 (100%)   | 51 (100%)  | 0        | 100         | 100 |
| 3   | 10    | 386/406 (95%)  | 375 (97%)  | 11 (3%)  | 38          | 60  |
| 4   | 11    | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 5   | 12    | 94/113 (83%)   | 94 (100%)  | 0        | 100         | 100 |
| 6   | 17    | 828/834 (99%)  | 801 (97%)  | 27 (3%)  | 33          | 55  |
| 7   | 2     | 35/35 (100%)   | 35 (100%)  | 0        | 100         | 100 |
| 14  | 9     | 699/699 (100%) | 678 (97%)  | 21 (3%)  | 36          | 57  |
| 15  | A     | 238/262 (91%)  | 235 (99%)  | 3 (1%)   | 61          | 74  |
| 16  | AA    | 125/178 (70%)  | 123 (98%)  | 2 (2%)   | 55          | 70  |
| 18  | AC    | 35/86 (41%)    | 35 (100%)  | 0        | 100         | 100 |
| 18  | x     | 44/86 (51%)    | 43 (98%)   | 1 (2%)   | 44          | 64  |
| 19  | C     | 182/183 (100%) | 180 (99%)  | 2 (1%)   | 65          | 76  |
| 20  | E     | 165/196 (84%)  | 165 (100%) | 0        | 100         | 100 |
| 21  | F     | 132/132 (100%) | 132 (100%) | 0        | 100         | 100 |
| 22  | G     | 123/124 (99%)  | 121 (98%)  | 2 (2%)   | 55          | 70  |
| 23  | H     | 112/115 (97%)  | 112 (100%) | 0        | 100         | 100 |
| 24  | I     | 97/99 (98%)    | 97 (100%)  | 0        | 100         | 100 |
| 25  | J     | 91/97 (94%)    | 91 (100%)  | 0        | 100         | 100 |
| 26  | K     | 117/120 (98%)  | 113 (97%)  | 4 (3%)   | 32          | 54  |
| 27  | L     | 102/105 (97%)  | 102 (100%) | 0        | 100         | 100 |
| 28  | M     | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |
| 29  | N     | 77/78 (99%)    | 76 (99%)   | 1 (1%)   | 61          | 74  |
| 30  | O     | 76/82 (93%)    | 76 (100%)  | 0        | 100         | 100 |
| 31  | P     | 75/75 (100%)   | 75 (100%)  | 0        | 100         | 100 |
| 32  | Q     | 62/94 (66%)    | 62 (100%)  | 0        | 100         | 100 |
| 33  | R     | 76/77 (99%)    | 75 (99%)   | 1 (1%)   | 61          | 74  |
| 34  | S     | 71/77 (92%)    | 69 (97%)   | 2 (3%)   | 38          | 60  |
| 35  | T     | 55/56 (98%)    | 55 (100%)  | 0        | 100         | 100 |
| 36  | W     | 187/232 (81%)  | 186 (100%) | 1 (0%)   | 81          | 83  |
| 38  | Z     | 2/2 (100%)     | 2 (100%)   | 0        | 100         | 100 |
| 39  | a     | 241/243 (99%)  | 233 (97%)  | 8 (3%)   | 33          | 55  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 40  | b     | 188/233 (81%)     | 183 (97%)   | 5 (3%)   | 39          | 61 |
| 41  | c     | 183/184 (100%)    | 174 (95%)   | 9 (5%)   | 22          | 43 |
| 42  | d     | 153/154 (99%)     | 148 (97%)   | 5 (3%)   | 33          | 55 |
| 43  | e     | 153/159 (96%)     | 149 (97%)   | 4 (3%)   | 40          | 62 |
| 44  | f     | 133/134 (99%)     | 127 (96%)   | 6 (4%)   | 24          | 46 |
| 45  | g     | 100/129 (78%)     | 98 (98%)    | 2 (2%)   | 48          | 66 |
| 46  | h     | 102/110 (93%)     | 97 (95%)    | 5 (5%)   | 22          | 43 |
| 47  | i     | 126/128 (98%)     | 122 (97%)   | 4 (3%)   | 34          | 56 |
| 48  | j     | 103/103 (100%)    | 100 (97%)   | 3 (3%)   | 37          | 58 |
| 49  | k     | 125/126 (99%)     | 119 (95%)   | 6 (5%)   | 23          | 44 |
| 50  | l     | 113/115 (98%)     | 111 (98%)   | 2 (2%)   | 51          | 68 |
| 51  | m     | 105/109 (96%)     | 103 (98%)   | 2 (2%)   | 50          | 67 |
| 52  | n     | 99/99 (100%)      | 95 (96%)    | 4 (4%)   | 28          | 49 |
| 53  | o     | 104/105 (99%)     | 101 (97%)   | 3 (3%)   | 37          | 58 |
| 54  | p     | 104/108 (96%)     | 102 (98%)   | 2 (2%)   | 50          | 67 |
| 55  | q     | 90/91 (99%)       | 84 (93%)    | 6 (7%)   | 15          | 36 |
| 56  | r     | 118/132 (89%)     | 116 (98%)   | 2 (2%)   | 53          | 69 |
| 57  | s     | 84/169 (50%)      | 79 (94%)    | 5 (6%)   | 17          | 39 |
| 58  | t     | 96/96 (100%)      | 92 (96%)    | 4 (4%)   | 26          | 48 |
| 59  | u     | 70/85 (82%)       | 68 (97%)    | 2 (3%)   | 37          | 58 |
| 60  | v     | 59/60 (98%)       | 56 (95%)    | 3 (5%)   | 21          | 42 |
| 61  | w     | 97/98 (99%)       | 93 (96%)    | 4 (4%)   | 27          | 49 |
| 62  | y     | 48/49 (98%)       | 47 (98%)    | 1 (2%)   | 47          | 65 |
| 63  | z     | 47/50 (94%)       | 44 (94%)    | 3 (6%)   | 16          | 37 |
| 64  | 13    | 1068/1069 (100%)  | 1050 (98%)  | 18 (2%)  | 53          | 69 |
| 65  | 14    | 1128/1129 (100%)  | 1102 (98%)  | 26 (2%)  | 44          | 64 |
| 66  | 15    | 1085/1086 (100%)  | 1049 (97%)  | 36 (3%)  | 33          | 55 |
| 67  | 16    | 240/241 (100%)    | 236 (98%)   | 4 (2%)   | 53          | 69 |
| 67  | 18    | 240/241 (100%)    | 237 (99%)   | 3 (1%)   | 61          | 74 |
| All | All   | 11091/11683 (95%) | 10826 (98%) | 265 (2%) | 43          | 64 |

All (265) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 10    | 91  | PRO  |
| 3   | 10    | 104 | THR  |
| 3   | 10    | 158 | THR  |
| 3   | 10    | 244 | PHE  |
| 3   | 10    | 254 | ILE  |
| 3   | 10    | 256 | GLN  |
| 3   | 10    | 258 | THR  |
| 3   | 10    | 290 | ILE  |
| 3   | 10    | 312 | THR  |
| 3   | 10    | 374 | THR  |
| 3   | 10    | 380 | ARG  |
| 6   | 17    | 13  | LEU  |
| 6   | 17    | 33  | SER  |
| 6   | 17    | 206 | LEU  |
| 6   | 17    | 218 | SER  |
| 6   | 17    | 250 | THR  |
| 6   | 17    | 337 | LEU  |
| 6   | 17    | 375 | THR  |
| 6   | 17    | 377 | ASP  |
| 6   | 17    | 385 | ASP  |
| 6   | 17    | 402 | ASP  |
| 6   | 17    | 500 | LEU  |
| 6   | 17    | 505 | LEU  |
| 6   | 17    | 508 | THR  |
| 6   | 17    | 509 | LEU  |
| 6   | 17    | 673 | HIS  |
| 6   | 17    | 693 | THR  |
| 6   | 17    | 710 | PHE  |
| 6   | 17    | 733 | THR  |
| 6   | 17    | 752 | LEU  |
| 6   | 17    | 797 | LEU  |
| 6   | 17    | 810 | LEU  |
| 6   | 17    | 821 | THR  |
| 6   | 17    | 824 | LEU  |
| 6   | 17    | 904 | LEU  |
| 6   | 17    | 934 | TRP  |
| 6   | 17    | 936 | SER  |
| 6   | 17    | 946 | THR  |
| 14  | 9     | 22  | LYS  |
| 14  | 9     | 75  | VAL  |
| 14  | 9     | 79  | THR  |
| 14  | 9     | 102 | MET  |
| 14  | 9     | 108 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | 9     | 132 | ASN  |
| 14  | 9     | 137 | GLN  |
| 14  | 9     | 141 | THR  |
| 14  | 9     | 252 | LYS  |
| 14  | 9     | 273 | ASN  |
| 14  | 9     | 276 | THR  |
| 14  | 9     | 310 | ARG  |
| 14  | 9     | 435 | ILE  |
| 14  | 9     | 439 | ASN  |
| 14  | 9     | 470 | GLU  |
| 14  | 9     | 529 | ARG  |
| 14  | 9     | 575 | MET  |
| 14  | 9     | 595 | ILE  |
| 14  | 9     | 720 | HIS  |
| 14  | 9     | 735 | VAL  |
| 14  | 9     | 753 | THR  |
| 15  | A     | 46  | GLU  |
| 15  | A     | 85  | VAL  |
| 15  | A     | 282 | LEU  |
| 16  | AA    | 67  | GLU  |
| 16  | AA    | 203 | LEU  |
| 19  | C     | 82  | ARG  |
| 19  | C     | 153 | ILE  |
| 22  | G     | 57  | PHE  |
| 22  | G     | 70  | VAL  |
| 26  | K     | 7   | LEU  |
| 26  | K     | 31  | LEU  |
| 26  | K     | 32  | ASN  |
| 26  | K     | 128 | SER  |
| 29  | N     | 15  | HIS  |
| 33  | R     | 78  | ARG  |
| 34  | S     | 36  | HIS  |
| 34  | S     | 75  | VAL  |
| 36  | W     | 58  | ILE  |
| 39  | a     | 37  | LEU  |
| 39  | a     | 100 | THR  |
| 39  | a     | 107 | SER  |
| 39  | a     | 200 | VAL  |
| 39  | a     | 202 | VAL  |
| 39  | a     | 227 | THR  |
| 39  | a     | 262 | HIS  |
| 39  | a     | 275 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | b     | 11  | VAL  |
| 40  | b     | 13  | MET  |
| 40  | b     | 39  | VAL  |
| 40  | b     | 217 | VAL  |
| 40  | b     | 220 | ILE  |
| 41  | c     | 7   | ILE  |
| 41  | c     | 21  | SER  |
| 41  | c     | 36  | ASP  |
| 41  | c     | 58  | VAL  |
| 41  | c     | 79  | THR  |
| 41  | c     | 178 | VAL  |
| 41  | c     | 180 | VAL  |
| 41  | c     | 183 | LEU  |
| 41  | c     | 203 | VAL  |
| 42  | d     | 4   | LEU  |
| 42  | d     | 50  | LEU  |
| 42  | d     | 66  | VAL  |
| 42  | d     | 119 | LEU  |
| 42  | d     | 179 | LYS  |
| 43  | e     | 34  | ILE  |
| 43  | e     | 101 | VAL  |
| 43  | e     | 108 | LEU  |
| 43  | e     | 135 | THR  |
| 44  | f     | 3   | VAL  |
| 44  | f     | 8   | ASP  |
| 44  | f     | 9   | VAL  |
| 44  | f     | 14  | LYS  |
| 44  | f     | 23  | ASP  |
| 44  | f     | 84  | HIS  |
| 45  | g     | 25  | VAL  |
| 45  | g     | 76  | ILE  |
| 46  | h     | 12  | ILE  |
| 46  | h     | 58  | TYR  |
| 46  | h     | 70  | THR  |
| 46  | h     | 100 | LYS  |
| 46  | h     | 121 | LEU  |
| 47  | i     | 20  | ILE  |
| 47  | i     | 62  | SER  |
| 47  | i     | 87  | ILE  |
| 47  | i     | 146 | SER  |
| 48  | j     | 19  | VAL  |
| 48  | j     | 28  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | j     | 116 | SER  |
| 49  | k     | 8   | SER  |
| 49  | k     | 31  | THR  |
| 49  | k     | 56  | THR  |
| 49  | k     | 78  | VAL  |
| 49  | k     | 108 | SER  |
| 49  | k     | 139 | VAL  |
| 50  | l     | 35  | VAL  |
| 50  | l     | 127 | VAL  |
| 51  | m     | 10  | THR  |
| 51  | m     | 23  | SER  |
| 52  | n     | 40  | SER  |
| 52  | n     | 47  | SER  |
| 52  | n     | 60  | LEU  |
| 52  | n     | 89  | VAL  |
| 53  | o     | 33  | VAL  |
| 53  | o     | 98  | ARG  |
| 53  | o     | 115 | LYS  |
| 54  | p     | 76  | SER  |
| 54  | p     | 99  | ILE  |
| 55  | q     | 5   | VAL  |
| 55  | q     | 45  | ILE  |
| 55  | q     | 75  | SER  |
| 55  | q     | 78  | HIS  |
| 55  | q     | 90  | THR  |
| 55  | q     | 92  | LEU  |
| 56  | r     | 37  | SER  |
| 56  | r     | 39  | THR  |
| 57  | s     | 24  | THR  |
| 57  | s     | 47  | VAL  |
| 57  | s     | 58  | LEU  |
| 57  | s     | 64  | THR  |
| 57  | s     | 84  | THR  |
| 58  | t     | 36  | VAL  |
| 58  | t     | 47  | LYS  |
| 58  | t     | 92  | VAL  |
| 58  | t     | 95  | PRO  |
| 59  | u     | 81  | VAL  |
| 59  | u     | 96  | SER  |
| 60  | v     | 9   | LEU  |
| 60  | v     | 48  | ILE  |
| 60  | v     | 49  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | w     | 16   | VAL  |
| 61  | w     | 20   | ILE  |
| 61  | w     | 38   | LEU  |
| 61  | w     | 76   | THR  |
| 18  | x     | 27   | SER  |
| 62  | y     | 11   | HIS  |
| 63  | z     | 5    | ARG  |
| 63  | z     | 18   | ASN  |
| 63  | z     | 21   | THR  |
| 64  | 13    | 67   | THR  |
| 64  | 13    | 92   | SER  |
| 64  | 13    | 406  | LEU  |
| 64  | 13    | 419  | THR  |
| 64  | 13    | 453  | THR  |
| 64  | 13    | 454  | THR  |
| 64  | 13    | 467  | LEU  |
| 64  | 13    | 530  | THR  |
| 64  | 13    | 807  | LEU  |
| 64  | 13    | 876  | LEU  |
| 64  | 13    | 921  | THR  |
| 64  | 13    | 928  | VAL  |
| 64  | 13    | 965  | THR  |
| 64  | 13    | 982  | THR  |
| 64  | 13    | 1092 | VAL  |
| 64  | 13    | 1110 | LEU  |
| 64  | 13    | 1129 | THR  |
| 64  | 13    | 1164 | THR  |
| 65  | 14    | 154  | LEU  |
| 65  | 14    | 209  | VAL  |
| 65  | 14    | 345  | THR  |
| 65  | 14    | 361  | THR  |
| 65  | 14    | 374  | THR  |
| 65  | 14    | 377  | THR  |
| 65  | 14    | 430  | THR  |
| 65  | 14    | 432  | THR  |
| 65  | 14    | 443  | ASP  |
| 65  | 14    | 507  | ASP  |
| 65  | 14    | 655  | THR  |
| 65  | 14    | 757  | THR  |
| 65  | 14    | 791  | LEU  |
| 65  | 14    | 898  | THR  |
| 65  | 14    | 907  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 65  | 14    | 927  | ASP  |
| 65  | 14    | 987  | THR  |
| 65  | 14    | 999  | THR  |
| 65  | 14    | 1000 | THR  |
| 65  | 14    | 1002 | THR  |
| 65  | 14    | 1050 | THR  |
| 65  | 14    | 1058 | THR  |
| 65  | 14    | 1059 | LEU  |
| 65  | 14    | 1162 | THR  |
| 65  | 14    | 1168 | THR  |
| 65  | 14    | 1228 | THR  |
| 66  | 15    | 19   | LEU  |
| 66  | 15    | 73   | THR  |
| 66  | 15    | 87   | LEU  |
| 66  | 15    | 153  | THR  |
| 66  | 15    | 249  | THR  |
| 66  | 15    | 283  | SER  |
| 66  | 15    | 303  | LEU  |
| 66  | 15    | 344  | VAL  |
| 66  | 15    | 382  | THR  |
| 66  | 15    | 476  | THR  |
| 66  | 15    | 483  | THR  |
| 66  | 15    | 551  | SER  |
| 66  | 15    | 564  | THR  |
| 66  | 15    | 581  | THR  |
| 66  | 15    | 601  | THR  |
| 66  | 15    | 635  | THR  |
| 66  | 15    | 639  | THR  |
| 66  | 15    | 668  | LEU  |
| 66  | 15    | 741  | LEU  |
| 66  | 15    | 743  | THR  |
| 66  | 15    | 747  | THR  |
| 66  | 15    | 755  | THR  |
| 66  | 15    | 786  | LEU  |
| 66  | 15    | 829  | TRP  |
| 66  | 15    | 830  | THR  |
| 66  | 15    | 832  | ILE  |
| 66  | 15    | 869  | LEU  |
| 66  | 15    | 876  | LEU  |
| 66  | 15    | 1000 | THR  |
| 66  | 15    | 1050 | THR  |
| 66  | 15    | 1160 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 66  | 15    | 1173 | LEU  |
| 66  | 15    | 1231 | THR  |
| 66  | 15    | 1243 | THR  |
| 66  | 15    | 1259 | THR  |
| 66  | 15    | 1260 | LEU  |
| 67  | 18    | 84   | THR  |
| 67  | 18    | 180  | THR  |
| 67  | 18    | 233  | THR  |
| 67  | 16    | 84   | THR  |
| 67  | 16    | 134  | THR  |
| 67  | 16    | 180  | THR  |
| 67  | 16    | 233  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 10    | 56  | ASN  |
| 3   | 10    | 62  | GLN  |
| 3   | 10    | 81  | GLN  |
| 3   | 10    | 100 | GLN  |
| 3   | 10    | 265 | GLN  |
| 3   | 10    | 268 | GLN  |
| 3   | 10    | 285 | ASN  |
| 3   | 10    | 350 | ASN  |
| 3   | 10    | 411 | ASN  |
| 3   | 10    | 444 | GLN  |
| 3   | 10    | 459 | GLN  |
| 3   | 10    | 460 | GLN  |
| 4   | 11    | 5   | GLN  |
| 4   | 11    | 37  | GLN  |
| 5   | 12    | 81  | ASN  |
| 6   | 17    | 81  | ASN  |
| 6   | 17    | 215 | ASN  |
| 6   | 17    | 453 | ASN  |
| 6   | 17    | 641 | GLN  |
| 6   | 17    | 642 | GLN  |
| 6   | 17    | 658 | ASN  |
| 6   | 17    | 812 | ASN  |
| 6   | 17    | 819 | GLN  |
| 6   | 17    | 836 | GLN  |
| 6   | 17    | 868 | ASN  |
| 6   | 17    | 894 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 17    | 932 | ASN  |
| 6   | 17    | 959 | GLN  |
| 7   | 2     | 20  | HIS  |
| 7   | 2     | 32  | HIS  |
| 7   | 2     | 36  | GLN  |
| 14  | 9     | 5   | ASN  |
| 14  | 9     | 41  | GLN  |
| 14  | 9     | 56  | GLN  |
| 14  | 9     | 87  | GLN  |
| 14  | 9     | 127 | HIS  |
| 14  | 9     | 137 | GLN  |
| 14  | 9     | 278 | ASN  |
| 14  | 9     | 284 | ASN  |
| 14  | 9     | 289 | HIS  |
| 14  | 9     | 293 | ASN  |
| 14  | 9     | 332 | ASN  |
| 14  | 9     | 447 | HIS  |
| 14  | 9     | 611 | GLN  |
| 14  | 9     | 647 | ASN  |
| 14  | 9     | 665 | HIS  |
| 14  | 9     | 724 | HIS  |
| 14  | 9     | 762 | GLN  |
| 14  | 9     | 795 | GLN  |
| 14  | 9     | 801 | HIS  |
| 14  | 9     | 805 | ASN  |
| 15  | A     | 55  | HIS  |
| 15  | A     | 81  | GLN  |
| 15  | A     | 192 | ASN  |
| 15  | A     | 220 | HIS  |
| 15  | A     | 221 | GLN  |
| 18  | AC    | 67  | ASN  |
| 18  | AC    | 98  | ASN  |
| 20  | E     | 25  | GLN  |
| 21  | F     | 39  | GLN  |
| 23  | H     | 43  | ASN  |
| 23  | H     | 77  | GLN  |
| 23  | H     | 91  | GLN  |
| 26  | K     | 29  | ASN  |
| 26  | K     | 85  | HIS  |
| 27  | L     | 79  | HIS  |
| 33  | R     | 14  | HIS  |
| 33  | R     | 25  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | S     | 31  | ASN  |
| 34  | S     | 40  | ASN  |
| 36  | W     | 91  | GLN  |
| 36  | W     | 125 | ASN  |
| 36  | W     | 150 | ASN  |
| 36  | W     | 221 | HIS  |
| 40  | b     | 66  | GLN  |
| 40  | b     | 67  | GLN  |
| 40  | b     | 73  | ASN  |
| 40  | b     | 148 | GLN  |
| 40  | b     | 157 | GLN  |
| 40  | b     | 171 | HIS  |
| 40  | b     | 188 | ASN  |
| 41  | c     | 113 | HIS  |
| 41  | c     | 126 | HIS  |
| 41  | c     | 170 | GLN  |
| 42  | d     | 37  | ASN  |
| 43  | e     | 63  | GLN  |
| 44  | f     | 85  | ASN  |
| 44  | f     | 96  | GLN  |
| 47  | i     | 134 | ASN  |
| 49  | k     | 39  | GLN  |
| 49  | k     | 129 | HIS  |
| 50  | l     | 113 | GLN  |
| 51  | m     | 77  | GLN  |
| 52  | n     | 7   | GLN  |
| 52  | n     | 69  | ASN  |
| 54  | p     | 40  | GLN  |
| 54  | p     | 71  | GLN  |
| 54  | p     | 106 | ASN  |
| 55  | q     | 78  | HIS  |
| 56  | r     | 7   | GLN  |
| 58  | t     | 98  | ASN  |
| 59  | u     | 43  | GLN  |
| 59  | u     | 100 | HIS  |
| 61  | w     | 66  | GLN  |
| 18  | x     | 10  | GLN  |
| 64  | 13    | 6   | ASN  |
| 64  | 13    | 19  | GLN  |
| 64  | 13    | 22  | ASN  |
| 64  | 13    | 29  | GLN  |
| 64  | 13    | 117 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 64  | 13    | 122  | GLN  |
| 64  | 13    | 246  | ASN  |
| 64  | 13    | 254  | GLN  |
| 64  | 13    | 451  | ASN  |
| 64  | 13    | 578  | ASN  |
| 64  | 13    | 588  | HIS  |
| 64  | 13    | 604  | GLN  |
| 64  | 13    | 642  | GLN  |
| 64  | 13    | 662  | ASN  |
| 64  | 13    | 736  | ASN  |
| 64  | 13    | 786  | GLN  |
| 64  | 13    | 864  | ASN  |
| 64  | 13    | 905  | GLN  |
| 64  | 13    | 1002 | GLN  |
| 64  | 13    | 1154 | GLN  |
| 64  | 13    | 1191 | GLN  |
| 65  | 14    | 32   | GLN  |
| 65  | 14    | 85   | GLN  |
| 65  | 14    | 111  | GLN  |
| 65  | 14    | 181  | ASN  |
| 65  | 14    | 270  | GLN  |
| 65  | 14    | 454  | GLN  |
| 65  | 14    | 676  | ASN  |
| 65  | 14    | 736  | GLN  |
| 65  | 14    | 764  | GLN  |
| 65  | 14    | 928  | ASN  |
| 65  | 14    | 941  | ASN  |
| 65  | 14    | 1032 | GLN  |
| 65  | 14    | 1140 | ASN  |
| 65  | 14    | 1143 | GLN  |
| 65  | 14    | 1173 | GLN  |
| 66  | 15    | 13   | GLN  |
| 66  | 15    | 62   | ASN  |
| 66  | 15    | 130  | GLN  |
| 66  | 15    | 140  | ASN  |
| 66  | 15    | 220  | GLN  |
| 66  | 15    | 241  | ASN  |
| 66  | 15    | 295  | ASN  |
| 66  | 15    | 351  | GLN  |
| 66  | 15    | 396  | GLN  |
| 66  | 15    | 406  | ASN  |
| 66  | 15    | 407  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | 15    | 424 | HIS  |
| 66  | 15    | 428 | GLN  |
| 66  | 15    | 540 | ASN  |
| 66  | 15    | 556 | GLN  |
| 66  | 15    | 637 | ASN  |
| 66  | 15    | 676 | GLN  |
| 66  | 15    | 693 | GLN  |
| 66  | 15    | 701 | GLN  |
| 66  | 15    | 814 | GLN  |
| 66  | 15    | 834 | ASN  |
| 66  | 15    | 843 | ASN  |
| 66  | 15    | 900 | GLN  |
| 67  | 18    | 3   | ASN  |
| 67  | 18    | 66  | ASN  |
| 67  | 18    | 88  | GLN  |
| 67  | 18    | 106 | ASN  |
| 67  | 18    | 177 | HIS  |
| 67  | 18    | 179 | GLN  |
| 67  | 18    | 197 | ASN  |
| 67  | 18    | 204 | HIS  |
| 67  | 18    | 259 | GLN  |
| 67  | 16    | 3   | ASN  |
| 67  | 16    | 63  | ASN  |
| 67  | 16    | 66  | ASN  |
| 67  | 16    | 71  | GLN  |
| 67  | 16    | 106 | ASN  |
| 67  | 16    | 151 | GLN  |
| 67  | 16    | 177 | HIS  |
| 67  | 16    | 259 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | 5     | 1506/1523 (98%) | 255 (16%)         | 8 (0%)          |
| 11  | 6     | 1/1523 (0%)     | 0                 | 0               |
| 12  | 7     | 75/76 (98%)     | 19 (25%)          | 1 (1%)          |
| 13  | 8     | 75/76 (98%)     | 18 (24%)          | 1 (1%)          |
| 17  | AB    | 20/21 (95%)     | 11 (55%)          | 3 (15%)         |
| 37  | Y     | 5/21 (23%)      | 1 (20%)           | 0               |
| 8   | 3     | 2892/2907 (99%) | 505 (17%)         | 13 (0%)         |
| 9   | 4     | 107/108 (99%)   | 29 (27%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| All | All   | 4681/6255 (74%) | 838 (17%)         | 26 (0%)         |

