



## Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 12:03 AM UTC

PDB ID : 5ZLU / pdb\_00005zlu  
EMDB ID : EMD-6934  
Title : Ribosome Structure bound to ABC-F protein.  
Authors : Su, W.X.; Kumar, V.; Ero, R.; Andrew, S.W.W.; Jian, S.; Yong-Gui, G.  
Deposited on : 2018-03-29  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

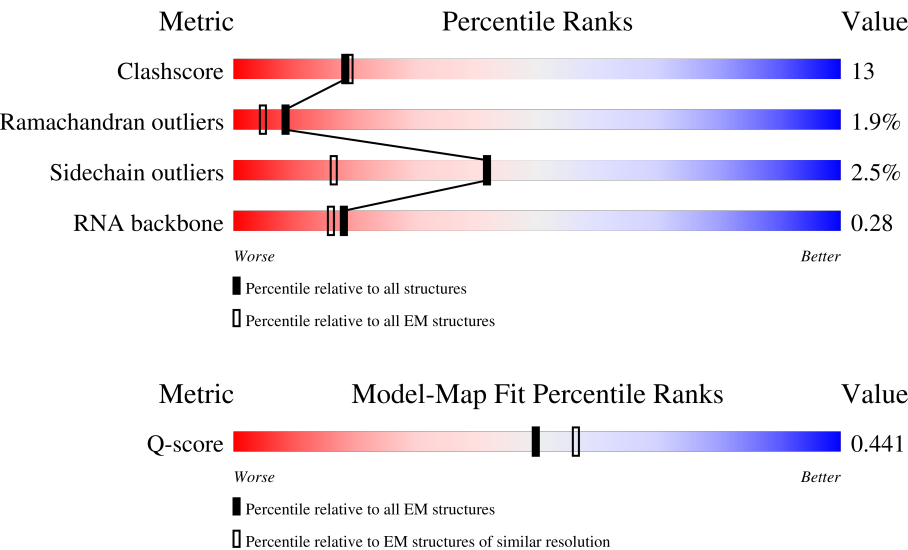
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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.



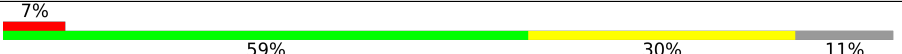
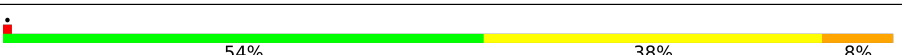
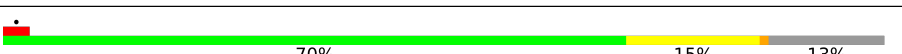
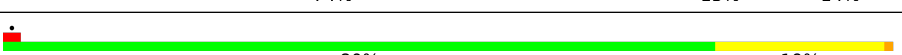
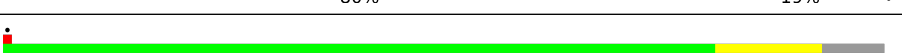
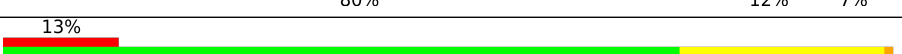
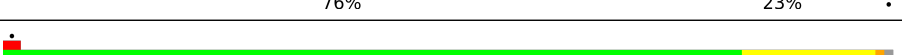
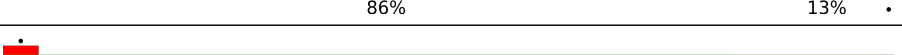
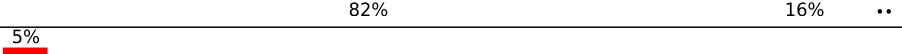
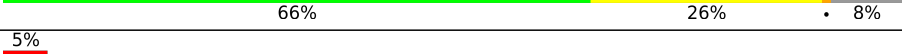
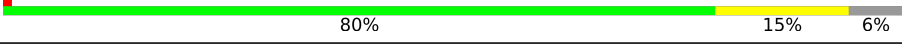
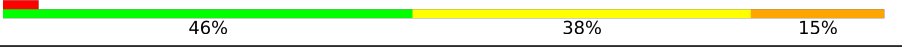
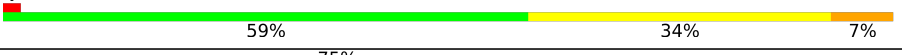
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 12797 ( 3.10 - 4.10 )                                    |

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   | W     | 25     |                  |
| 2   | A     | 104    |                  |
| 3   | B     | 73     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | C     | 106    |    |
| 5   | D     | 93     |    |
| 6   | E     | 105    |    |
| 7   | F     | 27     |    |
| 8   | G     | 1514   |    |
| 9   | H     | 256    |    |
| 10  | I     | 239    |    |
| 11  | J     | 209    |    |
| 12  | K     | 162    |    |
| 13  | L     | 101    |    |
| 14  | M     | 156    |    |
| 15  | N     | 138    |    |
| 16  | O     | 128    |   |
| 17  | P     | 129    |  |
| 18  | Q     | 132    |  |
| 19  | R     | 126    |  |
| 20  | S     | 61     |  |
| 21  | T     | 89     |  |
| 22  | U     | 88     |  |
| 23  | V     | 2875   |  |
| 24  | X     | 123    |  |
| 25  | Y     | 229    |  |
| 26  | Z     | 276    |  |
| 27  | a     | 206    |  |
| 28  | b     | 210    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | c     | 182    |                  |
| 30  | d     | 180    |                  |
| 31  | e     | 173    |                  |
| 32  | f     | 147    |                  |
| 33  | g     | 140    |                  |
| 34  | h     | 122    |                  |
| 35  | i     | 150    |                  |
| 36  | j     | 141    |                  |
| 37  | k     | 118    |                  |
| 38  | l     | 112    |                  |
| 39  | m     | 146    |                  |
| 40  | n     | 118    |                  |
| 41  | o     | 101    |                  |
| 42  | p     | 113    |                  |
| 43  | q     | 96     |                  |
| 44  | r     | 110    |                  |
| 45  | s     | 206    |                  |
| 46  | t     | 85     |                  |
| 47  | u     | 67     |                  |
| 48  | v     | 60     |                  |
| 49  | CC    | 71     |                  |
| 49  | w     | 71     |                  |
| 50  | x     | 60     |                  |
| 51  | y     | 54     |                  |
| 52  | z     | 49     |                  |

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| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 53  | AA    | 65     | <div><div></div><div>78%</div><div>15%</div><div></div><div></div></div>      |
| 54  | BB    | 37     | <div><div></div><div>65%</div><div>32%</div><div></div><div></div></div>      |
| 55  | DD    | 77     | <div><div>9%</div><div>44%</div><div>30%</div><div>22%</div><div></div></div> |
| 56  | EE    | 497    | <div><div>11%</div><div>91%</div><div>7%</div><div></div><div></div></div>    |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 150313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (25-mer).

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 1   | W     | 7        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 149   | 67 | 26 | 49 | 7 |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | A     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 519 | 149 | 138 | 2 |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 3   | B     | 73       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | C     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | D     | 82       | Total | C   | N   | O   | S | 0       | 1     |
|     |       |          | 656   | 419 | 121 | 113 | 3 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | E     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 794   | 499 | 156 | 138 | 1 |         |       |

- Molecule 7 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 7   | F     | 24       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |       |

- Molecule 8 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 8   | G     | 1514     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32534 | 14481 | 6019 | 10520 | 1514 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | H     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1810  | 1154 | 328 | 323 | 5 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | I     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | J     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | K     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | L     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | M     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | N     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | O     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |   |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | P     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | Q     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | R     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 565 | 189 | 158 | 2 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 20  | S     | 60       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | T     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | U     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 23  | V     | 2875     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 61917 | 27558 | 11575 | 19909 | 2875 |         |       |

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 24  | X     | 123      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2641  | 1175 | 488 | 855 | 123 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25  | Y     | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1742  | 1102 | 318 | 319 | 3 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | Z     | 273      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2126  | 1341 | 424 | 358 | 3 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | a     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 997 | 302 | 273 | 6 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | b     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1625  | 1034 | 303 | 286 | 2 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | c     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1455  | 929 | 266 | 256 | 4 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | d     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1335  | 847 | 250 | 237 | 1 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 31  | e     | 126      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 621   | 369 | 126 | 126 |  |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | f     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 993   | 632 | 175 | 181 | 5 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | g     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 931   | 603 | 171 | 154 | 3 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | h     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 932   | 587 | 171 | 170 | 4 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | i     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 689 | 226 | 191 | 2 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | j     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 688 | 204 | 183 | 5 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 37  | k     | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 38  | l     | 110      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |  |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | m     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 976   | 614 | 197 | 164 | 1 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | n     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | o     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | p     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 552 | 171 | 151 | 2 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | q     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 483 | 133 | 126 |   |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | r     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 844   | 539 | 158 | 141 | 6 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | s     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1435  | 916 | 256 | 260 | 3 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | t     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 629   | 389 | 132 | 107 | 1 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 47  | u     | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 567   | 350 | 116 | 99 | 2 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48  | v     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |   |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | w     | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |       |
| 49  | CC    | 32       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 157   | 93  | 32  | 32  |   |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | x     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 445   | 279 | 87 | 74 | 5 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | y     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 422   | 262 | 87 | 69 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| y     | 7       | LEU      | ILE    | see sequence details | UNP P35871 |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 52  | z     | 49       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 53  | AA    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 515   | 331 | 102 | 79 | 3 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | BB    | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |       |

- Molecule 55 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 55  | DD    | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1648  | 736 | 301 | 533 | 77 | 1 |         |       |

- Molecule 56 is a protein called Macrolide efflux protein.

| Mol | Chain | Residues | Atoms |      |     |     |    |  | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|--|---------|-------|
| 56  | EE    | 490      | Total | C    | N   | O   | S  |  | 0       | 0     |
|     |       |          | 3841  | 2415 | 668 | 742 | 16 |  |         |       |

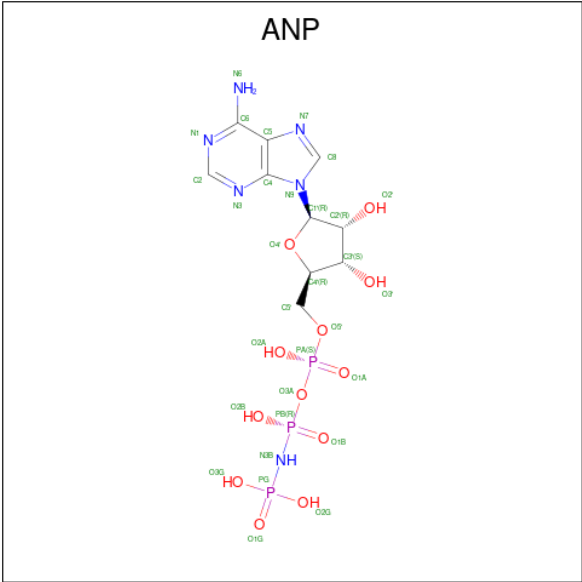
There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| EE    | 492     | HIS      | -      | expression tag | UNP A0A1I9WCL8 |
| EE    | 493     | HIS      | -      | expression tag | UNP A0A1I9WCL8 |
| EE    | 494     | HIS      | -      | expression tag | UNP A0A1I9WCL8 |
| EE    | 495     | HIS      | -      | expression tag | UNP A0A1I9WCL8 |
| EE    | 496     | HIS      | -      | expression tag | UNP A0A1I9WCL8 |
| EE    | 497     | HIS      | -      | expression tag | UNP A0A1I9WCL8 |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 57  | Z     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 57  | i     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 58 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

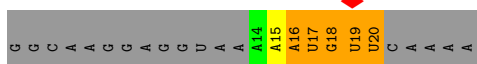


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 58  | EE    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |
| 58  | EE    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |

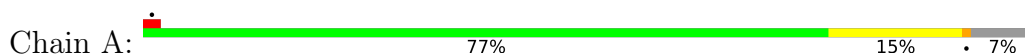
### 3 Residue-property plots [i](#)

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.