All (838) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 3     | 11  | U    |
| 8   | 3     | 12  | A    |
| 8   | 3     | 13  | C    |
| 8   | 3     | 14  | U    |
| 8   | 3     | 28  | G    |
| 8   | 3     | 37  | G    |
| 8   | 3     | 48  | G    |
| 8   | 3     | 64  | U    |
| 8   | 3     | 65  | A    |
| 8   | 3     | 73  | A    |
| 8   | 3     | 76  | A    |
| 8   | 3     | 77  | G    |
| 8   | 3     | 102 | A    |
| 8   | 3     | 103 | G    |
| 8   | 3     | 119 | A    |
| 8   | 3     | 121 | U    |
| 8   | 3     | 126 | C    |
| 8   | 3     | 132 | G    |
| 8   | 3     | 141 | A    |
| 8   | 3     | 142 | A    |
| 8   | 3     | 163 | A    |
| 8   | 3     | 180 | A    |
| 8   | 3     | 184 | A    |
| 8   | 3     | 187 | C    |
| 8   | 3     | 200 | A    |
| 8   | 3     | 203 | A    |
| 8   | 3     | 219 | G    |
| 8   | 3     | 220 | A    |
| 8   | 3     | 225 | A    |
| 8   | 3     | 226 | A    |
| 8   | 3     | 232 | A    |
| 8   | 3     | 234 | G    |
| 8   | 3     | 237 | A    |
| 8   | 3     | 245 | U    |
| 8   | 3     | 246 | G    |
| 8   | 3     | 252 | G    |
| 8   | 3     | 269 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 3     | 276 | A    |
| 8   | 3     | 284 | U    |
| 8   | 3     | 287 | G    |
| 8   | 3     | 295 | U    |
| 8   | 3     | 296 | U    |
| 8   | 3     | 297 | G    |
| 8   | 3     | 298 | U    |
| 8   | 3     | 299 | A    |
| 8   | 3     | 309 | A    |
| 8   | 3     | 310 | U    |
| 8   | 3     | 311 | G    |
| 8   | 3     | 315 | A    |
| 8   | 3     | 316 | C    |
| 8   | 3     | 317 | U    |
| 8   | 3     | 319 | G    |
| 8   | 3     | 325 | G    |
| 8   | 3     | 336 | C    |
| 8   | 3     | 345 | A    |
| 8   | 3     | 363 | G    |
| 8   | 3     | 364 | A    |
| 8   | 3     | 365 | U    |
| 8   | 3     | 402 | A    |
| 8   | 3     | 409 | A    |
| 8   | 3     | 410 | G    |
| 8   | 3     | 411 | U    |
| 8   | 3     | 418 | G    |
| 8   | 3     | 419 | A    |
| 8   | 3     | 424 | G    |
| 8   | 3     | 425 | U    |
| 8   | 3     | 426 | U    |
| 8   | 3     | 432 | G    |
| 8   | 3     | 437 | A    |
| 8   | 3     | 440 | C    |
| 8   | 3     | 460 | G    |
| 8   | 3     | 463 | U    |
| 8   | 3     | 483 | A    |
| 8   | 3     | 517 | G    |
| 8   | 3     | 539 | U    |
| 8   | 3     | 540 | A    |
| 8   | 3     | 548 | A    |
| 8   | 3     | 562 | C    |
| 8   | 3     | 565 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 3     | 566 | G    |
| 8   | 3     | 567 | U    |
| 8   | 3     | 573 | A    |
| 8   | 3     | 581 | A    |
| 8   | 3     | 583 | U    |
| 8   | 3     | 596 | G    |
| 8   | 3     | 598 | G    |
| 8   | 3     | 607 | U    |
| 8   | 3     | 608 | A    |
| 8   | 3     | 610 | G    |
| 8   | 3     | 620 | G    |
| 8   | 3     | 636 | U    |
| 8   | 3     | 637 | U    |
| 8   | 3     | 638 | A    |
| 8   | 3     | 648 | G    |
| 8   | 3     | 649 | A    |
| 8   | 3     | 650 | G    |
| 8   | 3     | 663 | A    |
| 8   | 3     | 670 | G    |
| 8   | 3     | 673 | A    |
| 8   | 3     | 681 | A    |
| 8   | 3     | 682 | A    |
| 8   | 3     | 689 | U    |
| 8   | 3     | 691 | G    |
| 8   | 3     | 705 | A    |
| 8   | 3     | 712 | A    |
| 8   | 3     | 716 | G    |
| 8   | 3     | 721 | G    |
| 8   | 3     | 722 | C    |
| 8   | 3     | 765 | A    |
| 8   | 3     | 775 | C    |
| 8   | 3     | 782 | U    |
| 8   | 3     | 792 | G    |
| 8   | 3     | 797 | U    |
| 8   | 3     | 800 | C    |
| 8   | 3     | 810 | G    |
| 8   | 3     | 811 | G    |
| 8   | 3     | 817 | A    |
| 8   | 3     | 819 | U    |
| 8   | 3     | 820 | U    |
| 8   | 3     | 824 | A    |
| 8   | 3     | 828 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 829  | A    |
| 8   | 3     | 840  | G    |
| 8   | 3     | 846  | U    |
| 8   | 3     | 847  | C    |
| 8   | 3     | 854  | A    |
| 8   | 3     | 862  | U    |
| 8   | 3     | 881  | A    |
| 8   | 3     | 882  | C    |
| 8   | 3     | 883  | A    |
| 8   | 3     | 901  | C    |
| 8   | 3     | 902  | U    |
| 8   | 3     | 903  | A    |
| 8   | 3     | 904  | C    |
| 8   | 3     | 906  | G    |
| 8   | 3     | 918  | G    |
| 8   | 3     | 924  | C    |
| 8   | 3     | 926  | U    |
| 8   | 3     | 927  | A    |
| 8   | 3     | 928  | G    |
| 8   | 3     | 930  | C    |
| 8   | 3     | 932  | U    |
| 8   | 3     | 934  | C    |
| 8   | 3     | 935  | U    |
| 8   | 3     | 936  | G    |
| 8   | 3     | 944  | U    |
| 8   | 3     | 947  | A    |
| 8   | 3     | 949  | C    |
| 8   | 3     | 951  | C    |
| 8   | 3     | 952  | U    |
| 8   | 3     | 953  | G    |
| 8   | 3     | 970  | U    |
| 8   | 3     | 981  | A    |
| 8   | 3     | 982  | G    |
| 8   | 3     | 994  | U    |
| 8   | 3     | 997  | G    |
| 8   | 3     | 998  | C    |
| 8   | 3     | 1008 | A    |
| 8   | 3     | 1010 | G    |
| 8   | 3     | 1016 | A    |
| 8   | 3     | 1019 | A    |
| 8   | 3     | 1026 | A    |
| 8   | 3     | 1032 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 1039 | G    |
| 8   | 3     | 1045 | A    |
| 8   | 3     | 1049 | U    |
| 8   | 3     | 1058 | U    |
| 8   | 3     | 1060 | G    |
| 8   | 3     | 1061 | A    |
| 8   | 3     | 1068 | U    |
| 8   | 3     | 1074 | A    |
| 8   | 3     | 1080 | A    |
| 8   | 3     | 1082 | A    |
| 8   | 3     | 1084 | C    |
| 8   | 3     | 1096 | U    |
| 8   | 3     | 1097 | G    |
| 8   | 3     | 1098 | G    |
| 8   | 3     | 1099 | C    |
| 8   | 3     | 1102 | A    |
| 8   | 3     | 1104 | A    |
| 8   | 3     | 1105 | A    |
| 8   | 3     | 1106 | G    |
| 8   | 3     | 1107 | C    |
| 8   | 3     | 1110 | C    |
| 8   | 3     | 1111 | C    |
| 8   | 3     | 1113 | U    |
| 8   | 3     | 1114 | C    |
| 8   | 3     | 1115 | G    |
| 8   | 3     | 1120 | A    |
| 8   | 3     | 1122 | G    |
| 8   | 3     | 1123 | A    |
| 8   | 3     | 1125 | U    |
| 8   | 3     | 1130 | A    |
| 8   | 3     | 1132 | C    |
| 8   | 3     | 1138 | A    |
| 8   | 3     | 1144 | C    |
| 8   | 3     | 1145 | G    |
| 8   | 3     | 1146 | A    |
| 8   | 3     | 1147 | G    |
| 8   | 3     | 1165 | U    |
| 8   | 3     | 1167 | U    |
| 8   | 3     | 1168 | A    |
| 8   | 3     | 1170 | C    |
| 8   | 3     | 1176 | U    |
| 8   | 3     | 1177 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 1178 | A    |
| 8   | 3     | 1204 | A    |
| 8   | 3     | 1208 | A    |
| 8   | 3     | 1209 | U    |
| 8   | 3     | 1210 | A    |
| 8   | 3     | 1212 | C    |
| 8   | 3     | 1215 | G    |
| 8   | 3     | 1234 | U    |
| 8   | 3     | 1235 | U    |
| 8   | 3     | 1236 | G    |
| 8   | 3     | 1242 | G    |
| 8   | 3     | 1246 | U    |
| 8   | 3     | 1250 | A    |
| 8   | 3     | 1251 | G    |
| 8   | 3     | 1253 | G    |
| 8   | 3     | 1256 | A    |
| 8   | 3     | 1257 | G    |
| 8   | 3     | 1266 | G    |
| 8   | 3     | 1268 | U    |
| 8   | 3     | 1280 | G    |
| 8   | 3     | 1281 | A    |
| 8   | 3     | 1283 | A    |
| 8   | 3     | 1285 | U    |
| 8   | 3     | 1286 | G    |
| 8   | 3     | 1292 | A    |
| 8   | 3     | 1301 | G    |
| 8   | 3     | 1304 | U    |
| 8   | 3     | 1313 | G    |
| 8   | 3     | 1325 | C    |
| 8   | 3     | 1328 | A    |
| 8   | 3     | 1329 | U    |
| 8   | 3     | 1330 | U    |
| 8   | 3     | 1369 | U    |
| 8   | 3     | 1378 | C    |
| 8   | 3     | 1380 | U    |
| 8   | 3     | 1388 | G    |
| 8   | 3     | 1393 | A    |
| 8   | 3     | 1406 | A    |
| 8   | 3     | 1407 | U    |
| 8   | 3     | 1412 | A    |
| 8   | 3     | 1423 | A    |
| 8   | 3     | 1424 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 1431 | A    |
| 8   | 3     | 1444 | C    |
| 8   | 3     | 1445 | U    |
| 8   | 3     | 1446 | G    |
| 8   | 3     | 1448 | U    |
| 8   | 3     | 1456 | C    |
| 8   | 3     | 1463 | G    |
| 8   | 3     | 1467 | U    |
| 8   | 3     | 1480 | A    |
| 8   | 3     | 1481 | U    |
| 8   | 3     | 1483 | G    |
| 8   | 3     | 1486 | U    |
| 8   | 3     | 1487 | U    |
| 8   | 3     | 1502 | A    |
| 8   | 3     | 1504 | G    |
| 8   | 3     | 1508 | G    |
| 8   | 3     | 1510 | A    |
| 8   | 3     | 1513 | A    |
| 8   | 3     | 1514 | U    |
| 8   | 3     | 1515 | A    |
| 8   | 3     | 1519 | A    |
| 8   | 3     | 1522 | U    |
| 8   | 3     | 1534 | A    |
| 8   | 3     | 1535 | A    |
| 8   | 3     | 1541 | A    |
| 8   | 3     | 1546 | U    |
| 8   | 3     | 1550 | G    |
| 8   | 3     | 1569 | A    |
| 8   | 3     | 1570 | A    |
| 8   | 3     | 1571 | G    |
| 8   | 3     | 1580 | G    |
| 8   | 3     | 1582 | G    |
| 8   | 3     | 1584 | U    |
| 8   | 3     | 1585 | A    |
| 8   | 3     | 1588 | A    |
| 8   | 3     | 1589 | A    |
| 8   | 3     | 1603 | A    |
| 8   | 3     | 1612 | U    |
| 8   | 3     | 1617 | U    |
| 8   | 3     | 1618 | U    |
| 8   | 3     | 1619 | A    |
| 8   | 3     | 1641 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 1642 | G    |
| 8   | 3     | 1643 | A    |
| 8   | 3     | 1644 | A    |
| 8   | 3     | 1645 | C    |
| 8   | 3     | 1650 | A    |
| 8   | 3     | 1651 | C    |
| 8   | 3     | 1661 | A    |
| 8   | 3     | 1668 | G    |
| 8   | 3     | 1680 | A    |
| 8   | 3     | 1681 | G    |
| 8   | 3     | 1682 | C    |
| 8   | 3     | 1688 | A    |
| 8   | 3     | 1694 | A    |
| 8   | 3     | 1708 | G    |
| 8   | 3     | 1727 | U    |
| 8   | 3     | 1737 | G    |
| 8   | 3     | 1748 | U    |
| 8   | 3     | 1749 | A    |
| 8   | 3     | 1764 | U    |
| 8   | 3     | 1769 | A    |
| 8   | 3     | 1770 | A    |
| 8   | 3     | 1771 | C    |
| 8   | 3     | 1780 | A    |
| 8   | 3     | 1789 | C    |
| 8   | 3     | 1791 | A    |
| 8   | 3     | 1807 | C    |
| 8   | 3     | 1808 | C    |
| 8   | 3     | 1809 | A    |
| 8   | 3     | 1816 | A    |
| 8   | 3     | 1823 | U    |
| 8   | 3     | 1836 | A    |
| 8   | 3     | 1854 | A    |
| 8   | 3     | 1855 | A    |
| 8   | 3     | 1866 | G    |
| 8   | 3     | 1869 | G    |
| 8   | 3     | 1878 | A    |
| 8   | 3     | 1886 | C    |
| 8   | 3     | 1910 | G    |
| 8   | 3     | 1913 | G    |
| 8   | 3     | 1920 | A    |
| 8   | 3     | 1936 | G    |
| 8   | 3     | 1937 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 1938 | U    |
| 8   | 3     | 1943 | A    |
| 8   | 3     | 1944 | A    |
| 8   | 3     | 1962 | U    |
| 8   | 3     | 1974 | U    |
| 8   | 3     | 1977 | A    |
| 8   | 3     | 1978 | U    |
| 8   | 3     | 1979 | G    |
| 8   | 3     | 1998 | U    |
| 8   | 3     | 1999 | G    |
| 8   | 3     | 2000 | U    |
| 8   | 3     | 2004 | G    |
| 8   | 3     | 2028 | G    |
| 8   | 3     | 2030 | A    |
| 8   | 3     | 2038 | A    |
| 8   | 3     | 2040 | A    |
| 8   | 3     | 2041 | C    |
| 8   | 3     | 2042 | A    |
| 8   | 3     | 2050 | G    |
| 8   | 3     | 2057 | C    |
| 8   | 3     | 2062 | C    |
| 8   | 3     | 2063 | G    |
| 8   | 3     | 2067 | A    |
| 8   | 3     | 2068 | G    |
| 8   | 3     | 2069 | A    |
| 8   | 3     | 2076 | G    |
| 8   | 3     | 2084 | A    |
| 8   | 3     | 2099 | U    |
| 8   | 3     | 2100 | G    |
| 8   | 3     | 2106 | G    |
| 8   | 3     | 2110 | U    |
| 8   | 3     | 2111 | U    |
| 8   | 3     | 2112 | A    |
| 8   | 3     | 2114 | C    |
| 8   | 3     | 2115 | A    |
| 8   | 3     | 2117 | G    |
| 8   | 3     | 2123 | A    |
| 8   | 3     | 2124 | A    |
| 8   | 3     | 2125 | U    |
| 8   | 3     | 2139 | C    |
| 8   | 3     | 2140 | G    |
| 8   | 3     | 2153 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 2154 | A    |
| 8   | 3     | 2164 | G    |
| 8   | 3     | 2166 | U    |
| 8   | 3     | 2171 | A    |
| 8   | 3     | 2180 | U    |
| 8   | 3     | 2181 | A    |
| 8   | 3     | 2193 | U    |
| 8   | 3     | 2195 | U    |
| 8   | 3     | 2196 | G    |
| 8   | 3     | 2197 | U    |
| 8   | 3     | 2198 | G    |
| 8   | 3     | 2199 | C    |
| 8   | 3     | 2200 | U    |
| 8   | 3     | 2201 | G    |
| 8   | 3     | 2202 | U    |
| 8   | 3     | 2207 | A    |
| 8   | 3     | 2211 | G    |
| 8   | 3     | 2212 | U    |
| 8   | 3     | 2219 | U    |
| 8   | 3     | 2220 | A    |
| 8   | 3     | 2221 | U    |
| 8   | 3     | 2227 | U    |
| 8   | 3     | 2228 | U    |
| 8   | 3     | 2233 | A    |
| 8   | 3     | 2246 | G    |
| 8   | 3     | 2247 | G    |
| 8   | 3     | 2274 | A    |
| 8   | 3     | 2276 | A    |
| 8   | 3     | 2287 | G    |
| 8   | 3     | 2291 | U    |
| 8   | 3     | 2295 | A    |
| 8   | 3     | 2298 | G    |
| 8   | 3     | 2305 | C    |
| 8   | 3     | 2311 | G    |
| 8   | 3     | 2313 | U    |
| 8   | 3     | 2316 | G    |
| 8   | 3     | 2319 | A    |
| 8   | 3     | 2327 | U    |
| 8   | 3     | 2329 | G    |
| 8   | 3     | 2333 | G    |
| 8   | 3     | 2335 | A    |
| 8   | 3     | 2336 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 2342 | U    |
| 8   | 3     | 2343 | A    |
| 8   | 3     | 2344 | A    |
| 8   | 3     | 2353 | G    |
| 8   | 3     | 2355 | C    |
| 8   | 3     | 2358 | U    |
| 8   | 3     | 2366 | A    |
| 8   | 3     | 2391 | G    |
| 8   | 3     | 2393 | C    |
| 8   | 3     | 2397 | G    |
| 8   | 3     | 2410 | C    |
| 8   | 3     | 2411 | C    |
| 8   | 3     | 2414 | U    |
| 8   | 3     | 2422 | G    |
| 8   | 3     | 2431 | U    |
| 8   | 3     | 2433 | A    |
| 8   | 3     | 2437 | G    |
| 8   | 3     | 2438 | A    |
| 8   | 3     | 2443 | A    |
| 8   | 3     | 2449 | U    |
| 8   | 3     | 2456 | A    |
| 8   | 3     | 2477 | A    |
| 8   | 3     | 2481 | U    |
| 8   | 3     | 2482 | U    |
| 8   | 3     | 2483 | C    |
| 8   | 3     | 2484 | A    |
| 8   | 3     | 2486 | A    |
| 8   | 3     | 2488 | C    |
| 8   | 3     | 2499 | U    |
| 8   | 3     | 2510 | G    |
| 8   | 3     | 2512 | U    |
| 8   | 3     | 2513 | G    |
| 8   | 3     | 2521 | A    |
| 8   | 3     | 2526 | A    |
| 8   | 3     | 2537 | G    |
| 8   | 3     | 2543 | G    |
| 8   | 3     | 2574 | A    |
| 8   | 3     | 2575 | G    |
| 8   | 3     | 2580 | A    |
| 8   | 3     | 2585 | A    |
| 8   | 3     | 2593 | U    |
| 8   | 3     | 2594 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 2605 | G    |
| 8   | 3     | 2610 | A    |
| 8   | 3     | 2611 | G    |
| 8   | 3     | 2617 | U    |
| 8   | 3     | 2618 | C    |
| 8   | 3     | 2621 | U    |
| 8   | 3     | 2623 | U    |
| 8   | 3     | 2637 | A    |
| 8   | 3     | 2638 | G    |
| 8   | 3     | 2654 | U    |
| 8   | 3     | 2668 | A    |
| 8   | 3     | 2669 | G    |
| 8   | 3     | 2697 | C    |
| 8   | 3     | 2698 | U    |
| 8   | 3     | 2722 | G    |
| 8   | 3     | 2734 | C    |
| 8   | 3     | 2737 | G    |
| 8   | 3     | 2741 | A    |
| 8   | 3     | 2752 | G    |
| 8   | 3     | 2756 | A    |
| 8   | 3     | 2760 | C    |
| 8   | 3     | 2764 | U    |
| 8   | 3     | 2765 | A    |
| 8   | 3     | 2773 | A    |
| 8   | 3     | 2786 | A    |
| 8   | 3     | 2798 | A    |
| 8   | 3     | 2799 | U    |
| 8   | 3     | 2804 | C    |
| 8   | 3     | 2806 | A    |
| 8   | 3     | 2807 | G    |
| 8   | 3     | 2808 | A    |
| 8   | 3     | 2810 | A    |
| 8   | 3     | 2813 | A    |
| 8   | 3     | 2822 | C    |
| 8   | 3     | 2824 | A    |
| 8   | 3     | 2829 | G    |
| 8   | 3     | 2839 | A    |
| 8   | 3     | 2853 | U    |
| 8   | 3     | 2862 | U    |
| 8   | 3     | 2863 | G    |
| 8   | 3     | 2871 | G    |
| 8   | 3     | 2876 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 2884 | C    |
| 8   | 3     | 2887 | A    |
| 8   | 3     | 2888 | U    |
| 8   | 3     | 2895 | A    |
| 8   | 3     | 2896 | G    |
| 8   | 3     | 2899 | C    |
| 9   | 4     | 9    | C    |
| 9   | 4     | 10   | C    |
| 9   | 4     | 11   | A    |
| 9   | 4     | 13   | G    |
| 9   | 4     | 14   | U    |
| 9   | 4     | 22   | G    |
| 9   | 4     | 23   | A    |
| 9   | 4     | 28   | C    |
| 9   | 4     | 33   | U    |
| 9   | 4     | 35   | C    |
| 9   | 4     | 39   | U    |
| 9   | 4     | 41   | C    |
| 9   | 4     | 48   | A    |
| 9   | 4     | 49   | G    |
| 9   | 4     | 54   | U    |
| 9   | 4     | 56   | A    |
| 9   | 4     | 60   | C    |
| 9   | 4     | 64   | G    |
| 9   | 4     | 65   | G    |
| 9   | 4     | 80   | G    |
| 9   | 4     | 82   | U    |
| 9   | 4     | 83   | U    |
| 9   | 4     | 84   | C    |
| 9   | 4     | 85   | A    |
| 9   | 4     | 88   | G    |
| 9   | 4     | 89   | A    |
| 9   | 4     | 99   | A    |
| 9   | 4     | 106  | A    |
| 9   | 4     | 108  | C    |
| 10  | 5     | 6    | C    |
| 10  | 5     | 10   | G    |
| 10  | 5     | 33   | A    |
| 10  | 5     | 40   | G    |
| 10  | 5     | 48   | C    |
| 10  | 5     | 49   | C    |
| 10  | 5     | 52   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | 5     | 57  | U    |
| 10  | 5     | 61  | A    |
| 10  | 5     | 106 | C    |
| 10  | 5     | 114 | C    |
| 10  | 5     | 115 | A    |
| 10  | 5     | 117 | U    |
| 10  | 5     | 120 | A    |
| 10  | 5     | 149 | G    |
| 10  | 5     | 154 | G    |
| 10  | 5     | 163 | G    |
| 10  | 5     | 167 | A    |
| 10  | 5     | 171 | A    |
| 10  | 5     | 173 | U    |
| 10  | 5     | 176 | G    |
| 10  | 5     | 180 | C    |
| 10  | 5     | 182 | C    |
| 10  | 5     | 185 | G    |
| 10  | 5     | 186 | A    |
| 10  | 5     | 189 | C    |
| 10  | 5     | 190 | A    |
| 10  | 5     | 197 | A    |
| 10  | 5     | 198 | A    |
| 10  | 5     | 199 | A    |
| 10  | 5     | 220 | U    |
| 10  | 5     | 223 | G    |
| 10  | 5     | 239 | A    |
| 10  | 5     | 241 | C    |
| 10  | 5     | 243 | G    |
| 10  | 5     | 247 | G    |
| 10  | 5     | 262 | G    |
| 10  | 5     | 263 | C    |
| 10  | 5     | 269 | A    |
| 10  | 5     | 275 | A    |
| 10  | 5     | 285 | G    |
| 10  | 5     | 301 | G    |
| 10  | 5     | 302 | A    |
| 10  | 5     | 324 | C    |
| 10  | 5     | 325 | A    |
| 10  | 5     | 326 | C    |
| 10  | 5     | 328 | G    |
| 10  | 5     | 341 | C    |
| 10  | 5     | 342 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | 5     | 344 | G    |
| 10  | 5     | 347 | G    |
| 10  | 5     | 348 | C    |
| 10  | 5     | 350 | G    |
| 10  | 5     | 359 | A    |
| 10  | 5     | 363 | U    |
| 10  | 5     | 368 | C    |
| 10  | 5     | 369 | A    |
| 10  | 5     | 370 | A    |
| 10  | 5     | 374 | G    |
| 10  | 5     | 380 | G    |
| 10  | 5     | 383 | U    |
| 10  | 5     | 394 | U    |
| 10  | 5     | 403 | A    |
| 10  | 5     | 408 | U    |
| 10  | 5     | 416 | U    |
| 10  | 5     | 418 | U    |
| 10  | 5     | 419 | A    |
| 10  | 5     | 422 | A    |
| 10  | 5     | 425 | G    |
| 10  | 5     | 426 | U    |
| 10  | 5     | 447 | G    |
| 10  | 5     | 449 | A    |
| 10  | 5     | 450 | U    |
| 10  | 5     | 452 | A    |
| 10  | 5     | 461 | G    |
| 10  | 5     | 462 | G    |
| 10  | 5     | 464 | A    |
| 10  | 5     | 468 | G    |
| 10  | 5     | 470 | U    |
| 10  | 5     | 475 | U    |
| 10  | 5     | 476 | U    |
| 10  | 5     | 477 | U    |
| 10  | 5     | 481 | U    |
| 10  | 5     | 482 | G    |
| 10  | 5     | 488 | U    |
| 10  | 5     | 489 | U    |
| 10  | 5     | 493 | A    |
| 10  | 5     | 494 | A    |
| 10  | 5     | 495 | U    |
| 10  | 5     | 507 | A    |
| 10  | 5     | 509 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | 5     | 510 | U    |
| 10  | 5     | 516 | C    |
| 10  | 5     | 517 | C    |
| 10  | 5     | 522 | G    |
| 10  | 5     | 525 | G7M  |
| 10  | 5     | 530 | A    |
| 10  | 5     | 531 | A    |
| 10  | 5     | 545 | A    |
| 10  | 5     | 557 | A    |
| 10  | 5     | 560 | U    |
| 10  | 5     | 562 | U    |
| 10  | 5     | 570 | A    |
| 10  | 5     | 571 | A    |
| 10  | 5     | 572 | A    |
| 10  | 5     | 574 | C    |
| 10  | 5     | 575 | A    |
| 10  | 5     | 579 | G    |
| 10  | 5     | 586 | G    |
| 10  | 5     | 594 | A    |
| 10  | 5     | 595 | G    |
| 10  | 5     | 628 | A    |
| 10  | 5     | 650 | A    |
| 10  | 5     | 661 | G    |
| 10  | 5     | 662 | G    |
| 10  | 5     | 683 | G    |
| 10  | 5     | 700 | G    |
| 10  | 5     | 715 | A    |
| 10  | 5     | 719 | G    |
| 10  | 5     | 720 | U    |
| 10  | 5     | 721 | G    |
| 10  | 5     | 728 | G    |
| 10  | 5     | 745 | U    |
| 10  | 5     | 752 | G    |
| 10  | 5     | 768 | G    |
| 10  | 5     | 790 | U    |
| 10  | 5     | 791 | A    |
| 10  | 5     | 811 | A    |
| 10  | 5     | 812 | A    |
| 10  | 5     | 814 | C    |
| 10  | 5     | 818 | A    |
| 10  | 5     | 825 | A    |
| 10  | 5     | 829 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | 5     | 836  | C    |
| 10  | 5     | 838  | A    |
| 10  | 5     | 839  | U    |
| 10  | 5     | 867  | A    |
| 10  | 5     | 883  | A    |
| 10  | 5     | 885  | U    |
| 10  | 5     | 908  | A    |
| 10  | 5     | 910  | C    |
| 10  | 5     | 911  | G    |
| 10  | 5     | 921  | G    |
| 10  | 5     | 922  | G    |
| 10  | 5     | 929  | C    |
| 10  | 5     | 930  | A    |
| 10  | 5     | 955  | U    |
| 10  | 5     | 964  | A    |
| 10  | 5     | 970  | A    |
| 10  | 5     | 971  | A    |
| 10  | 5     | 972  | A    |
| 10  | 5     | 982  | A    |
| 10  | 5     | 987  | U    |
| 10  | 5     | 988  | G    |
| 10  | 5     | 989  | A    |
| 10  | 5     | 994  | C    |
| 10  | 5     | 995  | U    |
| 10  | 5     | 996  | U    |
| 10  | 5     | 997  | G    |
| 10  | 5     | 998  | G    |
| 10  | 5     | 999  | C    |
| 10  | 5     | 1000 | A    |
| 10  | 5     | 1002 | A    |
| 10  | 5     | 1007 | U    |
| 10  | 5     | 1009 | G    |
| 10  | 5     | 1015 | U    |
| 10  | 5     | 1018 | U    |
| 10  | 5     | 1019 | G    |
| 10  | 5     | 1020 | G    |
| 10  | 5     | 1022 | G    |
| 10  | 5     | 1023 | G    |
| 10  | 5     | 1024 | U    |
| 10  | 5     | 1025 | U    |
| 10  | 5     | 1027 | A    |
| 10  | 5     | 1028 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | 5     | 1029 | C    |
| 10  | 5     | 1030 | G    |
| 10  | 5     | 1032 | G    |
| 10  | 5     | 1034 | G    |
| 10  | 5     | 1036 | C    |
| 10  | 5     | 1044 | G    |
| 10  | 5     | 1045 | C    |
| 10  | 5     | 1047 | U    |
| 10  | 5     | 1056 | U    |
| 10  | 5     | 1072 | G    |
| 10  | 5     | 1076 | U    |
| 10  | 5     | 1078 | G    |
| 10  | 5     | 1083 | A    |
| 10  | 5     | 1085 | G    |
| 10  | 5     | 1086 | U    |
| 10  | 5     | 1092 | A    |
| 10  | 5     | 1118 | A    |
| 10  | 5     | 1121 | U    |
| 10  | 5     | 1122 | U    |
| 10  | 5     | 1123 | G    |
| 10  | 5     | 1124 | U    |
| 10  | 5     | 1134 | C    |
| 10  | 5     | 1135 | U    |
| 10  | 5     | 1141 | U    |
| 10  | 5     | 1142 | G    |
| 10  | 5     | 1158 | A    |
| 10  | 5     | 1159 | A    |
| 10  | 5     | 1170 | C    |
| 10  | 5     | 1171 | A    |
| 10  | 5     | 1172 | A    |
| 10  | 5     | 1188 | A    |
| 10  | 5     | 1189 | U    |
| 10  | 5     | 1202 | A    |
| 10  | 5     | 1203 | A    |
| 10  | 5     | 1215 | U    |
| 10  | 5     | 1231 | U    |
| 10  | 5     | 1232 | C    |
| 10  | 5     | 1233 | G    |
| 10  | 5     | 1235 | C    |
| 10  | 5     | 1255 | A    |
| 10  | 5     | 1260 | U    |
| 10  | 5     | 1271 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | 5     | 1274 | G    |
| 10  | 5     | 1279 | G    |
| 10  | 5     | 1291 | C    |
| 10  | 5     | 1294 | U    |
| 10  | 5     | 1296 | C    |
| 10  | 5     | 1297 | G    |
| 10  | 5     | 1306 | A    |
| 10  | 5     | 1312 | G    |
| 10  | 5     | 1320 | A    |
| 10  | 5     | 1321 | G    |
| 10  | 5     | 1337 | U    |
| 10  | 5     | 1338 | A    |
| 10  | 5     | 1339 | U    |
| 10  | 5     | 1343 | G    |
| 10  | 5     | 1345 | G    |
| 10  | 5     | 1372 | C    |
| 10  | 5     | 1373 | A    |
| 10  | 5     | 1397 | G    |
| 10  | 5     | 1417 | U    |
| 10  | 5     | 1426 | U    |
| 10  | 5     | 1427 | U    |
| 10  | 5     | 1428 | A    |
| 10  | 5     | 1429 | G    |
| 10  | 5     | 1462 | G    |
| 10  | 5     | 1466 | U    |
| 10  | 5     | 1467 | A    |
| 10  | 5     | 1469 | G    |
| 10  | 5     | 1472 | G    |
| 10  | 5     | 1478 | A    |
| 10  | 5     | 1480 | G    |
| 10  | 5     | 1481 | U    |
| 10  | 5     | 1482 | A    |
| 10  | 5     | 1492 | G    |
| 10  | 5     | 1494 | MA6  |
| 10  | 5     | 1504 | G    |
| 10  | 5     | 1505 | G    |
| 10  | 5     | 1510 | C    |
| 10  | 5     | 1511 | C    |
| 12  | 7     | 4    | C    |
| 12  | 7     | 8    | 4SU  |
| 12  | 7     | 11   | C    |
| 12  | 7     | 13   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | 7     | 15  | G    |
| 12  | 7     | 16  | U    |
| 12  | 7     | 17  | C    |
| 12  | 7     | 19  | G    |
| 12  | 7     | 20  | U    |
| 12  | 7     | 21  | A    |
| 12  | 7     | 22  | G    |
| 12  | 7     | 46  | G7M  |
| 12  | 7     | 48  | C    |
| 12  | 7     | 49  | C    |
| 12  | 7     | 52  | G    |
| 12  | 7     | 58  | A    |
| 12  | 7     | 72  | C    |
| 12  | 7     | 74  | C    |
| 12  | 7     | 76  | A    |
| 13  | 8     | 4   | U    |
| 13  | 8     | 9   | A    |
| 13  | 8     | 10  | G    |
| 13  | 8     | 16  | U    |
| 13  | 8     | 17  | U    |
| 13  | 8     | 18  | G    |
| 13  | 8     | 19  | G    |
| 13  | 8     | 20  | U    |
| 13  | 8     | 21  | A    |
| 13  | 8     | 46  | G    |
| 13  | 8     | 48  | C    |
| 13  | 8     | 54  | 5MU  |
| 13  | 8     | 58  | A    |
| 13  | 8     | 60  | U    |
| 13  | 8     | 73  | A    |
| 13  | 8     | 74  | C    |
| 13  | 8     | 75  | C    |
| 13  | 8     | 76  | A    |
| 17  | AB    | 36  | U    |
| 17  | AB    | 37  | G    |
| 17  | AB    | 40  | U    |
| 17  | AB    | 47  | U    |
| 17  | AB    | 49  | U    |
| 17  | AB    | 50  | U    |
| 17  | AB    | 51  | C    |
| 17  | AB    | 52  | A    |
| 17  | AB    | 53  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | AB    | 54  | A    |
| 17  | AB    | 55  | A    |
| 37  | Y     | 43  | A    |