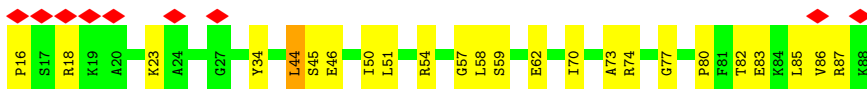
- Molecule 1: RNA (25-mer)



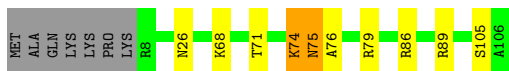
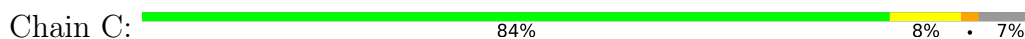
- Molecule 2: 30S ribosomal protein S17



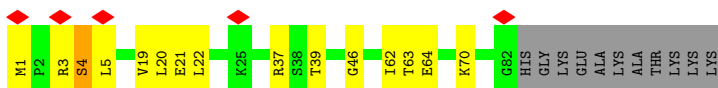
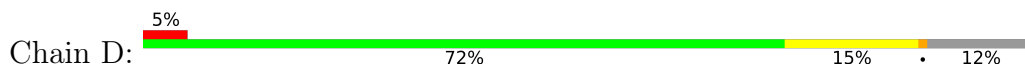
- Molecule 3: 30S ribosomal protein S18



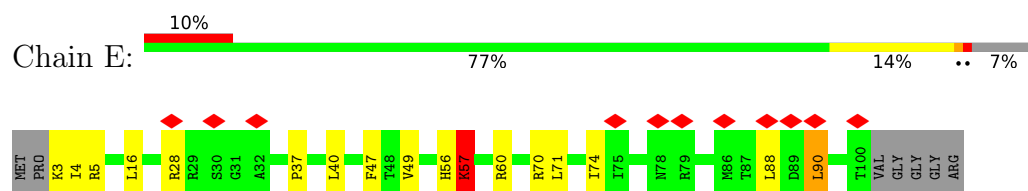
- Molecule 4: 30S ribosomal protein S20



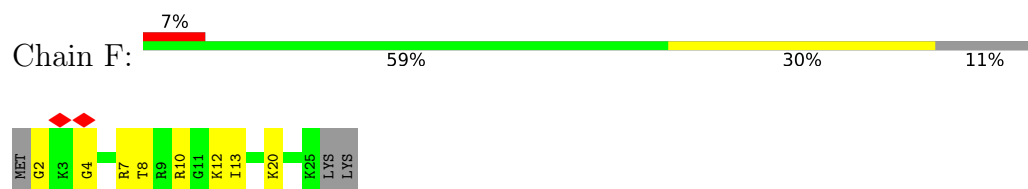
- Molecule 5: 30S ribosomal protein S19



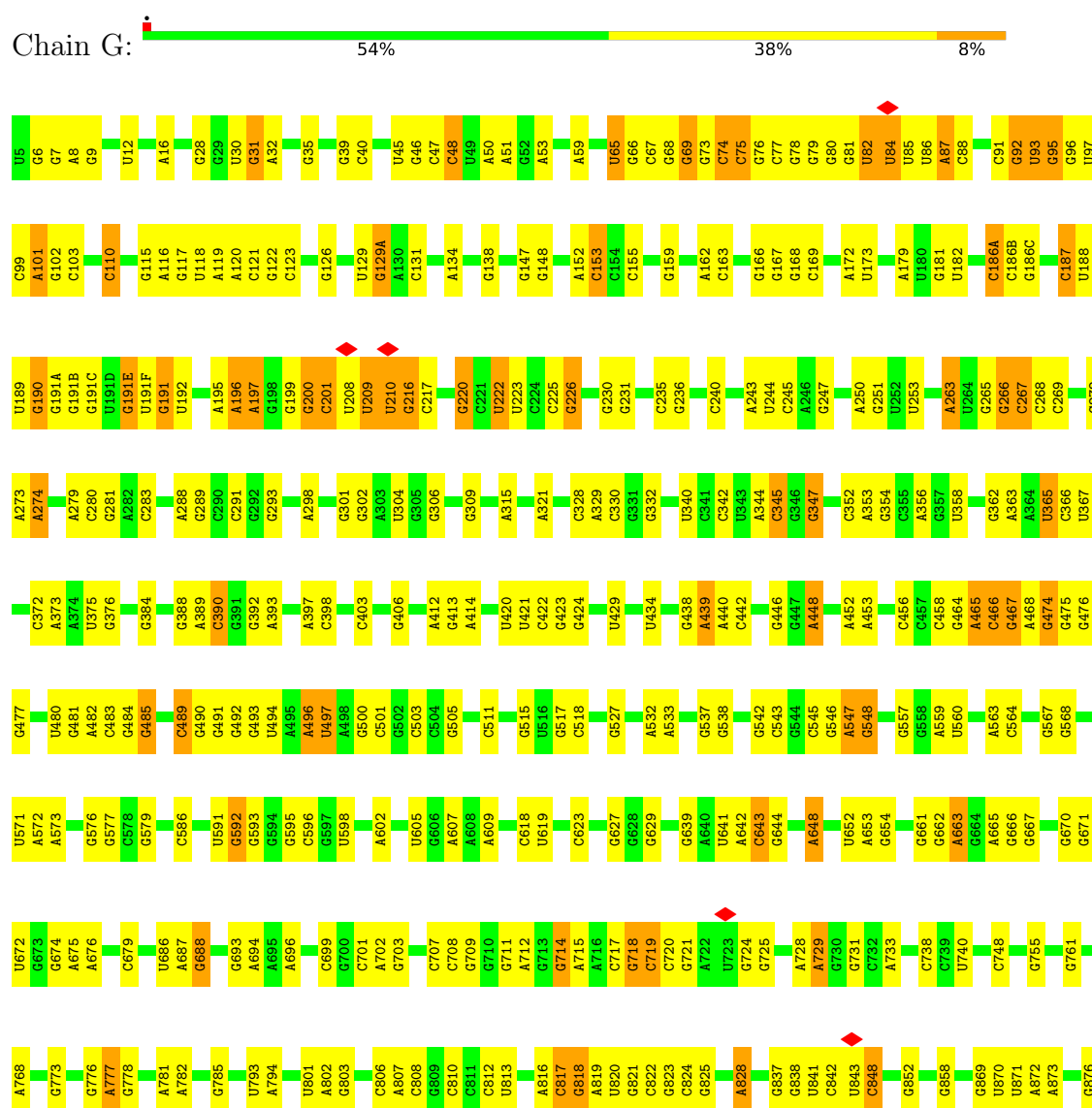
- Molecule 6: 30S ribosomal protein S10

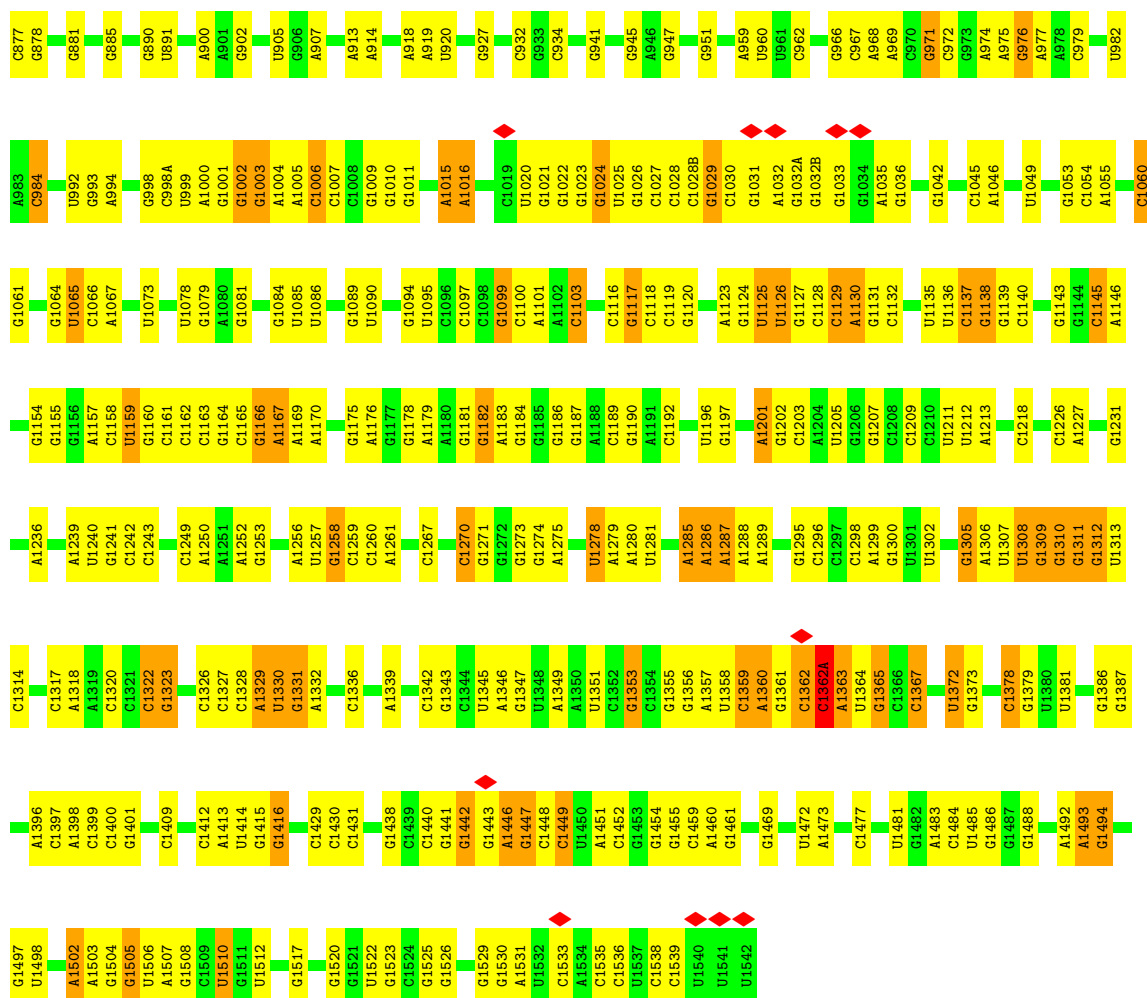


- Molecule 7: 30S ribosomal protein Thx

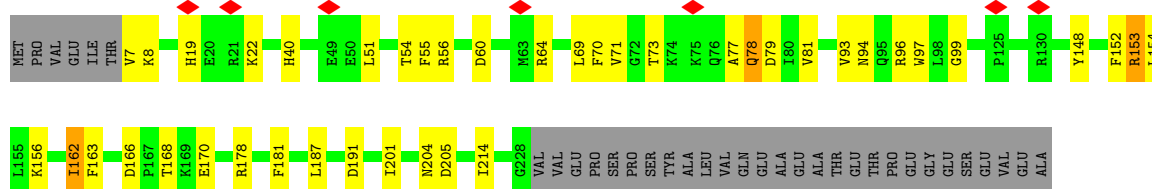


- Molecule 8: 16S ribosomal RNA

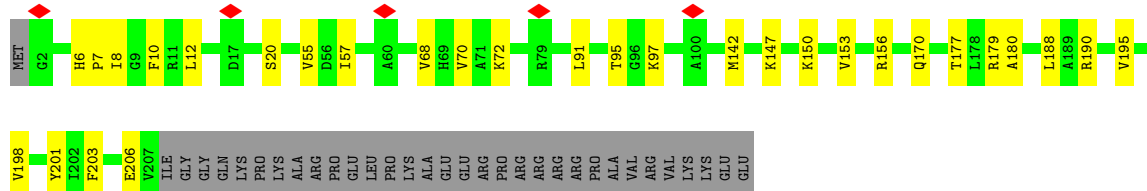




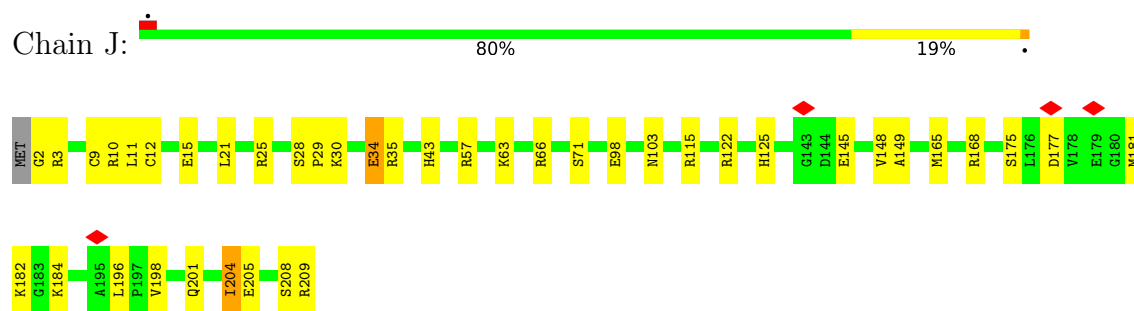
• Molecule 9: 30S ribosomal protein S2



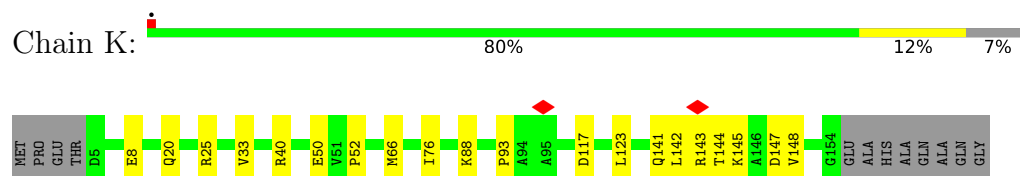
• Molecule 10: 30S ribosomal protein S3



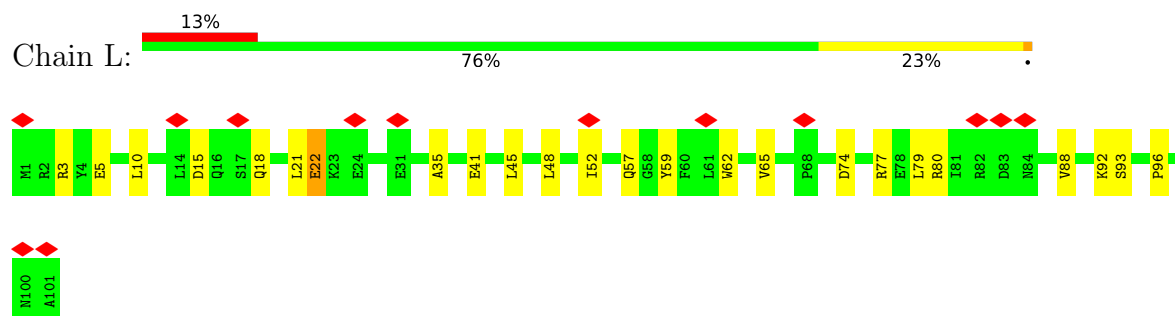
- Molecule 11: 30S ribosomal protein S4



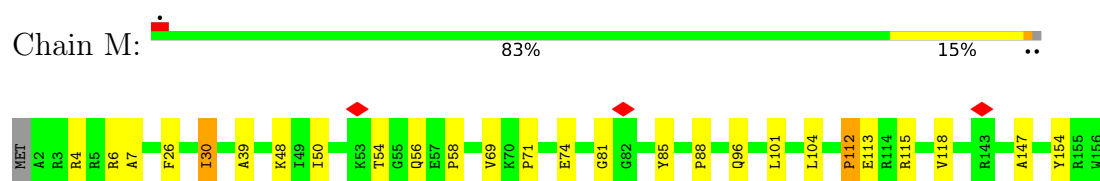
- Molecule 12: 30S ribosomal protein S5



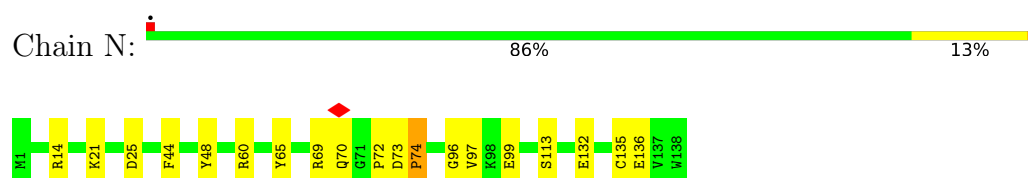
- Molecule 13: 30S ribosomal protein S6



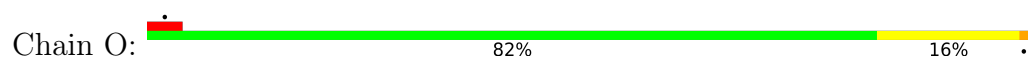
- Molecule 14: 30S ribosomal protein S7

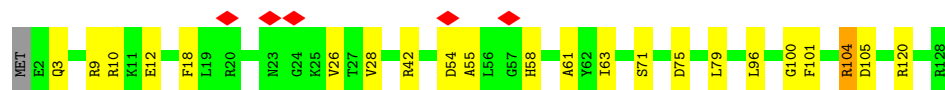


- Molecule 15: 30S ribosomal protein S8



- Molecule 16: 30S ribosomal protein S9

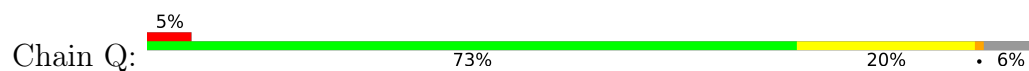




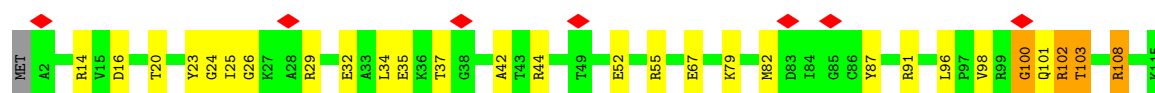
- Molecule 17: 30S ribosomal protein S11



- Molecule 18: 30S ribosomal protein S12



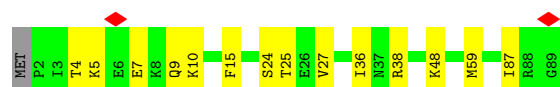
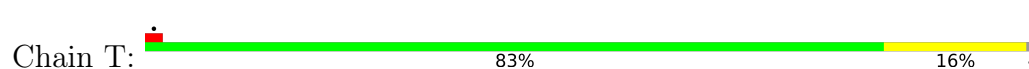
- Molecule 19: 30S ribosomal protein S13



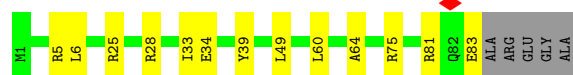
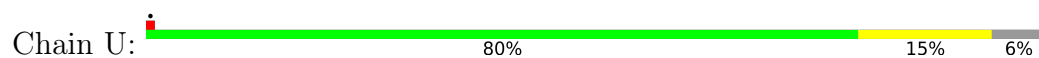
- Molecule 20: 30S ribosomal protein S14 type Z



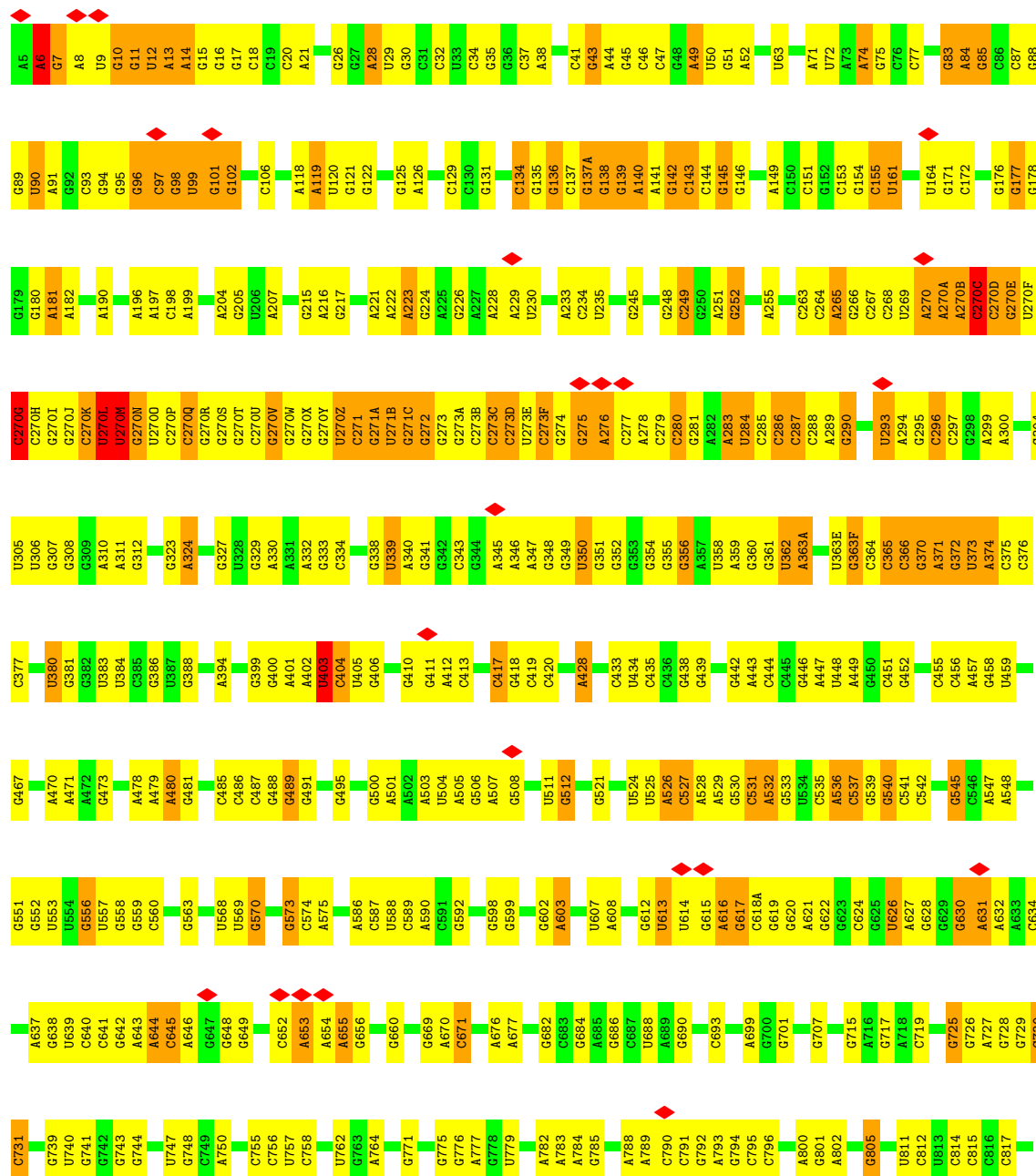
- Molecule 21: 30S ribosomal protein S15

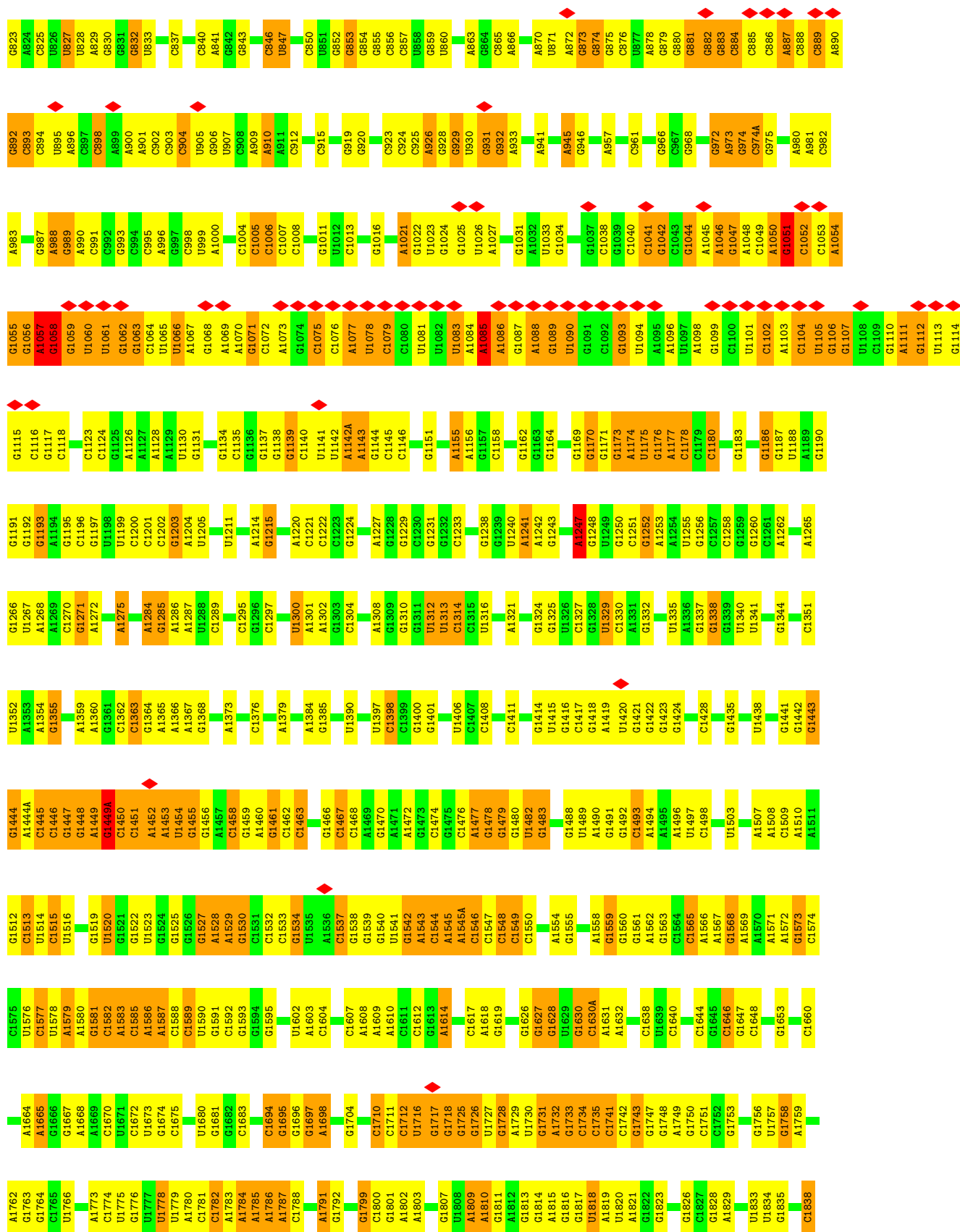


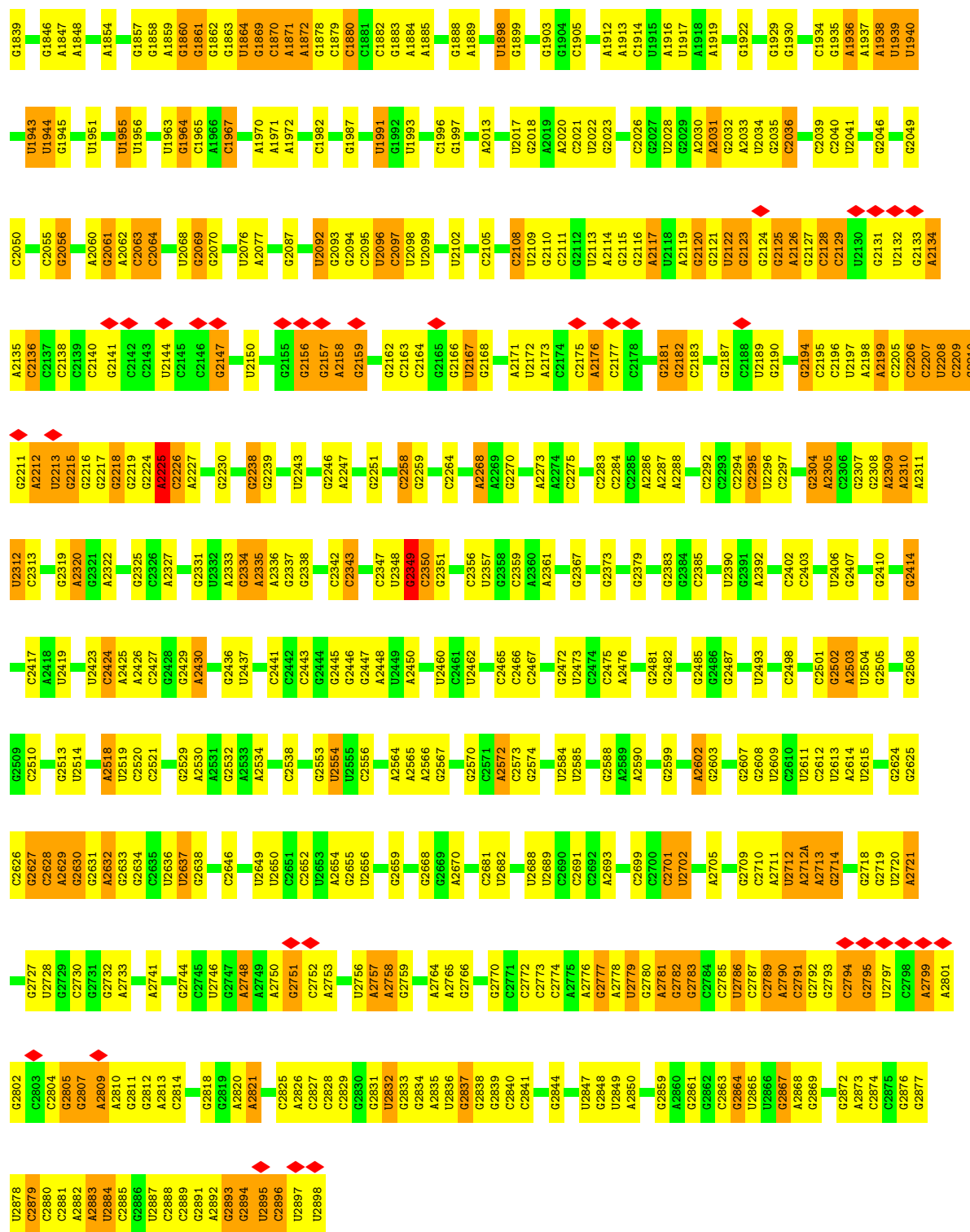
• Molecule 22: 30S ribosomal protein S16