All (26) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 3     | 315  | A    |
| 8   | 3     | 410  | G    |
| 8   | 3     | 881  | A    |
| 8   | 3     | 901  | C    |
| 8   | 3     | 902  | U    |
| 8   | 3     | 952  | U    |
| 8   | 3     | 1124 | G    |
| 8   | 3     | 1209 | U    |
| 8   | 3     | 1583 | G    |
| 8   | 3     | 1618 | U    |
| 8   | 3     | 2180 | U    |
| 8   | 3     | 2410 | C    |
| 8   | 3     | 2764 | U    |
| 10  | 5     | 196  | G    |
| 10  | 5     | 571  | A    |
| 10  | 5     | 994  | C    |
| 10  | 5     | 995  | U    |
| 10  | 5     | 1024 | U    |
| 10  | 5     | 1123 | G    |
| 10  | 5     | 1158 | A    |
| 10  | 5     | 1338 | A    |
| 12  | 7     | 10   | G    |
| 13  | 8     | 20   | U    |
| 17  | AB    | 49   | U    |
| 17  | AB    | 51   | C    |
| 17  | AB    | 54   | A    |

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

16 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 |
| 13  | PSU  | 8     | 55   | 13       | 18,21,22     | 4.70 | 8 (44%)  | 22,30,33    | 1.80 | 5 (22%)  |
| 12  | G7M  | 7     | 46   | 12       | 23,26,27     | 2.85 | 8 (34%)  | 35,39,42    | 1.93 | 8 (22%)  |
| 12  | PSU  | 7     | 32   | 12       | 18,21,22     | 4.68 | 8 (44%)  | 22,30,33    | 1.80 | 6 (27%)  |
| 13  | 3AU  | 8     | 47   | 13       | 24,28,29     | 2.88 | 8 (33%)  | 33,40,43    | 1.31 | 3 (9%)   |
| 12  | 3AU  | 7     | 47   | 12       | 24,28,29     | 2.86 | 7 (29%)  | 33,40,43    | 1.32 | 4 (12%)  |
| 13  | PSU  | 8     | 39   | 13       | 18,21,22     | 4.70 | 8 (44%)  | 22,30,33    | 1.79 | 5 (22%)  |
| 12  | PSU  | 7     | 55   | 12       | 18,21,22     | 4.68 | 8 (44%)  | 22,30,33    | 1.78 | 5 (22%)  |
| 13  | 5MU  | 8     | 54   | 13       | 19,22,23     | 1.46 | 6 (31%)  | 28,32,35    | 2.14 | 7 (25%)  |
| 12  | MIA  | 7     | 37   | 12       | 28,31,32     | 2.42 | 5 (17%)  | 40,44,47    | 2.94 | 16 (40%) |
| 10  | MA6  | 5     | 1494 | 10       | 23,26,27     | 1.23 | 3 (13%)  | 34,38,41    | 2.89 | 14 (41%) |
| 12  | 4SU  | 7     | 8    | 12       | 18,21,22     | 3.79 | 7 (38%)  | 26,30,33    | 2.23 | 5 (19%)  |
| 10  | MA6  | 5     | 1493 | 10       | 23,26,27     | 1.25 | 4 (17%)  | 34,38,41    | 2.88 | 14 (41%) |
| 12  | PSU  | 7     | 39   | 12       | 18,21,22     | 4.67 | 8 (44%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 13  | U8U  | 8     | 34   | 37,13,17 | 19,24,25     | 3.27 | 7 (36%)  | 23,34,37    | 1.13 | 2 (8%)   |
| 10  | G7M  | 5     | 525  | 10       | 23,26,27     | 3.63 | 12 (52%) | 35,39,42    | 1.67 | 7 (20%)  |
| 13  | T6A  | 8     | 37   | 13       | 31,34,35     | 2.00 | 7 (22%)  | 44,49,52    | 4.35 | 15 (34%) |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 13  | PSU  | 8     | 55   | 13   | -       | 0/7/25/26  | 0/2/2/2 |
| 12  | G7M  | 7     | 46   | 12   | -       | 4/7/25/26  | 0/3/3/3 |
| 12  | PSU  | 7     | 32   | 12   | -       | 0/7/25/26  | 0/2/2/2 |
| 13  | 3AU  | 8     | 47   | 13   | -       | 2/16/34/35 | 0/2/2/2 |
| 12  | 3AU  | 7     | 47   | 12   | -       | 4/16/34/35 | 0/2/2/2 |
| 13  | PSU  | 8     | 39   | 13   | -       | 0/7/25/26  | 0/2/2/2 |
| 12  | PSU  | 7     | 55   | 12   | -       | 0/7/25/26  | 0/2/2/2 |
| 13  | 5MU  | 8     | 54   | 13   | -       | 2/7/25/26  | 0/2/2/2 |
| 12  | MIA  | 7     | 37   | 12   | -       | 4/15/33/34 | 0/3/3/3 |
| 10  | MA6  | 5     | 1494 | 10   | -       | 3/11/29/30 | 0/3/3/3 |
| 12  | 4SU  | 7     | 8    | 12   | -       | 2/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 10  | MA6  | 5     | 1493 | 10       | -       | 0/11/29/30 | 0/3/3/3 |
| 12  | PSU  | 7     | 39   | 12       | -       | 0/7/25/26  | 0/2/2/2 |
| 13  | U8U  | 8     | 34   | 37,13,17 | -       | 1/9/28/29  | 0/2/2/2 |
| 10  | G7M  | 5     | 525  | 10       | -       | 2/7/25/26  | 0/3/3/3 |
| 13  | T6A  | 8     | 37   | 13       | -       | 4/23/41/42 | 0/3/3/3 |

All (114) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13  | 8     | 55  | PSU  | C6-C5  | 12.38 | 1.49        | 1.35     |
| 13  | 8     | 39  | PSU  | C6-C5  | 12.28 | 1.49        | 1.35     |
| 12  | 7     | 32  | PSU  | C6-C5  | 12.24 | 1.49        | 1.35     |
| 12  | 7     | 55  | PSU  | C6-C5  | 12.23 | 1.49        | 1.35     |
| 12  | 7     | 39  | PSU  | C6-C5  | 12.17 | 1.49        | 1.35     |
| 10  | 5     | 525 | G7M  | C8-N7  | 10.41 | 1.51        | 1.33     |
| 13  | 8     | 55  | PSU  | C2-N1  | 9.62  | 1.49        | 1.36     |
| 12  | 7     | 55  | PSU  | C2-N1  | 9.57  | 1.49        | 1.36     |
| 13  | 8     | 39  | PSU  | C2-N1  | 9.55  | 1.49        | 1.36     |
| 12  | 7     | 39  | PSU  | C2-N1  | 9.54  | 1.49        | 1.36     |
| 12  | 7     | 32  | PSU  | C2-N1  | 9.49  | 1.49        | 1.36     |
| 12  | 7     | 8   | 4SU  | C4-N3  | 8.83  | 1.47        | 1.37     |
| 13  | 8     | 39  | PSU  | C2-N3  | 8.37  | 1.51        | 1.37     |
| 12  | 7     | 32  | PSU  | C2-N3  | 8.32  | 1.51        | 1.37     |
| 12  | 7     | 55  | PSU  | C2-N3  | 8.28  | 1.51        | 1.37     |
| 13  | 8     | 55  | PSU  | C2-N3  | 8.25  | 1.51        | 1.37     |
| 12  | 7     | 47  | 3AU  | C2-N1  | 8.24  | 1.50        | 1.38     |
| 12  | 7     | 39  | PSU  | C2-N3  | 8.23  | 1.51        | 1.37     |
| 13  | 8     | 47  | 3AU  | C2-N1  | 8.18  | 1.50        | 1.38     |
| 12  | 7     | 37  | MIA  | C2-S10 | 7.96  | 1.82        | 1.75     |
| 12  | 7     | 37  | MIA  | C6-N6  | 7.88  | 1.46        | 1.34     |
| 12  | 7     | 8   | 4SU  | C2-N3  | 6.86  | 1.50        | 1.38     |
| 12  | 7     | 46  | G7M  | C4-N3  | 6.73  | 1.50        | 1.34     |
| 13  | 8     | 47  | 3AU  | C2-N3  | 6.66  | 1.50        | 1.38     |
| 12  | 7     | 46  | G7M  | C2-N2  | 6.55  | 1.49        | 1.34     |
| 12  | 7     | 47  | 3AU  | C2-N3  | 6.49  | 1.50        | 1.38     |
| 13  | 8     | 34  | U8U  | C6-N1  | 6.34  | 1.48        | 1.38     |
| 13  | 8     | 34  | U8U  | C2-N3  | 6.28  | 1.51        | 1.37     |
| 13  | 8     | 34  | U8U  | C2-S2  | -6.14 | 1.58        | 1.67     |
| 13  | 8     | 47  | 3AU  | C6-C5  | 6.05  | 1.49        | 1.35     |
| 12  | 7     | 47  | 3AU  | C6-C5  | 6.05  | 1.49        | 1.35     |
| 12  | 7     | 8   | 4SU  | C4-S4  | -6.02 | 1.57        | 1.68     |
| 12  | 7     | 46  | G7M  | C2-N3  | 5.94  | 1.47        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | 7     | 8   | 4SU  | C2-N1   | 5.88  | 1.47        | 1.38     |
| 12  | 7     | 39  | PSU  | C6-N1   | 5.86  | 1.46        | 1.36     |
| 13  | 8     | 55  | PSU  | C6-N1   | 5.84  | 1.45        | 1.36     |
| 13  | 8     | 39  | PSU  | C6-N1   | 5.84  | 1.45        | 1.36     |
| 10  | 5     | 525 | G7M  | C2-N3   | 5.84  | 1.47        | 1.33     |
| 12  | 7     | 8   | 4SU  | C6-C5   | 5.83  | 1.48        | 1.35     |
| 13  | 8     | 37  | T6A  | C10-N11 | 5.82  | 1.48        | 1.35     |
| 12  | 7     | 32  | PSU  | C6-N1   | 5.81  | 1.45        | 1.36     |
| 12  | 7     | 55  | PSU  | C6-N1   | 5.77  | 1.45        | 1.36     |
| 10  | 5     | 525 | G7M  | C8-N9   | 5.62  | 1.51        | 1.35     |
| 10  | 5     | 525 | G7M  | C4-N3   | 5.56  | 1.47        | 1.34     |
| 13  | 8     | 34  | U8U  | C6-C5   | 5.46  | 1.50        | 1.34     |
| 13  | 8     | 34  | U8U  | C4-N3   | 5.40  | 1.48        | 1.38     |
| 13  | 8     | 37  | T6A  | C10-N6  | 5.24  | 1.48        | 1.37     |
| 13  | 8     | 37  | T6A  | C6-N6   | 4.84  | 1.49        | 1.39     |
| 10  | 5     | 525 | G7M  | C2-N2   | 4.76  | 1.45        | 1.34     |
| 10  | 5     | 525 | G7M  | C5-N7   | 4.61  | 1.44        | 1.39     |
| 12  | 7     | 55  | PSU  | C4-N3   | 4.46  | 1.47        | 1.38     |
| 12  | 7     | 39  | PSU  | C4-N3   | 4.46  | 1.47        | 1.38     |
| 12  | 7     | 32  | PSU  | C4-N3   | 4.46  | 1.47        | 1.38     |
| 13  | 8     | 39  | PSU  | C4-N3   | 4.43  | 1.47        | 1.38     |
| 13  | 8     | 55  | PSU  | C4-N3   | 4.39  | 1.47        | 1.38     |
| 12  | 7     | 46  | G7M  | C5-N7   | -4.28 | 1.34        | 1.39     |
| 12  | 7     | 46  | G7M  | C5-C6   | 4.02  | 1.54        | 1.43     |
| 10  | 5     | 525 | G7M  | C2-N1   | 3.77  | 1.47        | 1.37     |
| 13  | 8     | 34  | U8U  | O4-C4   | -3.77 | 1.16        | 1.23     |
| 12  | 7     | 47  | 3AU  | C4-N3   | 3.71  | 1.46        | 1.40     |
| 13  | 8     | 47  | 3AU  | C4-N3   | 3.65  | 1.46        | 1.40     |
| 12  | 7     | 8   | 4SU  | C5-C4   | 3.53  | 1.47        | 1.42     |
| 10  | 5     | 525 | G7M  | C6-N1   | 3.44  | 1.45        | 1.38     |
| 12  | 7     | 8   | 4SU  | C6-N1   | 3.43  | 1.46        | 1.38     |
| 10  | 5     | 525 | G7M  | C5-C6   | 3.34  | 1.52        | 1.43     |
| 12  | 7     | 47  | 3AU  | C6-N1   | 3.28  | 1.45        | 1.38     |
| 13  | 8     | 47  | 3AU  | C6-N1   | 3.23  | 1.45        | 1.38     |
| 12  | 7     | 55  | PSU  | O4-C4   | -3.19 | 1.17        | 1.23     |
| 13  | 8     | 47  | 3AU  | C11-C10 | 3.16  | 1.59        | 1.52     |
| 13  | 8     | 39  | PSU  | O4-C4   | -3.15 | 1.17        | 1.23     |
| 13  | 8     | 55  | PSU  | O4-C4   | -3.12 | 1.17        | 1.23     |
| 12  | 7     | 32  | PSU  | O4-C4   | -3.12 | 1.17        | 1.23     |
| 12  | 7     | 39  | PSU  | O4-C4   | -3.09 | 1.17        | 1.23     |
| 12  | 7     | 47  | 3AU  | C11-C10 | 3.01  | 1.59        | 1.52     |
| 12  | 7     | 46  | G7M  | C2-N1   | 2.99  | 1.45        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12  | 7     | 46   | G7M  | C6-N1   | 2.96  | 1.44        | 1.38     |
| 10  | 5     | 1493 | MA6  | C6-N6   | 2.92  | 1.45        | 1.36     |
| 10  | 5     | 1494 | MA6  | C5-C4   | -2.88 | 1.33        | 1.39     |
| 12  | 7     | 55   | PSU  | C1'-C5  | 2.87  | 1.56        | 1.50     |
| 13  | 8     | 39   | PSU  | C1'-C5  | 2.86  | 1.56        | 1.50     |
| 12  | 7     | 32   | PSU  | C1'-C5  | 2.85  | 1.56        | 1.50     |
| 10  | 5     | 1494 | MA6  | C6-N6   | 2.84  | 1.45        | 1.36     |
| 12  | 7     | 39   | PSU  | C1'-C5  | 2.81  | 1.56        | 1.50     |
| 10  | 5     | 1493 | MA6  | C5-C4   | -2.80 | 1.33        | 1.39     |
| 13  | 8     | 47   | 3AU  | C5-C4   | 2.75  | 1.50        | 1.43     |
| 13  | 8     | 55   | PSU  | C1'-C5  | 2.74  | 1.56        | 1.50     |
| 13  | 8     | 54   | 5MU  | C6-C5   | 2.74  | 1.39        | 1.34     |
| 13  | 8     | 34   | U8U  | C-N     | -2.69 | 1.42        | 1.46     |
| 12  | 7     | 47   | 3AU  | C5-C4   | 2.67  | 1.50        | 1.43     |
| 13  | 8     | 54   | 5MU  | C4-N3   | -2.66 | 1.33        | 1.38     |
| 13  | 8     | 39   | PSU  | O2-C2   | -2.61 | 1.17        | 1.23     |
| 12  | 7     | 37   | MIA  | C5-N7   | -2.58 | 1.34        | 1.39     |
| 12  | 7     | 32   | PSU  | O2-C2   | -2.57 | 1.18        | 1.23     |
| 13  | 8     | 55   | PSU  | O2-C2   | -2.56 | 1.18        | 1.23     |
| 12  | 7     | 55   | PSU  | O2-C2   | -2.55 | 1.18        | 1.23     |
| 12  | 7     | 39   | PSU  | O2-C2   | -2.51 | 1.18        | 1.23     |
| 10  | 5     | 525  | G7M  | O6-C6   | -2.46 | 1.18        | 1.23     |
| 12  | 7     | 37   | MIA  | C5-C4   | -2.40 | 1.34        | 1.39     |
| 13  | 8     | 37   | T6A  | C5-C4   | -2.40 | 1.34        | 1.39     |
| 13  | 8     | 37   | T6A  | C5-N7   | -2.39 | 1.34        | 1.39     |
| 12  | 7     | 46   | G7M  | O6-C6   | -2.38 | 1.19        | 1.23     |
| 13  | 8     | 54   | 5MU  | C6-N1   | -2.35 | 1.34        | 1.38     |
| 10  | 5     | 525  | G7M  | C4-N9   | 2.32  | 1.44        | 1.38     |
| 13  | 8     | 54   | 5MU  | C2-N1   | 2.31  | 1.42        | 1.38     |
| 13  | 8     | 54   | 5MU  | C4-C5   | 2.27  | 1.48        | 1.44     |
| 10  | 5     | 1493 | MA6  | C5-N7   | -2.24 | 1.34        | 1.39     |
| 10  | 5     | 525  | G7M  | C5-C4   | 2.15  | 1.43        | 1.38     |
| 13  | 8     | 54   | 5MU  | C2-N3   | -2.15 | 1.34        | 1.38     |
| 13  | 8     | 37   | T6A  | C8-N9   | -2.13 | 1.33        | 1.37     |
| 10  | 5     | 1494 | MA6  | C5-N7   | -2.10 | 1.35        | 1.39     |
| 13  | 8     | 37   | T6A  | O10-C10 | -2.06 | 1.19        | 1.23     |
| 10  | 5     | 1493 | MA6  | C8-N9   | -2.05 | 1.33        | 1.37     |
| 13  | 8     | 47   | 3AU  | O4-C4   | -2.03 | 1.19        | 1.23     |
| 12  | 7     | 37   | MIA  | C8-N9   | -2.01 | 1.33        | 1.37     |

All (121) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 13  | 8     | 37   | T6A  | C5-C6-N6   | 16.61  | 162.62      | 118.71   |
| 13  | 8     | 37   | T6A  | N6-C6-N1   | -14.93 | 79.09       | 117.45   |
| 12  | 7     | 37   | MIA  | C11-S10-C2 | 11.16  | 110.60      | 102.27   |
| 13  | 8     | 37   | T6A  | N6-C10-N11 | 10.07  | 127.83      | 113.76   |
| 10  | 5     | 1493 | MA6  | N1-C6-N6   | -8.83  | 107.43      | 117.08   |
| 10  | 5     | 1494 | MA6  | N1-C6-N6   | -8.73  | 107.53      | 117.08   |
| 12  | 7     | 8    | 4SU  | C4-N3-C2   | -7.78  | 119.78      | 127.34   |
| 12  | 7     | 37   | MIA  | C5-C4-N3   | -6.85  | 119.49      | 127.19   |
| 13  | 8     | 37   | T6A  | C4-C5-C6   | 6.00   | 121.46      | 116.81   |
| 10  | 5     | 1494 | MA6  | N1-C2-N3   | -5.58  | 119.88      | 128.60   |
| 12  | 7     | 8    | 4SU  | C5-C4-N3   | 5.54   | 119.83      | 114.69   |
| 13  | 8     | 37   | T6A  | C5-C4-N3   | -5.48  | 119.60      | 126.75   |
| 10  | 5     | 1493 | MA6  | N1-C2-N3   | -5.47  | 120.05      | 128.60   |
| 13  | 8     | 54   | 5MU  | C4-N3-C2   | -5.25  | 120.56      | 127.35   |
| 13  | 8     | 37   | T6A  | N3-C2-N1   | -5.21  | 120.45      | 128.60   |
| 10  | 5     | 1493 | MA6  | C5-C4-N3   | -5.08  | 120.12      | 126.75   |
| 13  | 8     | 54   | 5MU  | N3-C2-N1   | 5.04   | 121.58      | 114.89   |
| 10  | 5     | 1494 | MA6  | C5-C4-N3   | -5.02  | 120.20      | 126.75   |
| 12  | 7     | 46   | G7M  | C2-N3-C4   | 4.95   | 121.13      | 112.30   |
| 13  | 8     | 37   | T6A  | O10-C10-N6 | -4.81  | 115.48      | 123.62   |
| 10  | 5     | 1494 | MA6  | N9-C8-N7   | -4.75  | 107.41      | 113.91   |
| 12  | 7     | 46   | G7M  | C5-C4-N3   | -4.73  | 119.07      | 128.15   |
| 12  | 7     | 39   | PSU  | C4-N3-C2   | -4.58  | 119.74      | 126.34   |
| 10  | 5     | 525  | G7M  | C2-N3-C4   | 4.57   | 120.44      | 112.30   |
| 10  | 5     | 1494 | MA6  | C1'-N9-C8  | -4.57  | 116.82      | 127.14   |
| 10  | 5     | 1493 | MA6  | C1'-N9-C8  | -4.55  | 116.85      | 127.14   |
| 12  | 7     | 55   | PSU  | C4-N3-C2   | -4.55  | 119.79      | 126.34   |
| 13  | 8     | 55   | PSU  | C4-N3-C2   | -4.53  | 119.82      | 126.34   |
| 10  | 5     | 1493 | MA6  | N9-C8-N7   | -4.52  | 107.73      | 113.91   |
| 13  | 8     | 39   | PSU  | C4-N3-C2   | -4.47  | 119.90      | 126.34   |
| 12  | 7     | 32   | PSU  | C4-N3-C2   | -4.43  | 119.96      | 126.34   |
| 13  | 8     | 54   | 5MU  | C5-C4-N3   | 4.37   | 119.04      | 115.31   |
| 12  | 7     | 37   | MIA  | N6-C6-N1   | -4.33  | 112.97      | 118.50   |
| 10  | 5     | 1493 | MA6  | C5-C6-N6   | 4.27   | 132.73      | 125.30   |
| 12  | 7     | 37   | MIA  | N9-C8-N7   | -4.23  | 108.13      | 113.91   |
| 10  | 5     | 1494 | MA6  | C5-C6-N6   | 4.18   | 132.59      | 125.30   |
| 12  | 7     | 39   | PSU  | N1-C2-N3   | 4.16   | 119.84      | 115.13   |
| 13  | 8     | 37   | T6A  | N9-C8-N7   | -4.09  | 108.33      | 113.91   |
| 12  | 7     | 46   | G7M  | C5-C6-N1   | 4.08   | 120.31      | 111.79   |
| 10  | 5     | 525  | G7M  | C5-C4-N3   | -4.04  | 120.41      | 128.15   |
| 12  | 7     | 37   | MIA  | C4-C5-C6   | 4.02   | 119.92      | 116.81   |
| 12  | 7     | 32   | PSU  | N1-C2-N3   | 4.01   | 119.68      | 115.13   |
| 13  | 8     | 39   | PSU  | N1-C2-N3   | 4.01   | 119.67      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | 7     | 37   | MIA  | N3-C4-N9    | 4.00  | 132.54      | 126.99   |
| 13  | 8     | 55   | PSU  | N1-C2-N3    | 3.98  | 119.64      | 115.13   |
| 12  | 7     | 55   | PSU  | N1-C2-N3    | 3.95  | 119.61      | 115.13   |
| 13  | 8     | 54   | 5MU  | C5-C6-N1    | -3.95 | 119.28      | 123.34   |
| 12  | 7     | 46   | G7M  | N9-C4-N3    | 3.93  | 133.83      | 125.94   |
| 13  | 8     | 47   | 3AU  | C4-N3-C2    | -3.91 | 119.73      | 124.63   |
| 10  | 5     | 525  | G7M  | C5-C6-N1    | 3.91  | 119.95      | 111.79   |
| 12  | 7     | 37   | MIA  | N3-C2-N1    | -3.84 | 119.92      | 126.95   |
| 12  | 7     | 8    | 4SU  | N3-C2-N1    | 3.77  | 119.89      | 114.89   |
| 13  | 8     | 37   | T6A  | C4-N9-C1'   | -3.76 | 117.63      | 126.59   |
| 12  | 7     | 47   | 3AU  | C4-N3-C2    | -3.70 | 119.99      | 124.63   |
| 13  | 8     | 54   | 5MU  | O4-C4-C5    | -3.68 | 120.64      | 124.90   |
| 10  | 5     | 1494 | MA6  | C2-N1-C6    | 3.63  | 120.33      | 111.75   |
| 13  | 8     | 37   | T6A  | N3-C4-N9    | 3.59  | 133.00      | 127.08   |
| 10  | 5     | 1493 | MA6  | C2-N1-C6    | 3.58  | 120.22      | 111.75   |
| 10  | 5     | 1494 | MA6  | C2-N3-C4    | 3.51  | 120.05      | 111.75   |
| 10  | 5     | 1493 | MA6  | C4-C5-C6    | 3.50  | 119.80      | 115.88   |
| 12  | 7     | 8    | 4SU  | C5-C4-S4    | -3.49 | 119.97      | 124.47   |
| 10  | 5     | 1493 | MA6  | C2-N3-C4    | 3.49  | 119.98      | 111.75   |
| 10  | 5     | 1493 | MA6  | C4-N9-C1'   | 3.42  | 134.74      | 126.59   |
| 13  | 8     | 47   | 3AU  | C5-C4-N3    | 3.40  | 119.99      | 115.50   |
| 10  | 5     | 1494 | MA6  | C5-N7-C8    | 3.40  | 108.33      | 103.51   |
| 12  | 7     | 46   | G7M  | O6-C6-C5    | -3.38 | 120.43      | 128.06   |
| 10  | 5     | 1494 | MA6  | C4-C5-C6    | 3.38  | 119.66      | 115.88   |
| 10  | 5     | 525  | G7M  | O6-C6-C5    | -3.37 | 120.46      | 128.06   |
| 10  | 5     | 1493 | MA6  | C5-N7-C8    | 3.34  | 108.26      | 103.51   |
| 10  | 5     | 1494 | MA6  | C4-N9-C1'   | 3.31  | 134.49      | 126.59   |
| 13  | 8     | 34   | U8U  | C5-C4-N3    | 3.27  | 119.57      | 114.97   |
| 12  | 7     | 37   | MIA  | C12-C13-C14 | -3.27 | 120.78      | 127.14   |
| 13  | 8     | 37   | T6A  | O10-C10-N11 | -3.26 | 116.69      | 122.62   |
| 12  | 7     | 47   | 3AU  | C5-C4-N3    | 3.25  | 119.78      | 115.50   |
| 12  | 7     | 37   | MIA  | C5-N7-C8    | 3.24  | 108.11      | 103.51   |
| 13  | 8     | 34   | U8U  | O4-C4-C5    | -3.16 | 120.25      | 124.96   |
| 13  | 8     | 37   | T6A  | C2-N3-C4    | 3.16  | 119.22      | 111.75   |
| 13  | 8     | 37   | T6A  | C1'-N9-C8   | 3.15  | 134.24      | 127.14   |
| 12  | 7     | 46   | G7M  | C2-N1-C6    | -3.14 | 119.37      | 125.10   |
| 12  | 7     | 37   | MIA  | C4-N9-C1'   | -3.13 | 119.13      | 126.59   |
| 13  | 8     | 37   | T6A  | C5-N7-C8    | 3.12  | 107.94      | 103.51   |
| 12  | 7     | 37   | MIA  | C2-N3-C4    | 3.10  | 120.52      | 112.35   |
| 12  | 7     | 39   | PSU  | C6-C5-C4    | 3.06  | 120.34      | 118.20   |
| 12  | 7     | 37   | MIA  | C5-C6-N6    | 3.05  | 126.91      | 121.76   |
| 10  | 5     | 1493 | MA6  | N3-C4-N9    | 3.01  | 132.05      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | 5     | 1494 | MA6  | N3-C4-N9    | 2.99  | 132.01      | 127.08   |
| 12  | 7     | 32   | PSU  | C6-N1-C2    | -2.97 | 119.64      | 122.68   |
| 12  | 7     | 39   | PSU  | C6-N1-C2    | -2.92 | 119.70      | 122.68   |
| 13  | 8     | 55   | PSU  | C6-C5-C4    | 2.91  | 120.23      | 118.20   |
| 13  | 8     | 39   | PSU  | C6-C5-C4    | 2.84  | 120.18      | 118.20   |
| 13  | 8     | 39   | PSU  | C6-N1-C2    | -2.83 | 119.79      | 122.68   |
| 10  | 5     | 525  | G7M  | C2-N1-C6    | -2.83 | 119.94      | 125.10   |
| 12  | 7     | 37   | MIA  | S10-C2-N3   | 2.78  | 125.64      | 116.01   |
| 12  | 7     | 46   | G7M  | CN7-N7-C5   | 2.77  | 130.21      | 126.77   |
| 12  | 7     | 55   | PSU  | C6-N1-C2    | -2.74 | 119.88      | 122.68   |
| 10  | 5     | 1494 | MA6  | C4-N9-C8    | 2.73  | 108.69      | 105.73   |
| 12  | 7     | 55   | PSU  | C6-C5-C4    | 2.72  | 120.10      | 118.20   |
| 12  | 7     | 32   | PSU  | C6-C5-C4    | 2.71  | 120.09      | 118.20   |
| 13  | 8     | 55   | PSU  | C6-N1-C2    | -2.66 | 119.96      | 122.68   |
| 12  | 7     | 37   | MIA  | C1'-N9-C8   | 2.59  | 132.99      | 127.14   |
| 12  | 7     | 32   | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 12  | 7     | 39   | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 10  | 5     | 1493 | MA6  | C4-N9-C8    | 2.47  | 108.40      | 105.73   |
| 13  | 8     | 55   | PSU  | O2-C2-N1    | -2.42 | 120.12      | 122.79   |
| 12  | 7     | 37   | MIA  | C16-C14-C15 | 2.41  | 119.94      | 114.60   |
| 13  | 8     | 39   | PSU  | O2-C2-N1    | -2.40 | 120.15      | 122.79   |
| 10  | 5     | 1494 | MA6  | C4-C5-N7    | -2.33 | 107.78      | 110.62   |
| 10  | 5     | 1493 | MA6  | C4-C5-N7    | -2.33 | 107.78      | 110.62   |
| 12  | 7     | 55   | PSU  | O2-C2-N1    | -2.32 | 120.24      | 122.79   |
| 10  | 5     | 525  | G7M  | N9-C8-N7    | -2.31 | 106.50      | 112.21   |
| 12  | 7     | 37   | MIA  | C4-C5-N7    | -2.22 | 107.92      | 110.62   |
| 13  | 8     | 47   | 3AU  | C10-N3-C2   | 2.21  | 120.98      | 117.67   |
| 13  | 8     | 37   | T6A  | C4-N9-C8    | 2.21  | 108.12      | 105.73   |
| 12  | 7     | 47   | 3AU  | C1'-N1-C2   | 2.14  | 120.61      | 116.99   |
| 12  | 7     | 47   | 3AU  | C6-N1-C2    | -2.12 | 119.89      | 121.79   |
| 13  | 8     | 54   | 5MU  | C3'-C2'-C1' | 2.11  | 105.43      | 101.43   |
| 13  | 8     | 54   | 5MU  | O2-C2-N1    | -2.07 | 120.03      | 122.79   |
| 12  | 7     | 32   | PSU  | O4'-C1'-C2' | 2.05  | 108.04      | 105.14   |
| 12  | 7     | 8    | 4SU  | O2-C2-N1    | -2.03 | 120.09      | 122.79   |
| 10  | 5     | 525  | G7M  | C5-C4-N9    | 2.02  | 110.33      | 105.89   |
| 12  | 7     | 46   | G7M  | CN7-N7-C8   | -2.01 | 121.74      | 124.84   |

There are no chirality outliers.