• Molecule 23: 23S ribosomal RNA

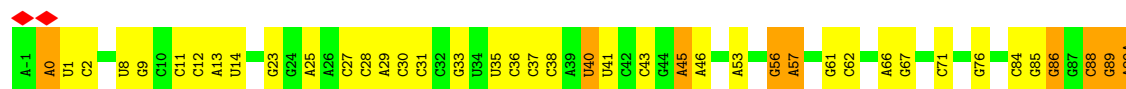


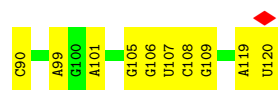




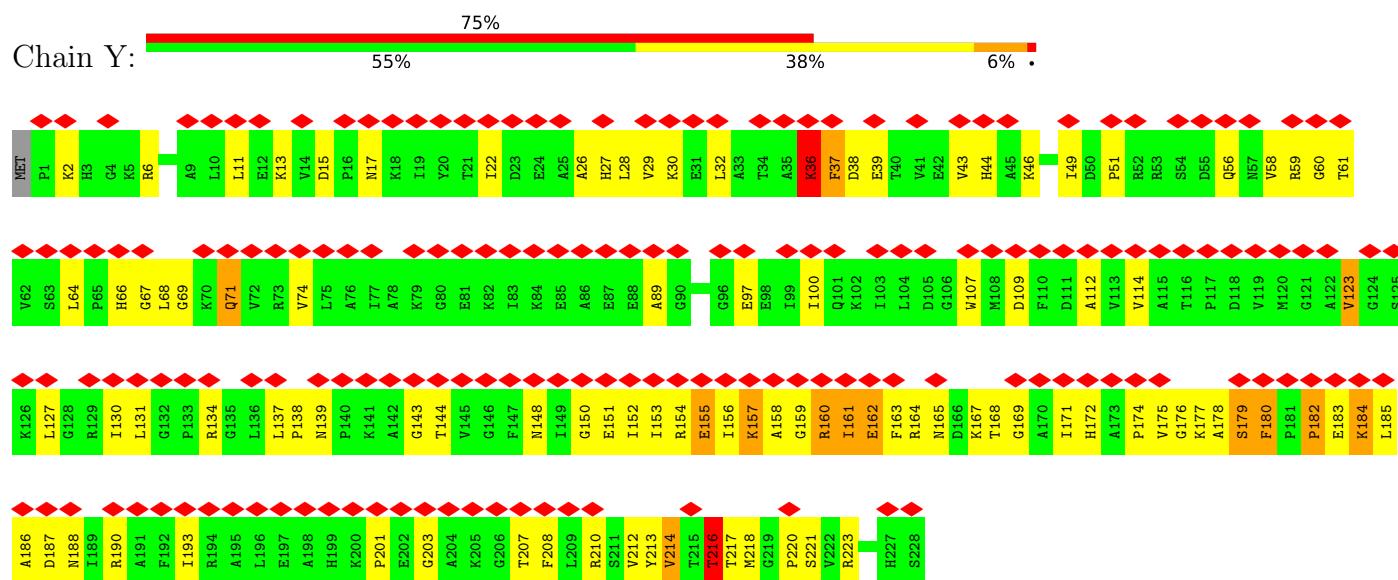
• Molecule 24: 5S ribosomal RNA

Chain X:

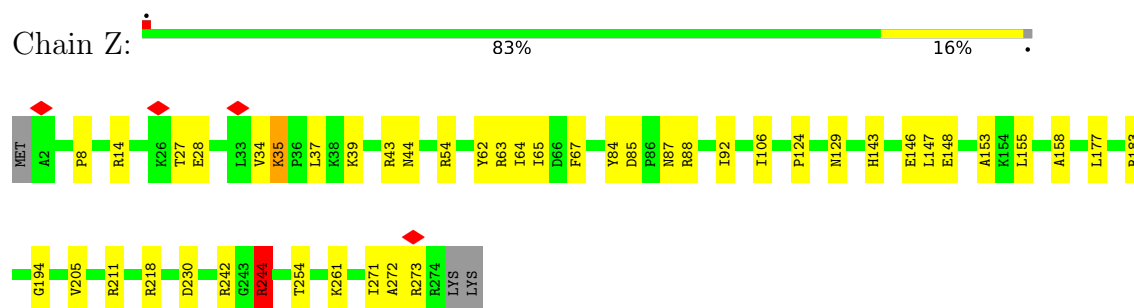




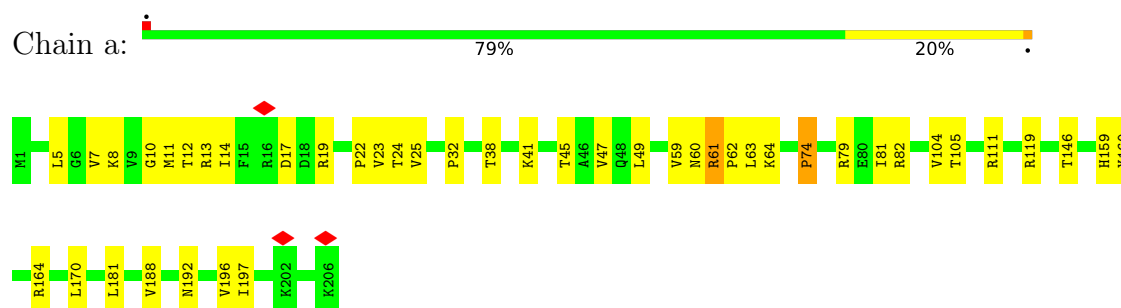
• Molecule 25: 50S ribosomal protein L1



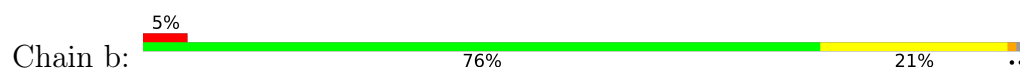
• Molecule 26: 50S ribosomal protein L2

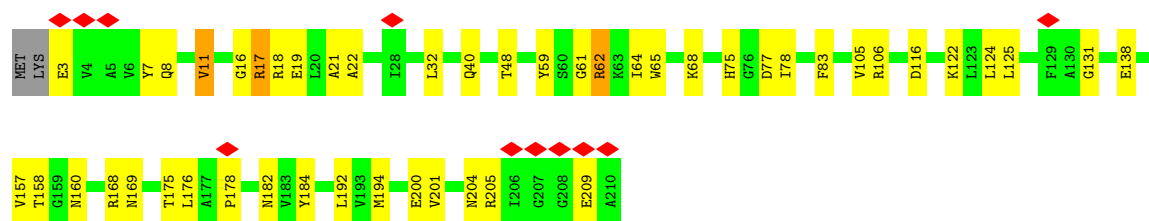


• Molecule 27: 50S ribosomal protein L3

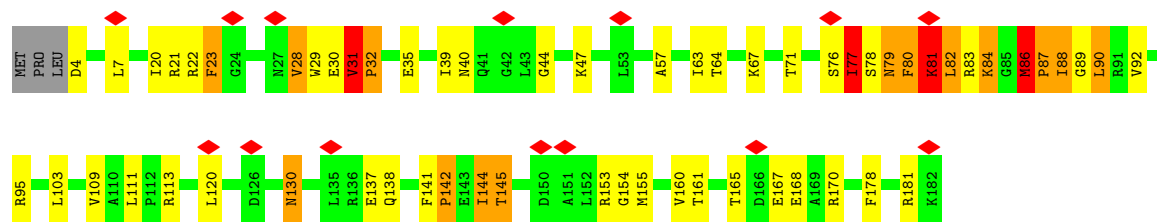


• Molecule 28: 50S ribosomal protein L4

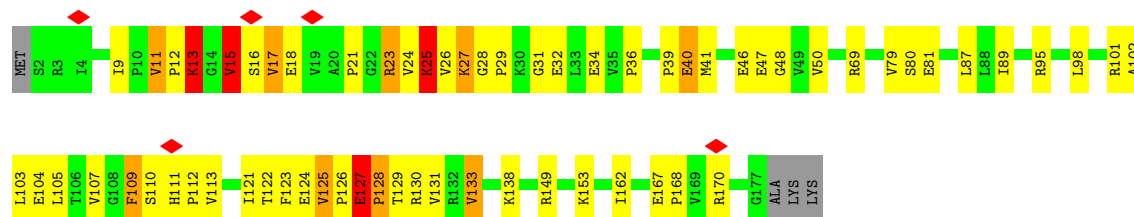




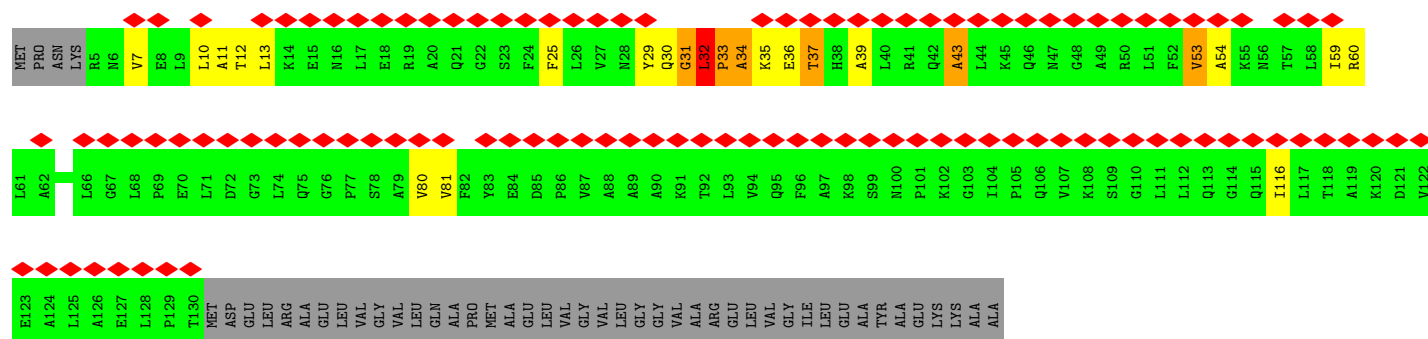
• Molecule 29: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L6

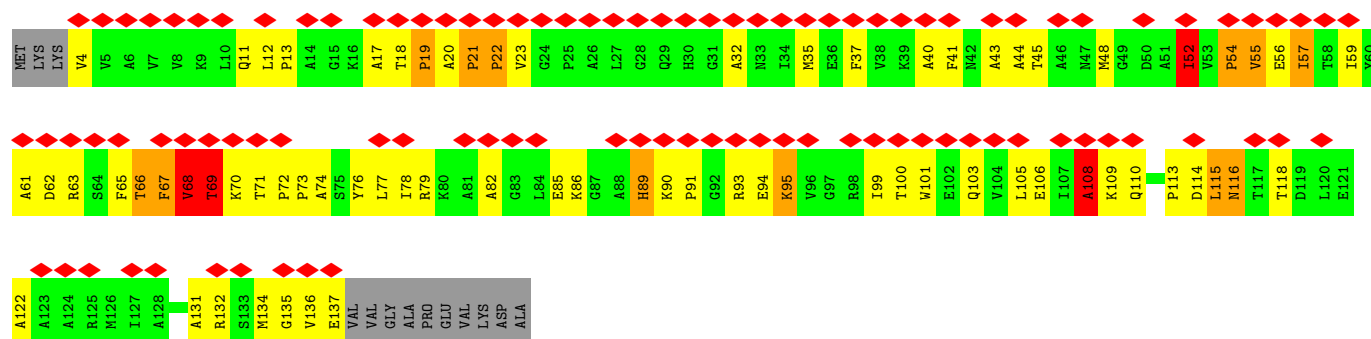


• Molecule 31: 50S ribosomal protein L10

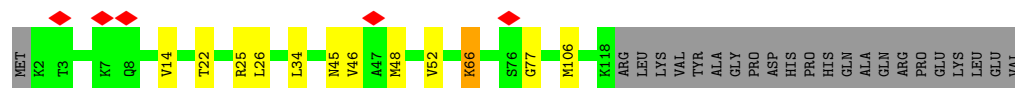
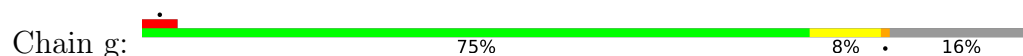


• Molecule 32: 50S ribosomal protein L11

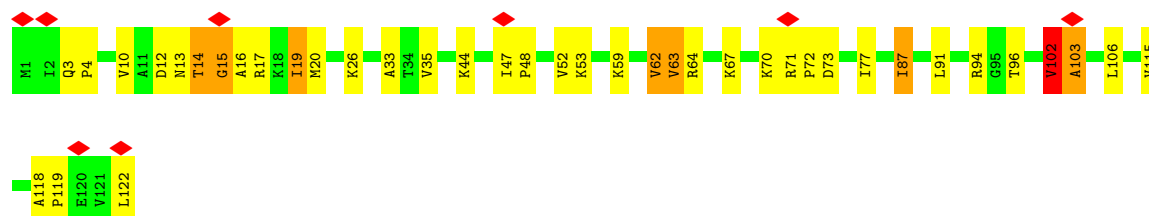




• Molecule 33: 50S ribosomal protein L13



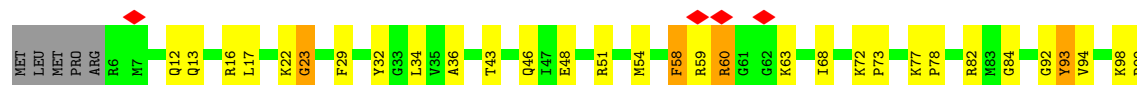
• Molecule 34: 50S ribosomal protein L14