All (28) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | 5     | 525 | G7M  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | 5     | 525  | G7M  | C3'-C4'-C5'-O5' |
| 10  | 5     | 1494 | MA6  | O4'-C4'-C5'-O5' |
| 12  | 7     | 8    | 4SU  | O4'-C4'-C5'-O5' |
| 12  | 7     | 37   | MIA  | C5-C6-N6-C12    |
| 12  | 7     | 37   | MIA  | N1-C2-S10-C11   |
| 12  | 7     | 37   | MIA  | N3-C2-S10-C11   |
| 12  | 7     | 47   | 3AU  | C2'-C1'-N1-C2   |
| 12  | 7     | 47   | 3AU  | C2'-C1'-N1-C6   |
| 13  | 8     | 34   | U8U  | N-C-C5-C4       |
| 10  | 5     | 1494 | MA6  | C3'-C4'-C5'-O5' |
| 12  | 7     | 8    | 4SU  | C3'-C4'-C5'-O5' |
| 13  | 8     | 37   | T6A  | N11-C12-C13-ODA |
| 13  | 8     | 37   | T6A  | N11-C12-C13-ODB |
| 12  | 7     | 37   | MIA  | N1-C6-N6-C12    |
| 10  | 5     | 1494 | MA6  | C5-C6-N6-C10    |
| 12  | 7     | 46   | G7M  | C2'-C1'-N9-C4   |
| 13  | 8     | 54   | 5MU  | O4'-C4'-C5'-O5' |
| 13  | 8     | 47   | 3AU  | C10-C11-C12-N40 |
| 13  | 8     | 54   | 5MU  | C3'-C4'-C5'-O5' |
| 13  | 8     | 37   | T6A  | C14-C12-C13-ODA |
| 12  | 7     | 47   | 3AU  | O4'-C1'-N1-C6   |
| 12  | 7     | 46   | G7M  | C4'-C5'-O5'-P   |
| 13  | 8     | 37   | T6A  | C14-C12-C13-ODB |
| 12  | 7     | 47   | 3AU  | O4'-C1'-N1-C2   |
| 12  | 7     | 46   | G7M  | O4'-C4'-C5'-O5' |
| 13  | 8     | 47   | 3AU  | C11-C10-N3-C4   |
| 12  | 7     | 46   | G7M  | C2'-C1'-N9-C8   |

There are no ring outliers.

10 monomers are involved in 22 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 13  | 8     | 55   | PSU  | 2       | 0            |
| 13  | 8     | 47   | 3AU  | 1       | 0            |
| 13  | 8     | 54   | 5MU  | 2       | 0            |
| 12  | 7     | 37   | MIA  | 6       | 0            |
| 12  | 7     | 8    | 4SU  | 1       | 0            |
| 10  | 5     | 1493 | MA6  | 1       | 0            |
| 12  | 7     | 39   | PSU  | 1       | 0            |
| 13  | 8     | 34   | U8U  | 6       | 0            |
| 10  | 5     | 525  | G7M  | 1       | 0            |
| 13  | 8     | 37   | T6A  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 337 ligands modelled in this entry, 325 are monoatomic - leaving 12 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 | $\# Z  > 2$ |
| 70  | PUT  | 3     | 3219 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.55 | 0           |
| 70  | PUT  | 3     | 3180 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.55 | 0           |
| 70  | PUT  | 3     | 3205 | -    | 5,5,5        | 0.24 | 0           | 4,4,4       | 0.54 | 0           |
| 70  | PUT  | 3     | 3210 | -    | 5,5,5        | 0.24 | 0           | 4,4,4       | 0.53 | 0           |
| 70  | PUT  | 5     | 1607 | -    | 5,5,5        | 0.24 | 0           | 4,4,4       | 0.53 | 0           |
| 70  | PUT  | 5     | 1631 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.54 | 0           |
| 70  | PUT  | 3     | 3214 | -    | 5,5,5        | 0.24 | 0           | 4,4,4       | 0.51 | 0           |
| 70  | PUT  | 5     | 1602 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.52 | 0           |
| 70  | PUT  | 3     | 3215 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.51 | 0           |
| 70  | PUT  | b     | 302  | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.52 | 0           |
| 70  | PUT  | 5     | 1605 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.54 | 0           |
| 70  | PUT  | 5     | 1635 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.55 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 70  | PUT  | 3     | 3219 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 3     | 3180 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 3     | 3205 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 3     | 3210 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 5     | 1607 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 5     | 1631 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 3     | 3214 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 5     | 1602 | -    | -       | 0/3/3/3  | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 70  | PUT  | 3     | 3215 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | b     | 302  | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 5     | 1605 | -    | -       | 0/3/3/3  | -     |
| 70  | PUT  | 5     | 1635 | -    | -       | 0/3/3/3  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 70  | 3     | 3214 | PUT  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 40  | b     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | b     | 229:ALA   | C      | 230:PRO   | N      | 3.19         |

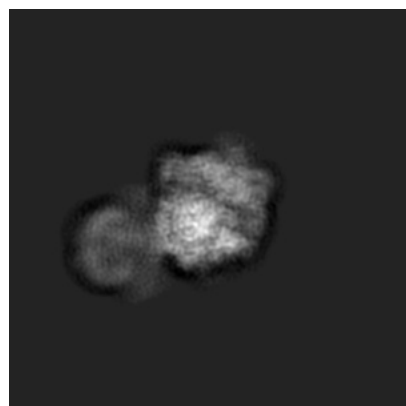
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55029. These allow visual inspection of the internal detail of the map and identification of artifacts.

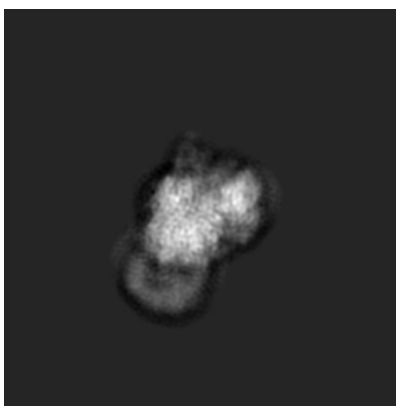
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

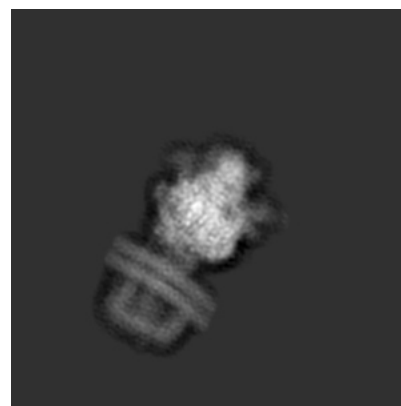
#### 6.1.1 Primary map



X

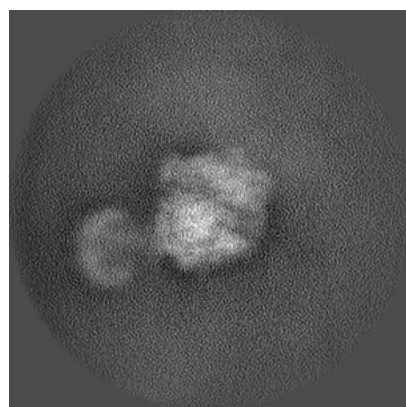


Y

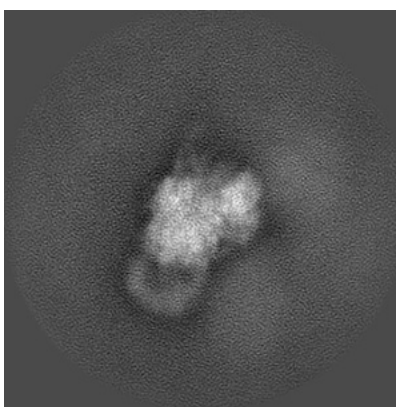


Z

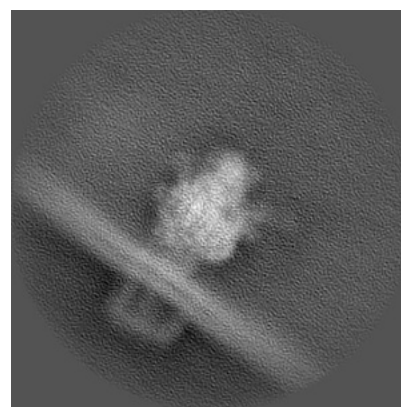
#### 6.1.2 Raw map



X



Y

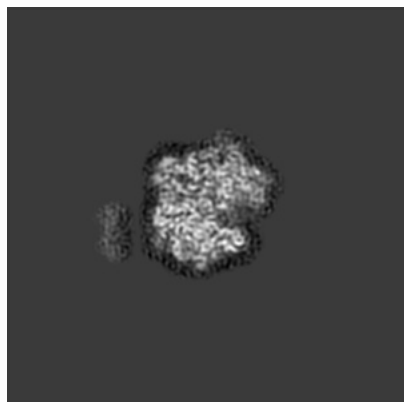


Z

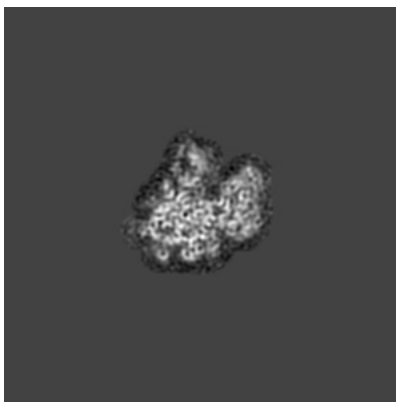
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

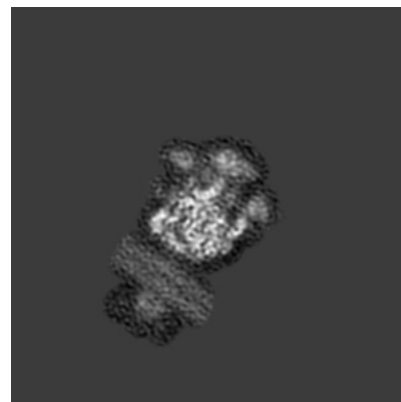
### 6.2.1 Primary map



X Index: 128

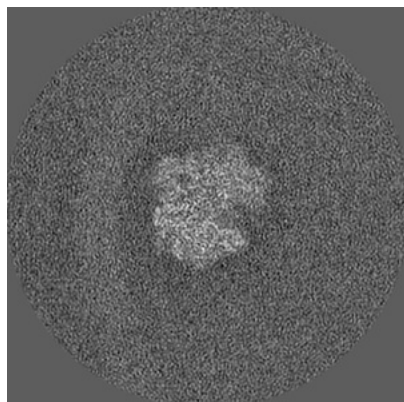


Y Index: 128

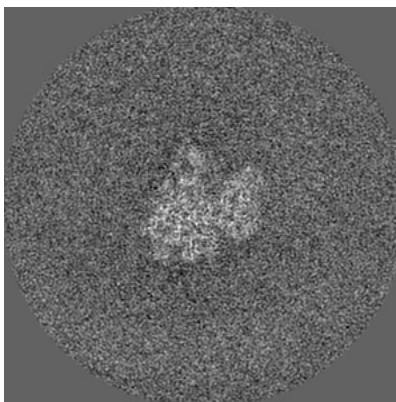


Z Index: 128

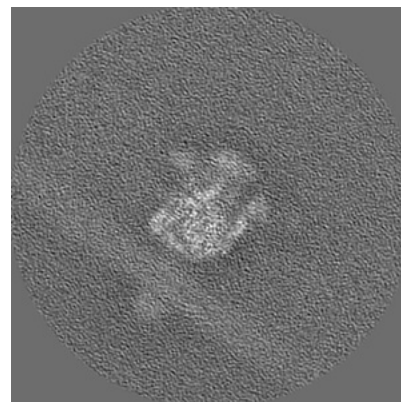
### 6.2.2 Raw map



X Index: 128



Y Index: 128

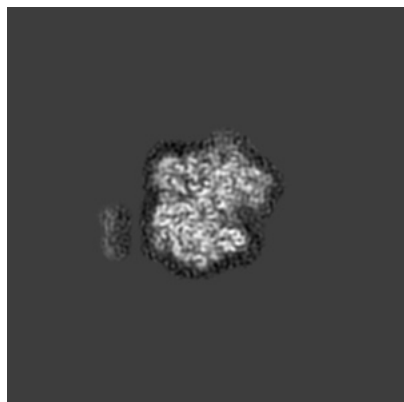


Z Index: 128

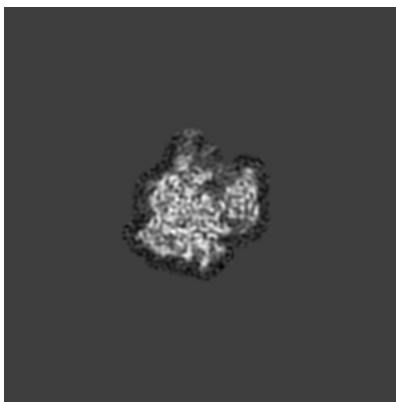
The images above show central slices of the map in three orthogonal directions.

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

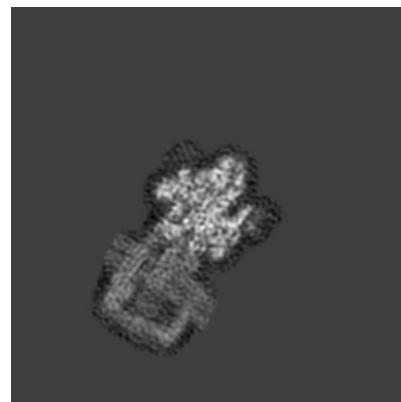
### 6.3.1 Primary map



X Index: 129

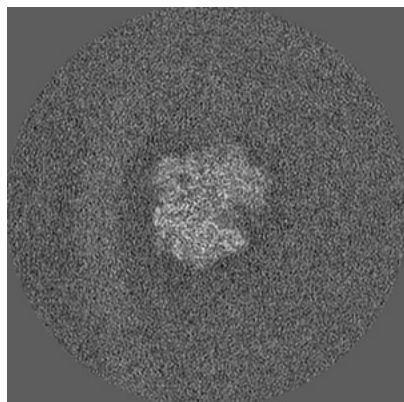


Y Index: 119

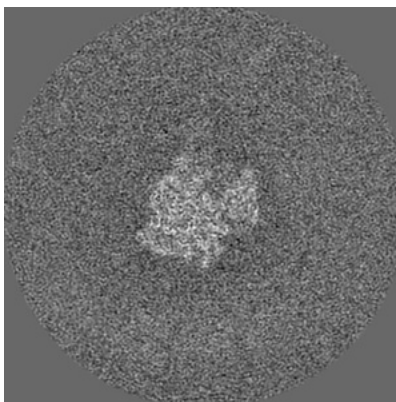


Z Index: 108

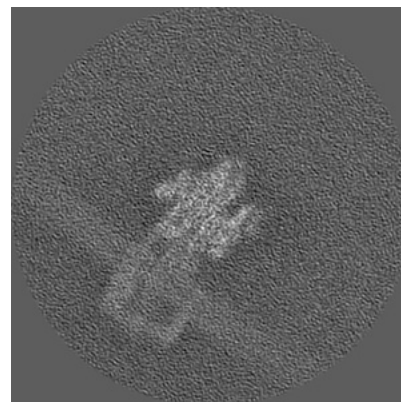
### 6.3.2 Raw map



X Index: 128



Y Index: 119

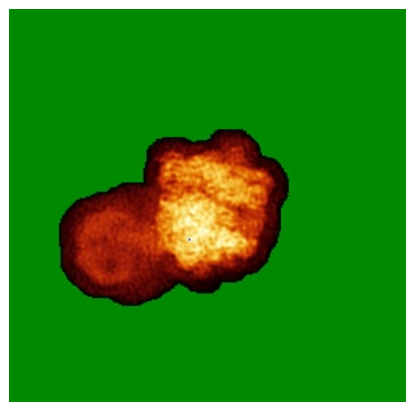


Z Index: 109

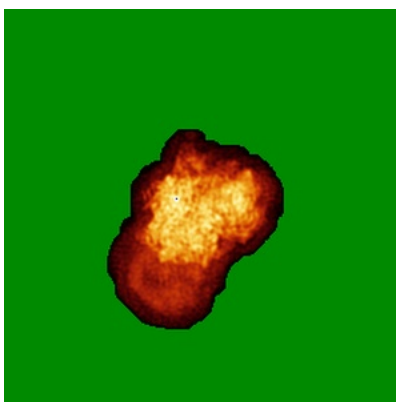
The images above show the largest variance slices of the map in three orthogonal directions.

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

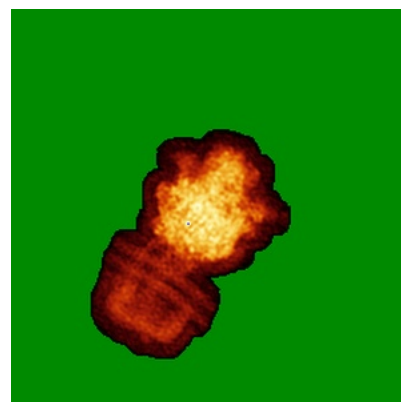
### 6.4.1 Primary map



X

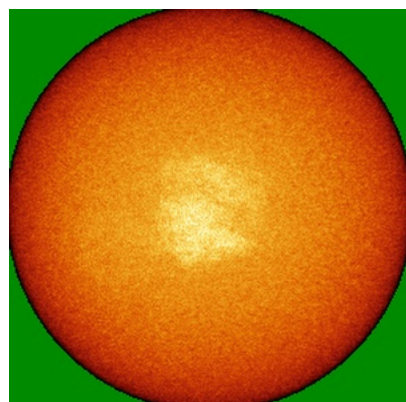


Y

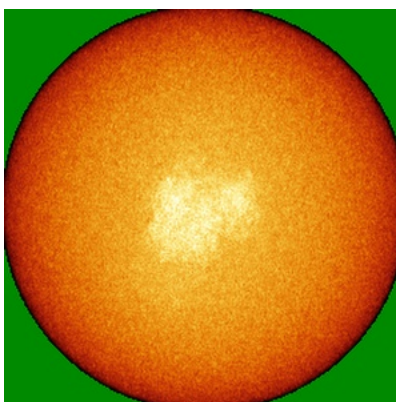


Z

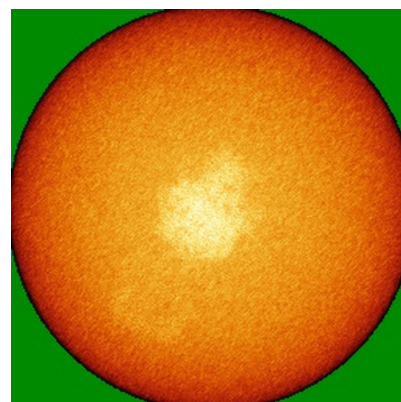
### 6.4.2 Raw map



X



Y

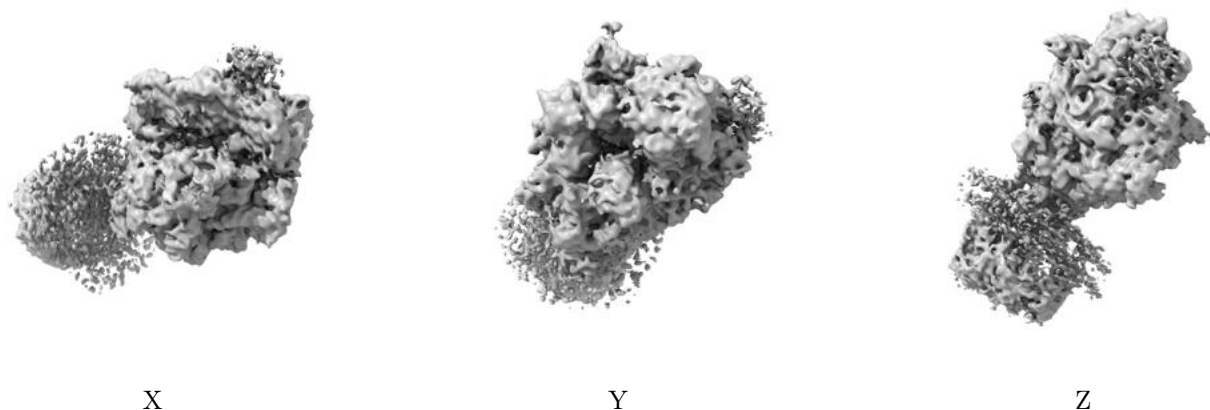


Z

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

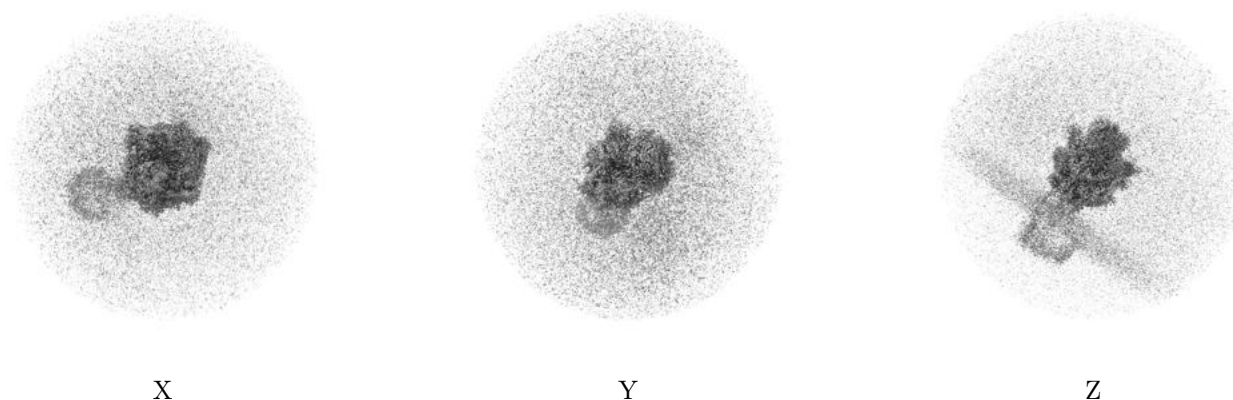
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

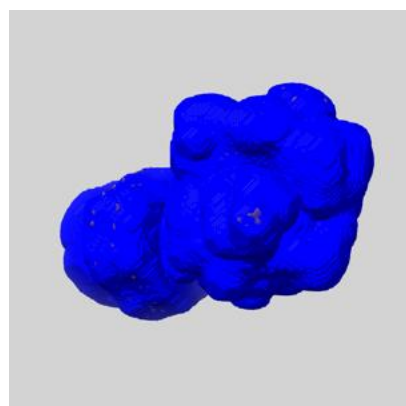
## 6.6 Mask visualisation [i](#)

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

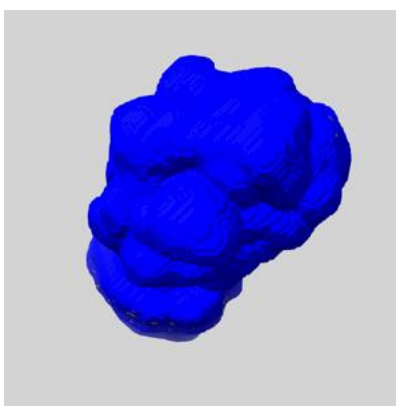
A mask typically either:

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

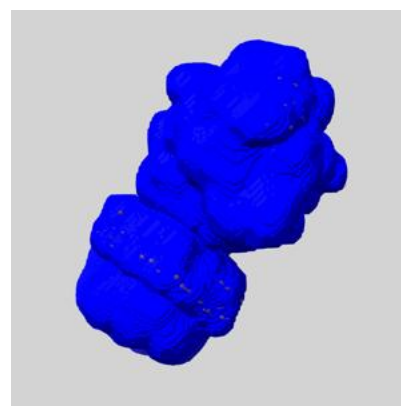
### 6.6.1 emd\_55029\_msk\_1.map [i](#)



X



Y

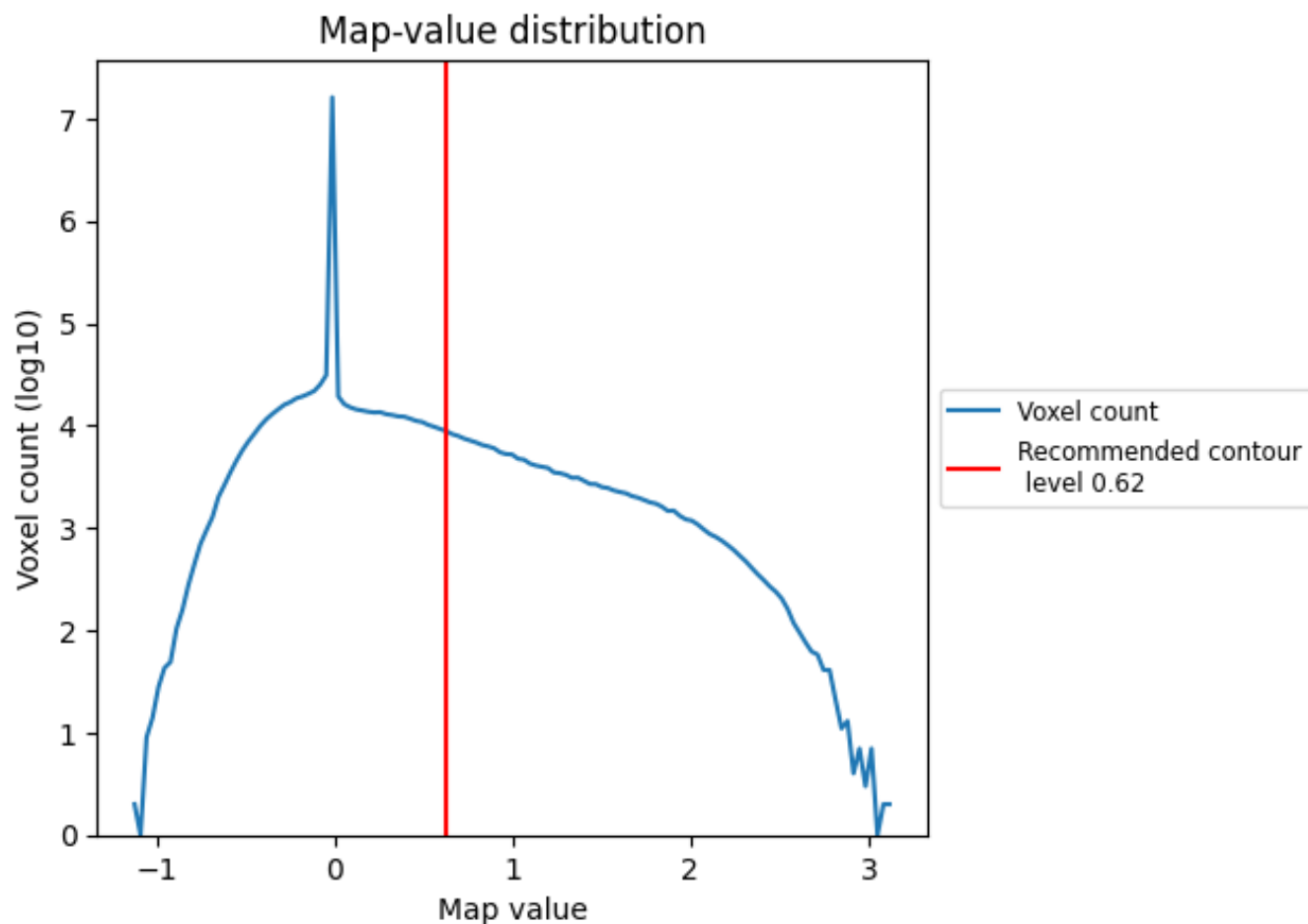


Z

## 7 Map analysis [i](#)

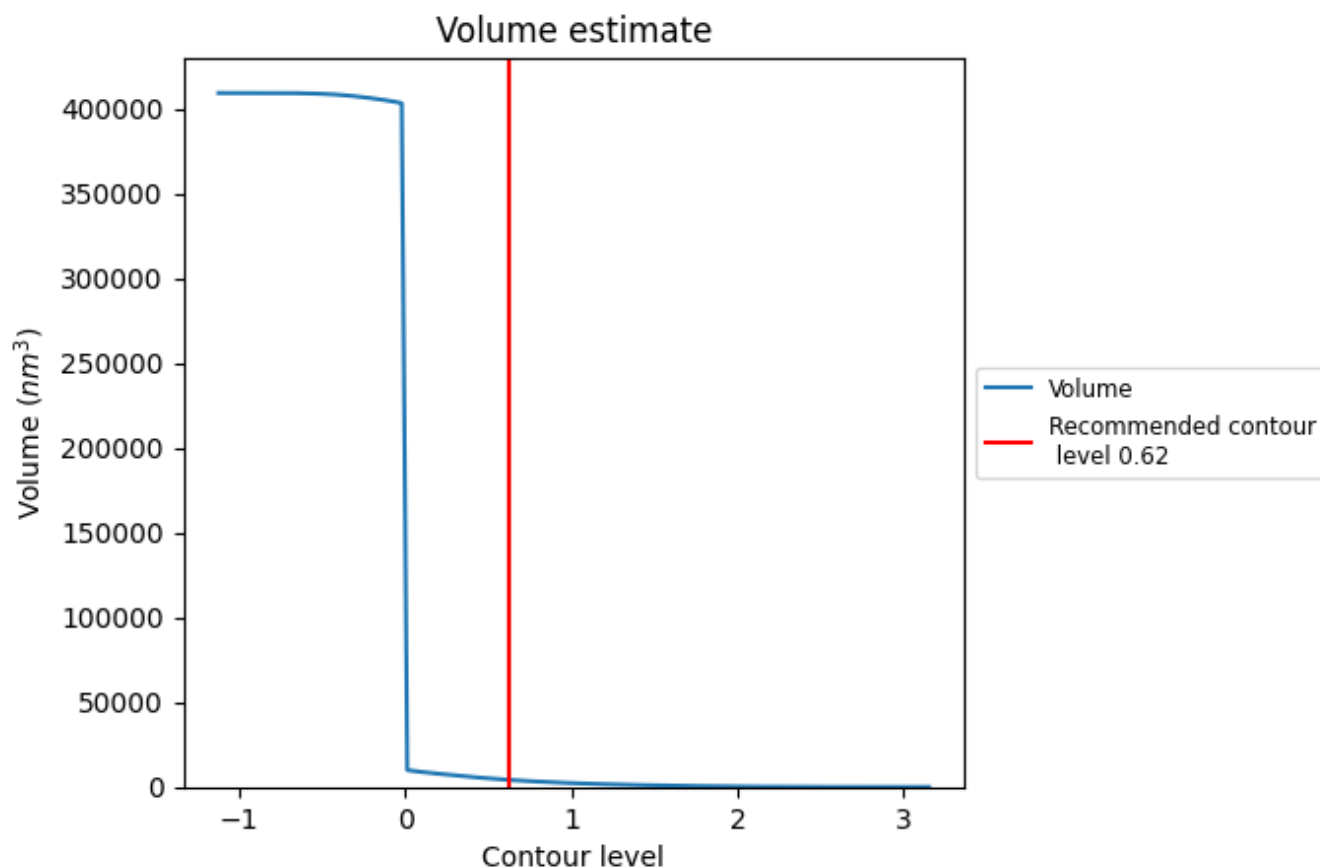
This section contains the results of statistical analysis of the map.