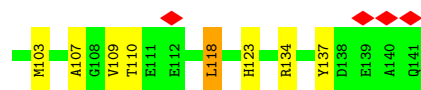


• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16





- Molecule 37: 50S ribosomal protein L17

Chain k: 86% 14%



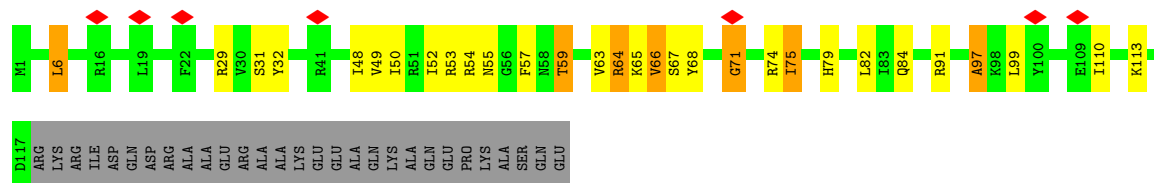
- Molecule 38: 50S ribosomal protein L18

Chain l: 55% 34% 9%



- Molecule 39: 50S ribosomal protein L19

Chain m: 5% 60% 16% 5% 20%



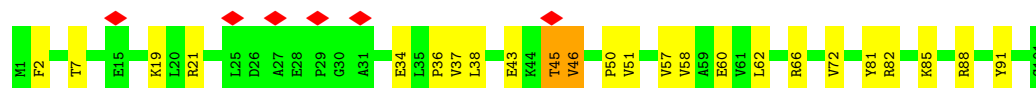
- Molecule 40: 50S ribosomal protein L20

Chain n: 88% 10%



- Molecule 41: 50S ribosomal protein L21

Chain o: 6% 76% 22%

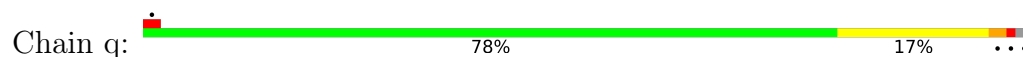


- Molecule 42: 50S ribosomal protein L22

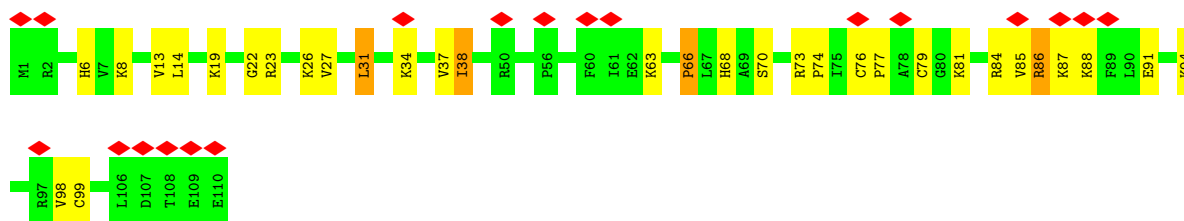
Chain p: 88% 10%



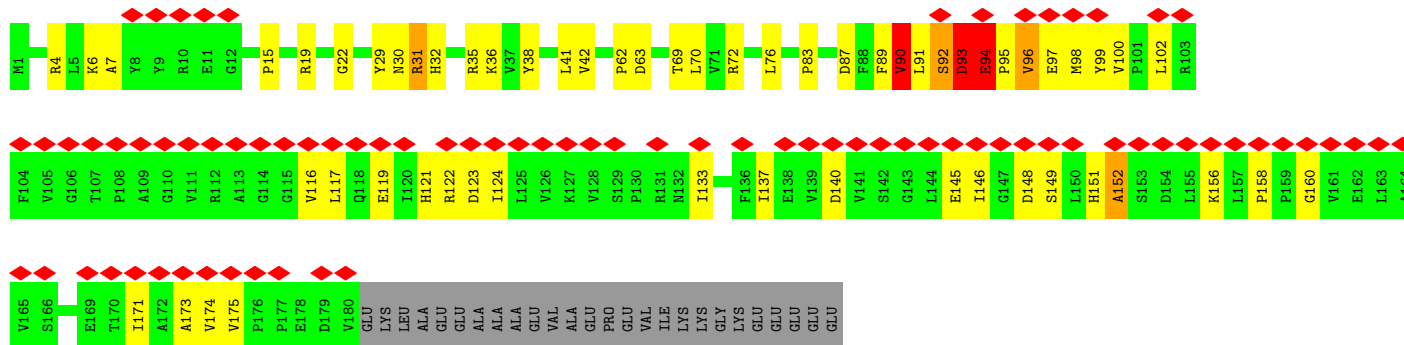
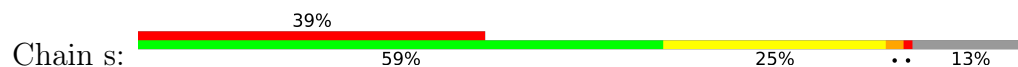
- Molecule 43: 50S ribosomal protein L23



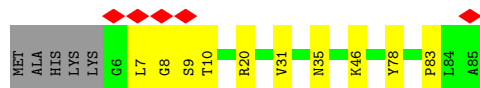
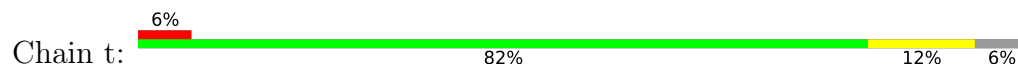
- Molecule 44: 50S ribosomal protein L24



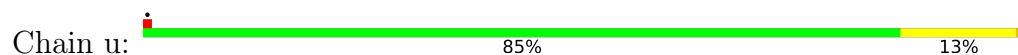
- Molecule 45: 50S ribosomal protein L25

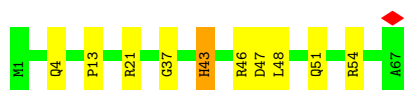


- Molecule 46: 50S ribosomal protein L27

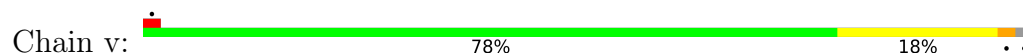


- Molecule 47: 50S ribosomal protein L29

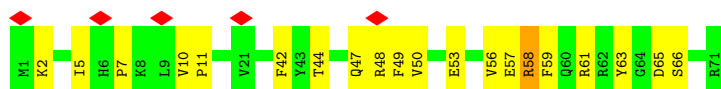




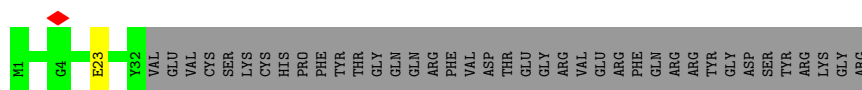
- Molecule 48: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L31



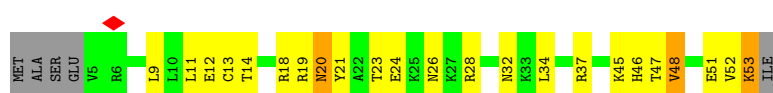
- Molecule 49: 50S ribosomal protein L31



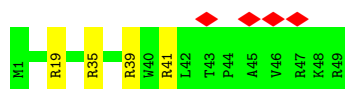
- Molecule 50: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34



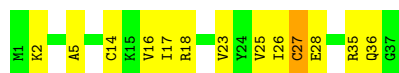
- Molecule 53: 50S ribosomal protein L35

Chain AA:  78% 15% . . .



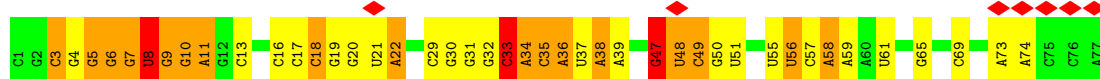
- Molecule 54: 50S ribosomal protein L36

Chain BB:  65% 32% .

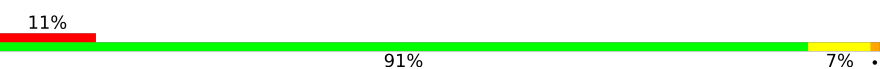


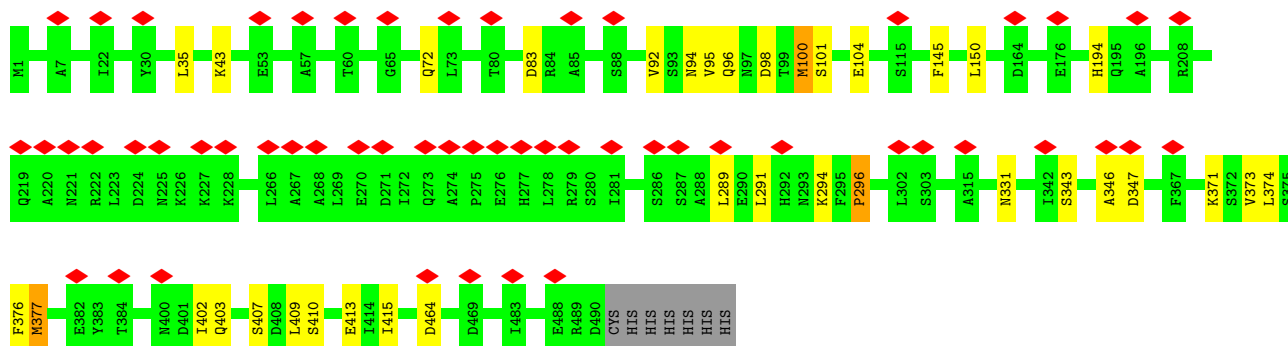
- Molecule 55: P-site tRNA

Chain DD:  9% 44% 30% 22% .



- Molecule 56: Macrolide efflux protein

Chain EE:  11% 91% 7% ..



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 127778                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.568                                   | Depositor |
| Minimum map value                    | -0.339                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.021                                   | Depositor |
| Recommended contour level            | 0.052                                   | Depositor |
| Map size (Å)                         | 396.0, 396.0, 396.0                     | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.1, 1.1, 1.1                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, MG, 5MU, 4SU, PSU, 7MG, ANP

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   | W     | 0.30         | 0/166          | 0.57        | 0/256            |
| 2   | A     | 0.30         | 0/821          | 0.70        | 0/1098           |
| 3   | B     | 0.29         | 0/603          | 0.80        | 2/799 (0.3%)     |
| 4   | C     | 0.28         | 0/765          | 0.68        | 0/1007           |
| 5   | D     | 0.36         | 0/670          | 0.70        | 0/903            |
| 6   | E     | 0.29         | 0/807          | 0.81        | 2/1085 (0.2%)    |
| 7   | F     | 0.27         | 0/212          | 0.61        | 0/277            |
| 8   | G     | 0.33         | 2/36416 (0.0%) | 0.51        | 4/56835 (0.0%)   |
| 9   | H     | 0.28         | 0/1842         | 0.77        | 0/2479           |
| 10  | I     | 0.28         | 0/1636         | 0.67        | 0/2205           |
| 11  | J     | 0.32         | 0/1733         | 0.79        | 7/2318 (0.3%)    |
| 12  | K     | 0.33         | 0/1162         | 0.72        | 0/1564           |
| 13  | L     | 0.29         | 0/856          | 0.74        | 0/1154           |
| 14  | M     | 0.30         | 0/1276         | 0.75        | 1/1709 (0.1%)    |
| 15  | N     | 0.30         | 0/1136         | 0.74        | 1/1527 (0.1%)    |
| 16  | O     | 0.29         | 0/1029         | 0.74        | 0/1379           |
| 17  | P     | 0.27         | 0/900          | 0.68        | 0/1213           |
| 18  | Q     | 0.36         | 0/986          | 0.86        | 0/1320           |
| 19  | R     | 0.29         | 0/924          | 0.80        | 2/1238 (0.2%)    |
| 20  | S     | 0.27         | 0/501          | 0.71        | 0/664            |
| 21  | T     | 0.29         | 0/745          | 0.64        | 0/992            |
| 22  | U     | 0.28         | 0/716          | 0.66        | 0/963            |
| 23  | V     | 0.43         | 2/69349 (0.0%) | 0.61        | 36/108263 (0.0%) |
| 24  | X     | 0.30         | 0/2954         | 0.51        | 1/4606 (0.0%)    |
| 25  | Y     | 0.46         | 1/1775 (0.1%)  | 0.90        | 5/2393 (0.2%)    |
| 26  | Z     | 0.44         | 0/2176         | 0.87        | 5/2933 (0.2%)    |
| 27  | a     | 0.44         | 0/1611         | 0.95        | 1/2171 (0.0%)    |
| 28  | b     | 0.40         | 0/1660         | 0.85        | 2/2247 (0.1%)    |
| 29  | c     | 0.31         | 0/1479         | 0.90        | 4/1989 (0.2%)    |
| 30  | d     | 0.32         | 0/1360         | 0.92        | 6/1838 (0.3%)    |
| 31  | e     | 0.53         | 0/620          | 1.05        | 6/861 (0.7%)     |
| 32  | f     | 0.35         | 0/1012         | 1.01        | 7/1373 (0.5%)    |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 33  | g     | 0.37         | 0/952           | 0.87        | 2/1283 (0.2%)     |
| 34  | h     | 0.42         | 0/942           | 1.06        | 4/1268 (0.3%)     |
| 35  | i     | 0.40         | 0/1125          | 1.01        | 4/1497 (0.3%)     |
| 36  | j     | 0.44         | 0/1100          | 1.01        | 1/1470 (0.1%)     |
| 37  | k     | 0.39         | 0/974           | 0.80        | 0/1302            |
| 38  | l     | 0.30         | 0/887           | 0.76        | 0/1180            |
| 39  | m     | 0.42         | 0/990           | 0.99        | 2/1325 (0.2%)     |
| 40  | n     | 0.42         | 0/982           | 0.74        | 0/1306            |
| 41  | o     | 0.38         | 0/790           | 1.03        | 5/1057 (0.5%)     |
| 42  | p     | 0.39         | 0/886           | 0.74        | 2/1189 (0.2%)     |
| 43  | q     | 0.35         | 0/756           | 0.91        | 2/1015 (0.2%)     |
| 44  | r     | 0.36         | 0/857           | 1.08        | 5/1142 (0.4%)     |
| 45  | s     | 0.36         | 0/1467          | 0.81        | 4/1992 (0.2%)     |
| 46  | t     | 0.33         | 0/637           | 0.69        | 0/848             |
| 47  | u     | 0.33         | 0/569           | 0.76        | 0/751             |
| 48  | v     | 0.40         | 0/474           | 0.87        | 0/635             |
| 49  | CC    | 0.19         | 0/156           | 0.62        | 0/215             |
| 49  | w     | 0.51         | 0/594           | 1.14        | 0/795             |
| 50  | x     | 0.39         | 0/459           | 0.92        | 0/621             |
| 51  | y     | 0.46         | 0/429           | 1.05        | 3/572 (0.5%)      |
| 52  | z     | 0.53         | 0/438           | 1.03        | 0/575             |
| 53  | AA    | 0.47         | 0/523           | 1.05        | 4/690 (0.6%)      |
| 54  | BB    | 0.37         | 0/310           | 0.89        | 1/407 (0.2%)      |
| 55  | DD    | 0.29         | 0/1724          | 0.52        | 1/2687 (0.0%)     |
| 56  | EE    | 0.31         | 0/3892          | 0.76        | 2/5224 (0.0%)     |
| All | All   | 0.38         | 5/162811 (0.0%) | 0.66        | 134/242705 (0.1%) |

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   | B     | 0                   | 3                   |
| 4   | C     | 0                   | 1                   |
| 5   | D     | 0                   | 1                   |
| 6   | E     | 0                   | 4                   |
| 9   | H     | 0                   | 2                   |
| 11  | J     | 0                   | 2                   |
| 12  | K     | 0                   | 1                   |
| 13  | L     | 0                   | 2                   |
| 14  | M     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 15  | N     | 0                   | 1                   |
| 16  | O     | 0                   | 2                   |
| 18  | Q     | 0                   | 1                   |
| 19  | R     | 0                   | 1                   |
| 23  | V     | 0                   | 6                   |
| 25  | Y     | 0                   | 4                   |
| 26  | Z     | 0                   | 8                   |
| 27  | a     | 0                   | 2                   |
| 28  | b     | 0                   | 5                   |
| 29  | c     | 0                   | 4                   |
| 30  | d     | 0                   | 2                   |
| 31  | e     | 0                   | 8                   |
| 32  | f     | 0                   | 2                   |
| 33  | g     | 0                   | 2                   |
| 34  | h     | 0                   | 10                  |
| 35  | i     | 0                   | 8                   |
| 36  | j     | 0                   | 6                   |
| 38  | l     | 0                   | 1                   |
| 39  | m     | 0                   | 8                   |
| 41  | o     | 0                   | 4                   |
| 43  | q     | 0                   | 2                   |
| 44  | r     | 0                   | 7                   |
| 46  | t     | 0                   | 1                   |
| 47  | u     | 0                   | 2                   |
| 48  | v     | 0                   | 1                   |
| 49  | w     | 0                   | 2                   |
| 50  | x     | 0                   | 1                   |
| 51  | y     | 0                   | 1                   |
| 52  | z     | 0                   | 1                   |
| 53  | AA    | 0                   | 2                   |
| 56  | EE    | 0                   | 6                   |
| All | All   | 0                   | 129                 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res     | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 23  | V     | 1449(A) | G    | O3'-P | -12.49 | 1.42        | 1.61     |
| 23  | V     | 1146    | C    | O3'-P | 9.51   | 1.75        | 1.61     |
| 8   | G     | 93      | U    | O3'-P | -7.18  | 1.50        | 1.61     |
| 8   | G     | 1167    | A    | O3'-P | -6.22  | 1.51        | 1.61     |
| 25  | Y     | 180     | PHE  | C-N   | 5.13   | 1.39        | 1.33     |

All (134) bond angle outliers are listed below:

| Mol | Chain | Res     | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|--------|-------------|----------|
| 23  | V     | 1449(A) | G    | O3'-P-O5'   | -24.54 | 67.19       | 104.00   |
| 23  | V     | 155     | C    | O3'-P-O5'   | -22.82 | 69.77       | 104.00   |
| 30  | d     | 11      | VAL  | C-N-CD      | -12.70 | 72.92       | 125.00   |
| 26  | Z     | 244     | ARG  | C-N-CD      | -11.75 | 94.75       | 120.60   |
| 26  | Z     | 244     | ARG  | CA-C-N      | 11.29  | 154.11      | 127.00   |
| 26  | Z     | 244     | ARG  | C-N-CA      | 11.29  | 154.11      | 127.00   |
| 8   | G     | 93      | U    | O3'-P-O5'   | -11.00 | 87.50       | 104.00   |
| 23  | V     | 1146    | C    | O3'-P-O5'   | 10.57  | 119.85      | 104.00   |
| 30  | d     | 127     | GLU  | C-N-CD      | -10.49 | 82.00       | 125.00   |
| 23  | V     | 1060    | U    | OP1-P-O3'   | -10.09 | 77.72       | 108.00   |
| 23  | V     | 1060    | U    | OP2-P-O3'   | -9.91  | 78.27       | 108.00   |
| 23  | V     | 920     | G    | OP1-P-O3'   | -9.43  | 79.71       | 108.00   |
| 32  | f     | 108     | ALA  | CA-C-N      | 9.34   | 137.60      | 122.10   |
| 32  | f     | 108     | ALA  | C-N-CA      | 9.34   | 137.60      | 122.10   |
| 32  | f     | 22      | PRO  | CA-N-CD     | -9.23  | 99.07       | 112.00   |
| 56  | EE    | 296     | PRO  | CA-N-CD     | -9.19  | 99.14       | 112.00   |
| 23  | V     | 1061    | U    | OP1-P-OP2   | 9.15   | 147.06      | 119.60   |
| 29  | c     | 86      | MET  | C-N-CD      | -8.85  | 88.71       | 125.00   |
| 23  | V     | 155     | C    | OP2-P-O3'   | 8.56   | 133.69      | 108.00   |
| 23  | V     | 1449(A) | G    | C2'-C3'-O3' | 8.15   | 121.72      | 109.50   |
| 23  | V     | 403     | U    | C2'-C3'-O3' | 8.14   | 121.70      | 109.50   |
| 23  | V     | 6       | A    | C2'-C3'-O3' | 8.12   | 121.67      | 109.50   |
| 30  | d     | 109     | PHE  | CA-C-N      | 7.66   | 136.17      | 121.54   |
| 30  | d     | 109     | PHE  | C-N-CA      | 7.66   | 136.17      | 121.54   |
| 8   | G     | 1362(A) | C    | C2'-C3'-O3' | 7.54   | 120.81      | 109.50   |
| 11  | J     | 9       | CYS  | CA-CB-SG    | 7.46   | 131.56      | 114.40   |
| 31  | e     | 34      | ALA  | N-CA-C      | 7.43   | 120.44      | 111.82   |
| 29  | c     | 31      | VAL  | C-N-CD      | -7.18  | 95.57       | 125.00   |
| 23  | V     | 1057    | A    | O3'-P-O5'   | 7.12   | 114.68      | 104.00   |
| 45  | s     | 31      | ARG  | CA-C-N      | 7.01   | 134.93      | 121.54   |
| 45  | s     | 31      | ARG  | C-N-CA      | 7.01   | 134.93      | 121.54   |
| 23  | V     | 136     | G    | C2'-C3'-O3' | 6.95   | 124.12      | 113.70   |
| 23  | V     | 1085    | A    | P-O3'-C3'   | 6.84   | 130.46      | 120.20   |
| 33  | g     | 66      | LYS  | CA-C-N      | 6.80   | 134.53      | 121.54   |
| 33  | g     | 66      | LYS  | C-N-CA      | 6.80   | 134.53      | 121.54   |
| 54  | BB    | 27      | CYS  | CA-CB-SG    | 6.79   | 130.01      | 114.40   |
| 23  | V     | 920     | G    | OP2-P-O3'   | -6.73  | 87.82       | 108.00   |
| 44  | r     | 85      | VAL  | CA-C-N      | 6.63   | 134.20      | 121.54   |
| 44  | r     | 85      | VAL  | C-N-CA      | 6.63   | 134.20      | 121.54   |
| 23  | V     | 1052    | C    | O5'-C5'-C4' | 6.62   | 121.43      | 111.50   |
| 43  | q     | 87      | GLN  | CA-C-N      | 6.56   | 134.07      | 121.54   |
| 43  | q     | 87      | GLN  | C-N-CA      | 6.56   | 134.07      | 121.54   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 35  | i     | 69     | GLY  | CA-C-N      | -6.46 | 109.20      | 121.54   |
| 35  | i     | 69     | GLY  | C-N-CA      | -6.46 | 109.20      | 121.54   |
| 31  | e     | 31     | GLY  | N-CA-C      | 6.43  | 128.42      | 113.18   |
| 23  | V     | 136    | G    | C3'-C2'-O2' | 6.42  | 120.33      | 110.70   |
| 32  | f     | 18     | THR  | C-N-CD      | -6.36 | 98.91       | 125.00   |
| 35  | i     | 35     | HIS  | CA-C-N      | 6.32  | 133.61      | 121.54   |
| 35  | i     | 35     | HIS  | C-N-CA      | 6.32  | 133.61      | 121.54   |
| 23  | V     | 1052   | C    | C5'-C4'-C3' | 6.31  | 125.46      | 116.00   |
| 31  | e     | 59     | ILE  | CA-C-N      | 6.20  | 133.38      | 121.54   |
| 31  | e     | 59     | ILE  | C-N-CA      | 6.20  | 133.38      | 121.54   |
| 11  | J     | 29     | PRO  | CA-C-N      | 6.13  | 131.37      | 122.36   |
| 11  | J     | 29     | PRO  | C-N-CA      | 6.13  | 131.37      | 122.36   |
| 25  | Y     | 180    | PHE  | CA-C-N      | -6.13 | 114.07      | 120.38   |
| 25  | Y     | 180    | PHE  | C-N-CA      | -6.13 | 114.07      | 120.38   |
| 30  | d     | 25     | LYS  | N-CA-C      | 6.12  | 118.72      | 109.23   |
| 23  | V     | 1051   | G    | P-O3'-C3'   | 6.07  | 129.30      | 120.20   |
| 23  | V     | 1057   | A    | C3'-C2'-C1' | 6.06  | 107.36      | 101.30   |
| 23  | V     | 270(M) | U    | C2'-C3'-O3' | -6.01 | 100.49      | 109.50   |
| 27  | a     | 61     | ARG  | CA-CB-CG    | 6.00  | 126.09      | 114.10   |
| 14  | M     | 147    | ALA  | N-CA-C      | -5.98 | 106.62      | 114.04   |
| 44  | r     | 66     | PRO  | CA-C-N      | 5.96  | 135.46      | 121.52   |
| 44  | r     | 66     | PRO  | C-N-CA      | 5.96  | 135.46      | 121.52   |
| 23  | V     | 270(L) | U    | C2'-C3'-O3' | 5.95  | 118.43      | 109.50   |
| 39  | m     | 64     | ARG  | CA-C-N      | 5.92  | 132.85      | 121.54   |
| 39  | m     | 64     | ARG  | C-N-CA      | 5.92  | 132.85      | 121.54   |
| 23  | V     | 1057   | A    | P-O3'-C3'   | 5.92  | 129.07      | 120.20   |
| 23  | V     | 155    | C    | P-O3'-C3'   | -5.89 | 111.36      | 120.20   |
| 8   | G     | 1446   | A    | C2'-C3'-O3' | 5.87  | 118.31      | 109.50   |
| 11  | J     | 12     | CYS  | CA-CB-SG    | 5.87  | 127.90      | 114.40   |
| 11  | J     | 34     | GLU  | CA-C-N      | 5.87  | 132.74      | 121.54   |
| 11  | J     | 34     | GLU  | C-N-CA      | 5.87  | 132.74      | 121.54   |
| 51  | y     | 18     | ARG  | CA-C-N      | 5.87  | 132.74      | 121.54   |
| 51  | y     | 18     | ARG  | C-N-CA      | 5.87  | 132.74      | 121.54   |
| 23  | V     | 1146   | C    | P-O3'-C3'   | -5.84 | 111.44      | 120.20   |
| 19  | R     | 103    | THR  | CA-C-N      | 5.82  | 132.65      | 121.54   |
| 19  | R     | 103    | THR  | C-N-CA      | 5.82  | 132.65      | 121.54   |
| 6   | E     | 56     | HIS  | CA-C-N      | 5.80  | 132.62      | 121.54   |
| 6   | E     | 56     | HIS  | C-N-CA      | 5.80  | 132.62      | 121.54   |
| 34  | h     | 12     | ASP  | CA-C-N      | 5.80  | 130.41      | 121.19   |
| 34  | h     | 12     | ASP  | C-N-CA      | 5.80  | 130.41      | 121.19   |
| 26  | Z     | 27     | THR  | CA-C-N      | 5.77  | 135.89      | 121.80   |
| 26  | Z     | 27     | THR  | C-N-CA      | 5.77  | 135.89      | 121.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | B     | 87   | ARG  | CA-C-N      | 5.75  | 132.05      | 121.70   |
| 3   | B     | 87   | ARG  | C-N-CA      | 5.75  | 132.05      | 121.70   |
| 45  | s     | 94   | GLU  | CA-C-N      | -5.71 | 114.08      | 119.90   |
| 45  | s     | 94   | GLU  | C-N-CA      | -5.71 | 114.08      | 119.90   |
| 23  | V     | 2238 | G    | P-O3'-C3'   | 5.66  | 128.70      | 120.20   |
| 42  | p     | 89   | ALA  | CA-C-N      | 5.63  | 132.30      | 121.54   |
| 42  | p     | 89   | ALA  | C-N-CA      | 5.63  | 132.30      | 121.54   |
| 23  | V     | 846  | C    | P-O3'-C3'   | 5.57  | 128.55      | 120.20   |
| 36  | j     | 23   | GLY  | N-CA-C      | 5.52  | 126.26      | 113.18   |
| 30  | d     | 125  | VAL  | C-N-CD      | -5.49 | 102.50      | 125.00   |
| 41  | o     | 81   | TYR  | CA-C-N      | 5.49  | 130.42      | 122.36   |
| 41  | o     | 81   | TYR  | C-N-CA      | 5.49  | 130.42      | 122.36   |
| 23  | V     | 2349 | G    | C4-N9-C1'   | 5.47  | 142.92      | 126.50   |
| 23  | V     | 1247 | A    | P-O3'-C3'   | 5.47  | 128.41      | 120.20   |
| 23  | V     | 2225 | A    | C4'-C3'-O3' | 5.47  | 117.61      | 109.40   |
| 53  | AA    | 13   | ARG  | CA-C-N      | 5.42  | 131.72      | 121.97   |
| 53  | AA    | 13   | ARG  | C-N-CA      | 5.42  | 131.72      | 121.97   |
| 41  | o     | 82   | ARG  | N-CA-C      | 5.41  | 119.30      | 111.56   |
| 34  | h     | 102  | VAL  | CA-C-N      | 5.40  | 131.85      | 121.54   |
| 34  | h     | 102  | VAL  | C-N-CA      | 5.40  | 131.85      | 121.54   |
| 32  | f     | 109  | LYS  | N-CA-C      | -5.36 | 101.15      | 108.38   |
| 23  | V     | 2158 | A    | P-O3'-C3'   | 5.36  | 128.23      | 120.20   |
| 56  | EE    | 377  | MET  | N-CA-C      | -5.35 | 105.45      | 111.28   |
| 51  | y     | 23   | THR  | N-CA-C      | 5.35  | 122.20      | 110.80   |
| 23  | V     | 119  | A    | C2'-C3'-O3' | 5.33  | 117.50      | 109.50   |
| 8   | G     | 1065 | U    | P-O3'-C3'   | 5.30  | 128.16      | 120.20   |
| 31  | e     | 53   | VAL  | CA-C-N      | 5.28  | 131.62      | 121.54   |
| 31  | e     | 53   | VAL  | C-N-CA      | 5.28  | 131.62      | 121.54   |
| 28  | b     | 17   | ARG  | CA-C-N      | 5.27  | 131.61      | 121.54   |
| 28  | b     | 17   | ARG  | C-N-CA      | 5.27  | 131.61      | 121.54   |
| 23  | V     | 1085 | A    | C2'-C3'-O3' | 5.25  | 117.38      | 109.50   |
| 41  | o     | 45   | THR  | CA-C-N      | 5.25  | 131.41      | 121.97   |
| 41  | o     | 45   | THR  | C-N-CA      | 5.25  | 131.41      | 121.97   |
| 11  | J     | 196  | LEU  | CA-CB-CG    | 5.22  | 134.58      | 116.30   |
| 29  | c     | 145  | THR  | CA-C-N      | 5.21  | 131.50      | 121.54   |
| 29  | c     | 145  | THR  | C-N-CA      | 5.21  | 131.50      | 121.54   |
| 23  | V     | 1062 | G    | P-O3'-C3'   | 5.19  | 127.98      | 120.20   |
| 55  | DD    | 18   | C    | P-O3'-C3'   | 5.19  | 127.98      | 120.20   |
| 23  | V     | 119  | A    | P-O3'-C3'   | 5.16  | 127.94      | 120.20   |
| 25  | Y     | 216  | THR  | CB-CA-C     | 5.15  | 120.67      | 110.42   |
| 32  | f     | 116  | ASN  | CA-C-N      | 5.11  | 131.29      | 121.54   |
| 32  | f     | 116  | ASN  | C-N-CA      | 5.11  | 131.29      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 53  | AA    | 12   | LYS  | CA-C-N    | 5.09  | 131.26      | 121.54   |
| 53  | AA    | 12   | LYS  | C-N-CA    | 5.09  | 131.26      | 121.54   |
| 25  | Y     | 36   | LYS  | CA-C-N    | 5.08  | 131.24      | 121.54   |
| 25  | Y     | 36   | LYS  | C-N-CA    | 5.08  | 131.24      | 121.54   |
| 23  | V     | 1058 | G    | O5'-P-OP2 | -5.07 | 92.78       | 108.00   |
| 44  | r     | 31   | LEU  | CA-CB-CG  | 5.07  | 134.03      | 116.30   |
| 15  | N     | 44   | PHE  | N-CA-C    | 5.01  | 116.44      | 110.97   |
| 24  | X     | 56   | G    | P-O3'-C3' | 5.00  | 127.71      | 120.20   |