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



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

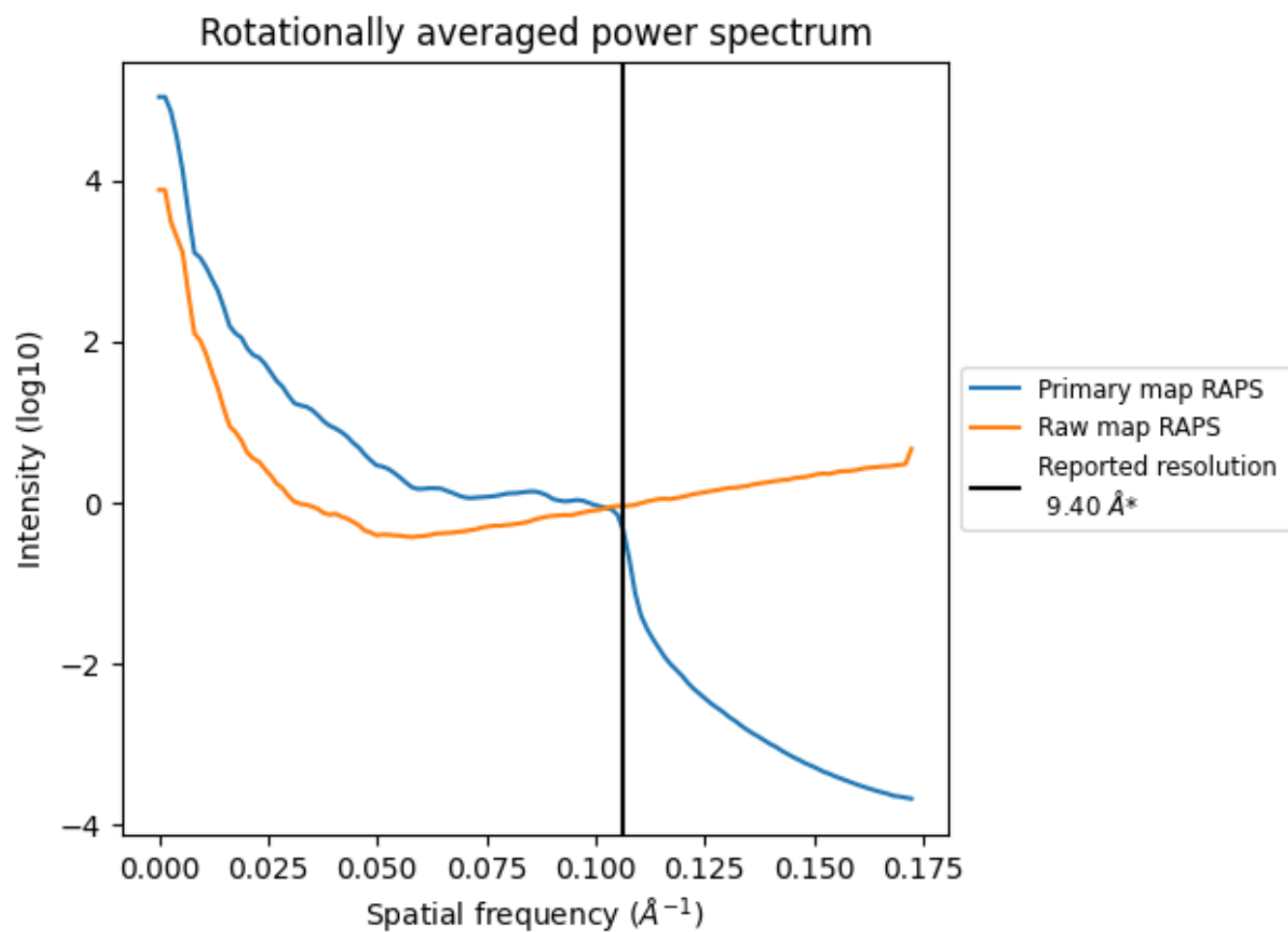
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4188  $\text{nm}^3$ ; this corresponds to an approximate mass of 3783 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 ⓘ

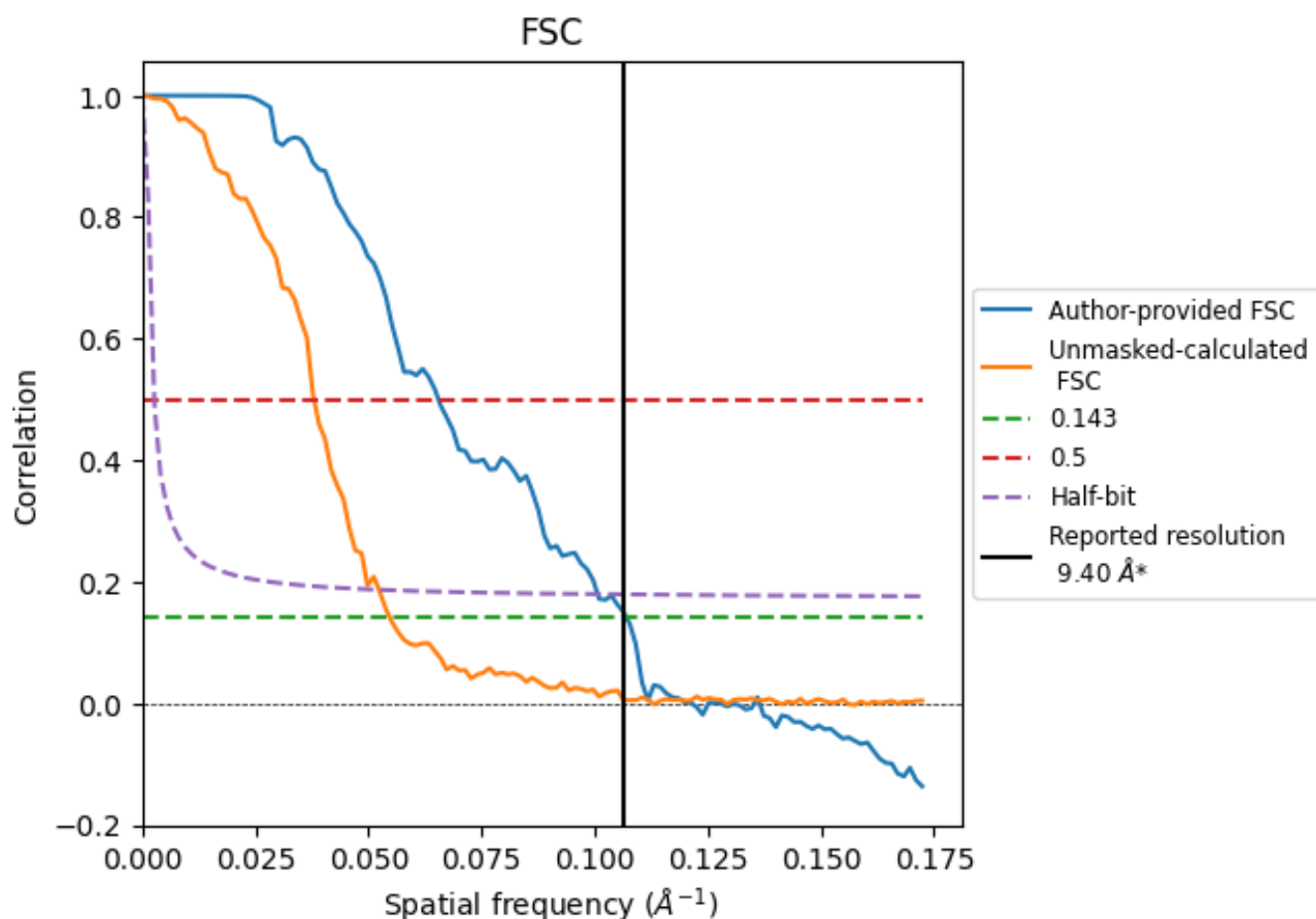


\*Reported resolution corresponds to spatial frequency of 0.106 Å<sup>-1</sup>

## 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 0.106 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

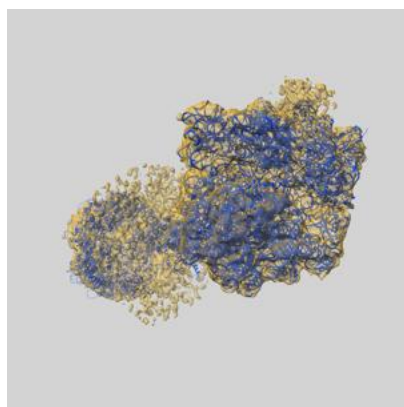
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 9.40                               | -     | -        |
| Author-provided FSC curve | 9.35                               | 15.27 | 9.93     |
| Unmasked-calculated*      | 18.32                              | 26.32 | 19.08    |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 18.32 differs from the reported value 9.4 by more than 10 %

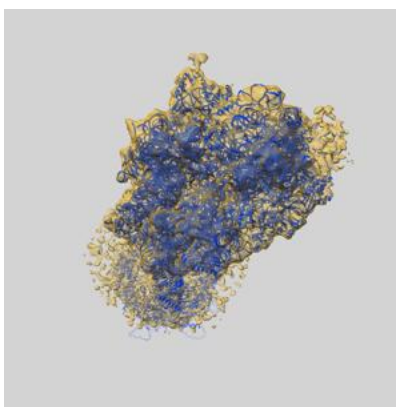
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55029 and PDB model 9SMD. Per-residue inclusion information can be found in section [3](#) on page [19](#).

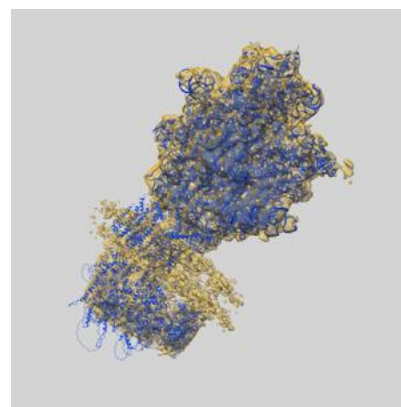
### 9.1 Map-model overlay [i](#)



X



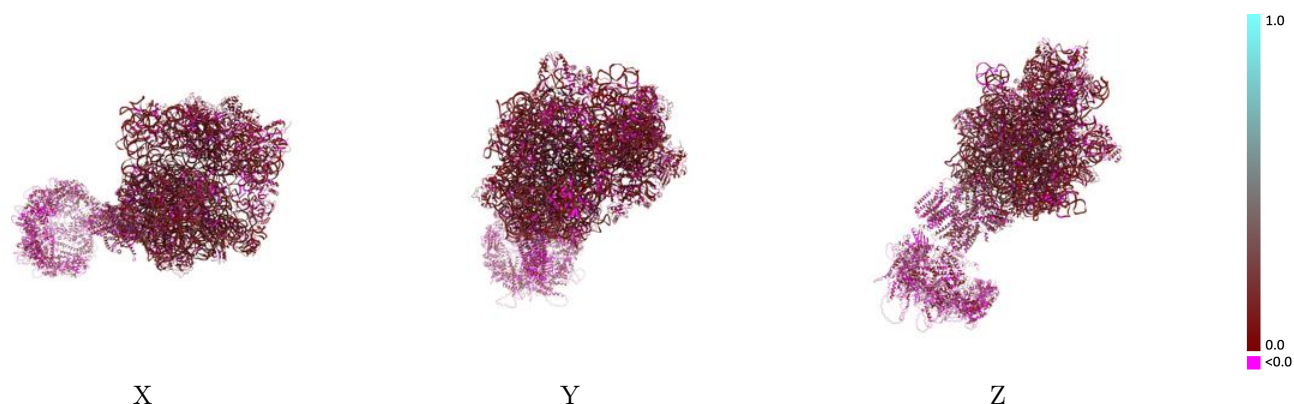
Y



Z

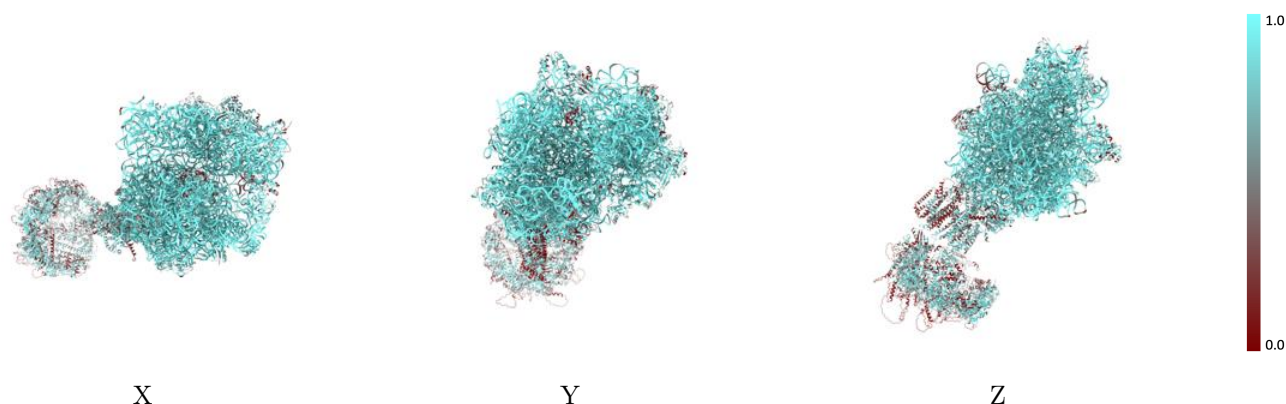
The images above show the 3D surface view of the map at the recommended contour level 0.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



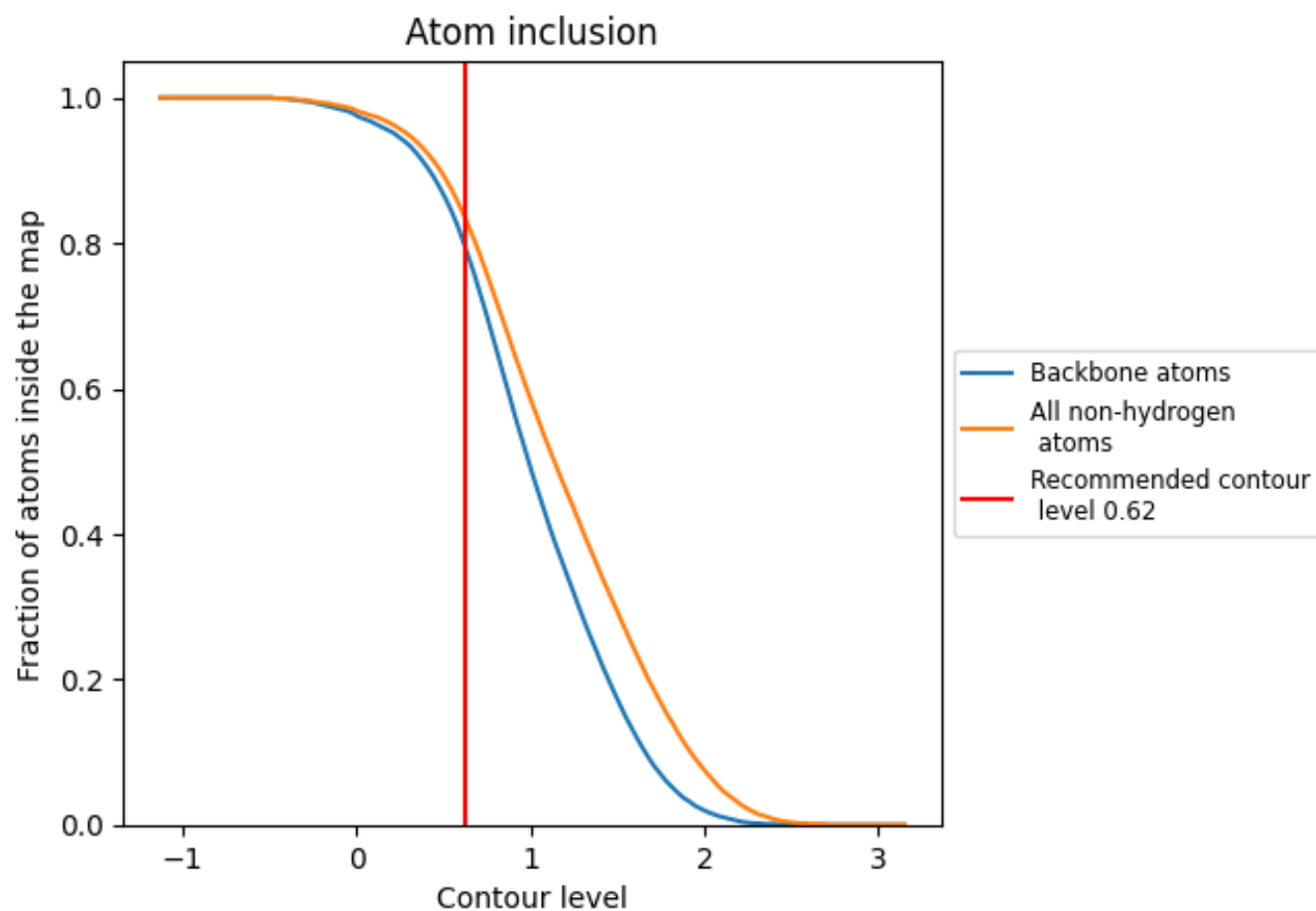
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.62).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 84% 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 (0.62) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8380   |  0.0990   |
| 0     |  0.9640   |  0.0770   |
| 1     |  0.9510   |  0.0760   |
| 10    |  0.6260   |  0.0850   |
| 11    |  0.5660   |  0.0800   |
| 12    |  0.4200   |  0.0840   |
| 13    |  0.5870   |  0.0280   |
| 14    |  0.5730   |  0.0480   |
| 15    |  0.5590   |  0.0390   |
| 16    |  0.3780   |  0.0120   |
| 17    |  0.4410   |  0.0140   |
| 18    |  0.5300   |  0.0090   |
| 2     |  0.9560   |  0.0490   |
| 3     |  0.9820   |  0.1380   |
| 4     |  0.9940  |  0.1530  |
| 5     |  0.9750 |  0.1220 |
| 6     |  1.0000 |  0.0500 |
| 7     |  0.9720 |  0.1250 |
| 8     |  0.7490 |  0.0980 |
| 9     |  0.7650 |  0.0930 |
| A     |  0.7710 |  0.1100 |
| AA    |  0.8940 |  0.0830 |
| AB    |  0.8850 |  0.1010 |
| AC    |  0.6850 |  0.1020 |
| C     |  0.8180 |  0.0840 |
| E     |  0.6920 |  0.1040 |
| F     |  0.9310 |  0.0930 |
| G     |  0.8790 |  0.1080 |
| H     |  0.8760 |  0.0670 |
| I     |  0.7590 |  0.0600 |
| J     |  0.7820 |  0.0720 |
| K     |  0.9100 |  0.0780 |
| L     |  0.7900 |  0.0700 |
| M     |  0.9560 |  0.0330 |
| N     |  0.8740 |  0.0980 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| O     |  0.8960   |  0.0780   |
| P     |  0.7960   |  0.0660   |
| Q     |  0.8560   |  0.0870   |
| R     |  0.7540   |  0.0410   |
| S     |  0.9330   |  0.1120   |
| T     |  0.7920   |  0.0980   |
| W     |  0.8410   |  0.0800   |
| Y     |  1.0000   |  0.1870   |
| Z     |  0.8340   |  0.0360   |
| a     |  0.9440   |  0.0720   |
| b     |  0.8980   |  0.0790   |
| c     |  0.8780   |  0.0950   |
| d     |  0.9260   |  0.1110   |
| e     |  0.8190   |  0.1150   |
| f     |  0.3830   |  0.1020   |
| g     |  0.7490   |  0.0950   |
| h     |  0.5990   |  0.0740   |
| i     |  0.9080  |  0.0910  |
| j     |  0.8710 |  0.0820 |
| k     |  0.8880 |  0.0820 |
| l     |  0.9350 |  0.0920 |
| m     |  0.9290 |  0.0940 |
| n     |  0.9180 |  0.1000 |
| o     |  0.8950 |  0.1030 |
| p     |  0.8960 |  0.0920 |
| q     |  0.8220 |  0.0990 |
| r     |  0.9340 |  0.1100 |
| s     |  0.8530 |  0.0880 |
| t     |  0.8380 |  0.0820 |
| u     |  0.9170 |  0.0540 |
| v     |  0.9140 |  0.0930 |
| w     |  0.7930 |  0.1300 |
| x     |  0.7850 |  0.0980 |
| y     |  0.9410 |  0.0650 |
| z     |  0.9500 |  0.1040 |