There are no chirality outliers.

All (129) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 53  | AA    | 53  | PRO  | Peptide |
| 53  | AA    | 62  | LEU  | Peptide |
| 3   | B     | 44  | LEU  | Peptide |
| 3   | B     | 83  | GLU  | Peptide |
| 3   | B     | 86  | VAL  | Peptide |
| 4   | C     | 75  | ASN  | Peptide |
| 5   | D     | 4   | SER  | Peptide |
| 6   | E     | 28  | ARG  | Peptide |
| 6   | E     | 40  | LEU  | Peptide |
| 6   | E     | 57  | LYS  | Peptide |
| 6   | E     | 90  | LEU  | Peptide |
| 56  | EE    | 194 | HIS  | Peptide |
| 56  | EE    | 289 | LEU  | Peptide |
| 56  | EE    | 343 | SER  | Peptide |
| 56  | EE    | 346 | ALA  | Peptide |
| 56  | EE    | 464 | ASP  | Peptide |
| 56  | EE    | 83  | ASP  | Peptide |
| 9   | H     | 152 | PHE  | Peptide |
| 9   | H     | 99  | GLY  | Peptide |
| 11  | J     | 28  | SER  | Peptide |
| 11  | J     | 34  | GLU  | Peptide |
| 12  | K     | 143 | ARG  | Peptide |
| 13  | L     | 22  | GLU  | Peptide |
| 13  | L     | 41  | GLU  | Peptide |
| 14  | M     | 112 | PRO  | Peptide |
| 14  | M     | 7   | ALA  | Peptide |
| 15  | N     | 73  | ASP  | Peptide |
| 16  | O     | 104 | ARG  | Peptide |
| 16  | O     | 54  | ASP  | Peptide |

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| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 18  | Q     | 104    | VAL  | Peptide   |
| 19  | R     | 103    | THR  | Peptide   |
| 23  | V     | 270(C) | C    | Sidechain |
| 23  | V     | 270(D) | C    | Sidechain |
| 23  | V     | 270(G) | C    | Sidechain |
| 23  | V     | 270(Q) | C    | Sidechain |
| 23  | V     | 273(C) | C    | Sidechain |
| 23  | V     | 273(D) | C    | Sidechain |
| 25  | Y     | 11     | LEU  | Peptide   |
| 25  | Y     | 2      | LYS  | Peptide   |
| 25  | Y     | 214    | VAL  | Peptide   |
| 25  | Y     | 71     | GLN  | Peptide   |
| 26  | Z     | 148    | GLU  | Peptide   |
| 26  | Z     | 158    | ALA  | Peptide   |
| 26  | Z     | 211    | ARG  | Peptide   |
| 26  | Z     | 244    | ARG  | Peptide   |
| 26  | Z     | 271    | ILE  | Peptide   |
| 26  | Z     | 272    | ALA  | Peptide   |
| 26  | Z     | 28     | GLU  | Peptide   |
| 26  | Z     | 35     | LYS  | Peptide   |
| 27  | a     | 38     | THR  | Peptide   |
| 27  | a     | 74     | PRO  | Peptide   |
| 28  | b     | 125    | LEU  | Peptide   |
| 28  | b     | 176    | LEU  | Peptide   |
| 28  | b     | 19     | GLU  | Peptide   |
| 28  | b     | 59     | TYR  | Peptide   |
| 28  | b     | 61     | GLY  | Peptide   |
| 29  | c     | 130    | ASN  | Peptide   |
| 29  | c     | 145    | THR  | Peptide   |
| 29  | c     | 181    | ARG  | Peptide   |
| 29  | c     | 23     | PHE  | Peptide   |
| 30  | d     | 110    | SER  | Peptide   |
| 30  | d     | 40     | GLU  | Peptide   |
| 31  | e     | 29     | TYR  | Peptide   |
| 31  | e     | 32     | LEU  | Mainchain |
| 31  | e     | 33     | PRO  | Peptide   |
| 31  | e     | 36     | GLU  | Peptide   |
| 31  | e     | 37     | THR  | Peptide   |
| 31  | e     | 43     | ALA  | Peptide   |
| 31  | e     | 53     | VAL  | Peptide   |
| 31  | e     | 80     | VAL  | Peptide   |
| 32  | f     | 108    | ALA  | Peptide   |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 32  | f     | 118 | THR  | Peptide |
| 33  | g     | 34  | LEU  | Peptide |
| 33  | g     | 77  | GLY  | Peptide |
| 34  | h     | 102 | VAL  | Peptide |
| 34  | h     | 103 | ALA  | Peptide |
| 34  | h     | 118 | ALA  | Peptide |
| 34  | h     | 13  | ASN  | Peptide |
| 34  | h     | 26  | LYS  | Peptide |
| 34  | h     | 52  | VAL  | Peptide |
| 34  | h     | 62  | VAL  | Peptide |
| 34  | h     | 63  | VAL  | Peptide |
| 34  | h     | 73  | ASP  | Peptide |
| 34  | h     | 87  | ILE  | Peptide |
| 35  | i     | 108 | LYS  | Peptide |
| 35  | i     | 15  | ARG  | Peptide |
| 35  | i     | 18  | ARG  | Peptide |
| 35  | i     | 30  | THR  | Peptide |
| 35  | i     | 32  | THR  | Peptide |
| 35  | i     | 34  | GLY  | Peptide |
| 35  | i     | 57  | THR  | Peptide |
| 35  | i     | 9   | ASN  | Peptide |
| 36  | j     | 118 | LEU  | Peptide |
| 36  | j     | 123 | HIS  | Peptide |
| 36  | j     | 58  | PHE  | Peptide |
| 36  | j     | 77  | LYS  | Peptide |
| 36  | j     | 92  | GLY  | Peptide |
| 36  | j     | 93  | TYR  | Peptide |
| 38  | l     | 55  | ALA  | Peptide |
| 39  | m     | 49  | VAL  | Peptide |
| 39  | m     | 57  | PHE  | Peptide |
| 39  | m     | 59  | THR  | Peptide |
| 39  | m     | 6   | LEU  | Peptide |
| 39  | m     | 63  | VAL  | Peptide |
| 39  | m     | 71  | GLY  | Peptide |
| 39  | m     | 75  | ILE  | Peptide |
| 39  | m     | 97  | ALA  | Peptide |
| 41  | o     | 45  | THR  | Peptide |
| 41  | o     | 50  | PRO  | Peptide |
| 41  | o     | 51  | VAL  | Peptide |
| 41  | o     | 91  | TYR  | Peptide |
| 43  | q     | 62  | LYS  | Peptide |
| 43  | q     | 88  | LYS  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 44  | r     | 31  | LEU  | Peptide |
| 44  | r     | 37  | VAL  | Peptide |
| 44  | r     | 6   | HIS  | Peptide |
| 44  | r     | 70  | SER  | Peptide |
| 44  | r     | 79  | CYS  | Peptide |
| 44  | r     | 86  | ARG  | Peptide |
| 44  | r     | 98  | VAL  | Peptide |
| 46  | t     | 83  | PRO  | Peptide |
| 47  | u     | 37  | GLY  | Peptide |
| 47  | u     | 43  | HIS  | Peptide |
| 48  | v     | 27  | GLY  | Peptide |
| 49  | w     | 2   | LYS  | Peptide |
| 49  | w     | 53  | GLU  | Peptide |
| 50  | x     | 58  | LEU  | Peptide |
| 51  | y     | 20  | ASN  | Peptide |
| 52  | z     | 41  | ARG  | Peptide |

## 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   | W     | 149   | 0        | 75       | 18      | 0            |
| 2   | A     | 808   | 0        | 875      | 9       | 0            |
| 3   | B     | 597   | 0        | 668      | 15      | 0            |
| 4   | C     | 763   | 0        | 861      | 8       | 0            |
| 5   | D     | 656   | 0        | 684      | 11      | 0            |
| 6   | E     | 794   | 0        | 840      | 10      | 0            |
| 7   | F     | 208   | 0        | 221      | 10      | 0            |
| 8   | G     | 32534 | 0        | 16418    | 443     | 0            |
| 9   | H     | 1810  | 0        | 1861     | 26      | 0            |
| 10  | I     | 1612  | 0        | 1677     | 17      | 0            |
| 11  | J     | 1703  | 0        | 1763     | 20      | 0            |
| 12  | K     | 1146  | 0        | 1207     | 10      | 0            |
| 13  | L     | 843   | 0        | 857      | 15      | 0            |
| 14  | M     | 1257  | 0        | 1296     | 13      | 0            |
| 15  | N     | 1116  | 0        | 1177     | 11      | 0            |
| 16  | O     | 1010  | 0        | 1037     | 16      | 0            |
| 17  | P     | 885   | 0        | 904      | 23      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | Q     | 970   | 0        | 1057     | 19      | 0            |
| 19  | R     | 914   | 0        | 971      | 18      | 0            |
| 20  | S     | 492   | 0        | 533      | 65      | 0            |
| 21  | T     | 734   | 0        | 771      | 9       | 0            |
| 22  | U     | 700   | 0        | 720      | 14      | 0            |
| 23  | V     | 61917 | 0        | 31186    | 1550    | 0            |
| 24  | X     | 2641  | 0        | 1337     | 26      | 0            |
| 25  | Y     | 1742  | 0        | 1796     | 159     | 0            |
| 26  | Z     | 2126  | 0        | 2208     | 26      | 0            |
| 27  | a     | 1578  | 0        | 1646     | 43      | 0            |
| 28  | b     | 1625  | 0        | 1666     | 26      | 0            |
| 29  | c     | 1455  | 0        | 1511     | 101     | 0            |
| 30  | d     | 1335  | 0        | 1402     | 81      | 0            |
| 31  | e     | 621   | 0        | 301      | 18      | 0            |
| 32  | f     | 993   | 0        | 1030     | 149     | 0            |
| 33  | g     | 931   | 0        | 1002     | 6       | 0            |
| 34  | h     | 932   | 0        | 994      | 20      | 0            |
| 35  | i     | 1108  | 0        | 1182     | 45      | 0            |
| 36  | j     | 1080  | 0        | 1127     | 25      | 0            |
| 37  | k     | 960   | 0        | 1021     | 13      | 0            |
| 38  | l     | 877   | 0        | 936      | 86      | 0            |
| 39  | m     | 976   | 0        | 1033     | 19      | 0            |
| 40  | n     | 964   | 0        | 1022     | 9       | 0            |
| 41  | o     | 779   | 0        | 852      | 12      | 0            |
| 42  | p     | 876   | 0        | 941      | 5       | 0            |
| 43  | q     | 742   | 0        | 800      | 12      | 0            |
| 44  | r     | 844   | 0        | 930      | 15      | 0            |
| 45  | s     | 1435  | 0        | 1463     | 59      | 0            |
| 46  | t     | 629   | 0        | 650      | 4       | 0            |
| 47  | u     | 567   | 0        | 621      | 22      | 0            |
| 48  | v     | 469   | 0        | 518      | 8       | 0            |
| 49  | CC    | 157   | 0        | 69       | 1       | 0            |
| 49  | w     | 581   | 0        | 577      | 13      | 0            |
| 50  | x     | 445   | 0        | 459      | 15      | 0            |
| 51  | y     | 422   | 0        | 443      | 20      | 0            |
| 52  | z     | 430   | 0        | 480      | 2       | 0            |
| 53  | AA    | 515   | 0        | 587      | 11      | 0            |
| 54  | BB    | 307   | 0        | 335      | 9       | 0            |
| 55  | DD    | 1648  | 0        | 845      | 57      | 0            |
| 56  | EE    | 3841  | 0        | 3897     | 2       | 0            |
| 57  | Z     | 1     | 0        | 0        | 0       | 0            |
| 57  | i     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58  | EE    | 62     | 0        | 26       | 0       | 0            |
| All | All   | 150313 | 0        | 103366   | 3151    | 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 13.

All (3151) 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) |
|------------------|------------------|--------------------------|-------------------|
| 23:V:1084:A:H1'  | 23:V:1106:G:C6   | 1.34                     | 1.60              |
| 32:f:44:ALA:CB   | 32:f:67:PHE:HA   | 1.32                     | 1.57              |
| 32:f:44:ALA:HB2  | 32:f:67:PHE:CA   | 1.22                     | 1.57              |
| 23:V:1778:U:C4   | 23:V:1784:A:C2   | 1.93                     | 1.56              |
| 32:f:48:MET:HE3  | 32:f:69:THR:CG2  | 1.27                     | 1.54              |
| 23:V:1778:U:C5   | 23:V:1784:A:C2   | 1.93                     | 1.54              |
| 32:f:48:MET:HE3  | 32:f:69:THR:CB   | 1.41                     | 1.50              |
| 23:V:1778:U:C4   | 23:V:1784:A:H2   | 1.22                     | 1.49              |
| 20:S:29:ARG:CD   | 20:S:42:ILE:HD11 | 1.40                     | 1.49              |
| 8:G:1309:G:N2    | 8:G:1328:C:C5    | 1.81                     | 1.48              |
| 23:V:1169:G:H2'  | 23:V:1170:G:C8   | 1.47                     | 1.48              |
| 23:V:536:A:C2    | 23:V:558:G:C2    | 2.00                     | 1.47              |
| 23:V:2124:G:C8   | 25:Y:218:MET:N   | 1.79                     | 1.46              |
| 45:s:70:LEU:HD11 | 45:s:98:MET:CE   | 1.43                     | 1.46              |
| 23:V:96:G:H4'    | 47:u:43:HIS:CE1  | 1.53                     | 1.42              |
| 30:d:127:GLU:HB3 | 30:d:128:PRO:CD  | 1.49                     | 1.42              |
| 23:V:2124:G:C8   | 25:Y:217:THR:C   | 1.95                     | 1.40              |
| 29:c:67:LYS:NZ   | 29:c:90:LEU:HD13 | 1.22                     | 1.40              |
| 23:V:1786:A:C2   | 23:V:1938:A:N7   | 1.90                     | 1.39              |
| 8:G:1309:G:N2    | 8:G:1328:C:C4    | 1.85                     | 1.39              |
| 38:l:17:ARG:NH1  | 38:l:89:ARG:HD2  | 1.38                     | 1.38              |
| 23:V:96:G:O3'    | 47:u:43:HIS:CE1  | 1.74                     | 1.37              |
| 23:V:1067:A:H4'  | 32:f:21:PRO:CG   | 1.52                     | 1.37              |
| 38:l:25:ARG:HB3  | 38:l:87:PHE:CZ   | 1.59                     | 1.37              |
| 30:d:16:SER:O    | 30:d:17:VAL:CG2  | 1.74                     | 1.36              |
| 50:x:30:LEU:HB3  | 50:x:39:MET:SD   | 1.65                     | 1.34              |
| 23:V:96:G:O3'    | 47:u:43:HIS:ND1  | 1.61                     | 1.34              |
| 8:G:440:A:N6     | 8:G:493:G:N3     | 1.71                     | 1.33              |
| 23:V:974:G:C8    | 23:V:1187:G:O2'  | 1.79                     | 1.32              |
| 30:d:101:ARG:O   | 30:d:123:PHE:CD2 | 1.83                     | 1.31              |
| 32:f:48:MET:CE   | 32:f:69:THR:CG2  | 2.09                     | 1.31              |
| 30:d:13:LYS:CE   | 30:d:29:PRO:HD3  | 1.61                     | 1.30              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:V:974:G:O6    | 23:V:1187:G:N3   | 1.61                     | 1.30              |
| 23:V:1084:A:H1'  | 23:V:1106:G:C5   | 1.67                     | 1.30              |
| 8:G:69:G:N2      | 8:G:101:A:C6     | 1.97                     | 1.29              |
| 23:V:2124:G:N7   | 25:Y:217:THR:C   | 1.91                     | 1.29              |
| 23:V:2209:C:N4   | 23:V:2215:G:O6   | 1.66                     | 1.29              |
| 23:V:2209:C:N3   | 23:V:2216:G:N2   | 1.80                     | 1.28              |
| 35:i:47:ASP:O    | 35:i:49:ARG:N    | 1.64                     | 1.28              |
| 23:V:975:G:N2    | 23:V:990:A:N9    | 1.78                     | 1.28              |
| 23:V:41:C:O2     | 23:V:439:G:N2    | 1.64                     | 1.28              |
| 25:Y:177:LYS:N   | 25:Y:180:PHE:CD1 | 2.01                     | 1.28              |
| 29:c:67:LYS:NZ   | 29:c:90:LEU:CD1  | 1.94                     | 1.28              |
| 23:V:972:G:H3'   | 23:V:973:A:C2'   | 1.65                     | 1.27              |
| 23:V:2124:G:H5'  | 25:Y:217:THR:OG1 | 1.22                     | 1.27              |
| 23:V:2124:G:OP2  | 25:Y:218:MET:HB2 | 1.31                     | 1.26              |
| 29:c:31:VAL:CB   | 29:c:32:PRO:CD   | 2.13                     | 1.26              |
| 55:DD:47:7MG:O2' | 55:DD:48:U:H4'   | 1.31                     | 1.25              |
| 23:V:536:A:C6    | 23:V:558:G:N1    | 2.04                     | 1.25              |
| 23:V:96:G:C4'    | 47:u:43:HIS:HE1  | 1.48                     | 1.25              |
| 45:s:30:ASN:ND2  | 45:s:89:PHE:CE1  | 2.02                     | 1.25              |
| 23:V:2809:A:C6   | 27:a:60:ASN:ND2  | 2.05                     | 1.25              |
| 29:c:31:VAL:HB   | 29:c:32:PRO:CD   | 1.63                     | 1.25              |
| 8:G:222:U:N3     | 8:G:223:U:O4     | 1.68                     | 1.24              |
| 23:V:536:A:N1    | 23:V:558:G:N1    | 1.85                     | 1.24              |
| 23:V:923:C:C4    | 23:V:924:C:N4    | 2.04                     | 1.24              |
| 23:V:96:G:C4'    | 47:u:43:HIS:CE1  | 2.20                     | 1.24              |
| 23:V:1778:U:C6   | 23:V:1784:A:C2   | 2.24                     | 1.24              |
| 23:V:974:G:C6    | 23:V:1187:G:N3   | 2.07                     | 1.23              |
| 23:V:1084:A:O2'  | 23:V:1106:G:N7   | 1.72                     | 1.23              |
| 29:c:31:VAL:CB   | 29:c:32:PRO:HD2  | 1.68                     | 1.23              |
| 20:S:26:ARG:CD   | 20:S:43:CYS:HB2  | 1.69                     | 1.23              |
| 23:V:1778:U:N3   | 23:V:1784:A:H2   | 1.36                     | 1.23              |
| 1:W:16:A:H2      | 1:W:17:U:C2      | 1.57                     | 1.22              |
| 50:x:30:LEU:CB   | 50:x:39:MET:SD   | 2.26                     | 1.22              |
| 8:G:1306:A:H62   | 8:G:1331:G:N2    | 1.35                     | 1.22              |
| 8:G:500:G:C6     | 8:G:546:G:N2     | 2.08                     | 1.22              |
| 23:V:271(B):U:O4 | 23:V:404:C:N3    | 1.74                     | 1.21              |
| 23:V:1086:A:P    | 23:V:1104:C:O2'  | 1.96                     | 1.21              |
| 23:V:1442:G:N2   | 23:V:1550:C:C2   | 2.09                     | 1.21              |
| 23:V:527:C:O2    | 23:V:2779:U:C5   | 1.94                     | 1.21              |
| 30:d:127:GLU:CB  | 30:d:128:PRO:HD2 | 1.66                     | 1.20              |
| 1:W:16:A:C2      | 1:W:17:U:C2      | 2.30                     | 1.19              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:2809:A:N6    | 27:a:60:ASN:HD22  | 1.40                     | 1.19              |
| 23:V:536:A:N1     | 23:V:558:G:C6     | 2.11                     | 1.18              |
| 23:V:1084:A:C1'   | 23:V:1106:G:C6    | 2.26                     | 1.18              |
| 23:V:2209:C:C2    | 23:V:2216:G:N2    | 2.12                     | 1.18              |
| 35:i:51:PHE:HB3   | 35:i:57:THR:OG1   | 1.38                     | 1.18              |
| 23:V:1778:U:C6    | 23:V:1784:A:N1    | 2.11                     | 1.17              |
| 32:f:19:PRO:HA    | 32:f:22:PRO:HG2   | 1.20                     | 1.17              |
| 23:V:269:U:H5'    | 23:V:270(Y):G:H2' | 1.23                     | 1.17              |
| 32:f:93:ARG:HD2   | 32:f:135:GLY:O    | 1.37                     | 1.17              |
| 23:V:1086:A:OP1   | 23:V:1104:C:O2'   | 1.58                     | 1.17              |
| 30:d:18:GLU:HG3   | 30:d:24:VAL:HB    | 1.21                     | 1.17              |
| 23:V:270(C):C:H2' | 23:V:270(D):C:H6  | 1.10                     | 1.16              |
| 32:f:52:ILE:HG13  | 32:f:76:TYR:CG    | 1.79                     | 1.16              |
| 8:G:1306:A:N6     | 8:G:1331:G:N3     | 1.93                     | 1.16              |
| 45:s:70:LEU:CD1   | 45:s:98:MET:HE1   | 1.74                     | 1.16              |
| 23:V:1041:C:O2    | 23:V:1115:G:O6    | 1.64                     | 1.16              |
| 32:f:68:VAL:CG2   | 32:f:69:THR:H     | 1.51                     | 1.15              |
| 32:f:48:MET:CE    | 32:f:69:THR:HB    | 1.74                     | 1.15              |
| 23:V:1173:G:H1'   | 23:V:1177:A:N6    | 1.61                     | 1.15              |
| 29:c:31:VAL:CG1   | 29:c:32:PRO:HD3   | 1.75                     | 1.15              |
| 23:V:832:G:O2'    | 35:i:52:GLU:HG3   | 1.42                     | 1.14              |
| 32:f:48:MET:HE3   | 32:f:69:THR:HB    | 1.22                     | 1.14              |
| 8:G:1309:G:N2     | 8:G:1328:C:C6     | 2.15                     | 1.14              |
| 23:V:95:G:H2'     | 23:V:96:G:C1'     | 1.77                     | 1.14              |
| 23:V:2209:C:C5    | 23:V:2212:A:N1    | 2.14                     | 1.14              |
| 30:d:16:SER:C     | 30:d:17:VAL:HG23  | 1.72                     | 1.14              |
| 32:f:44:ALA:HB1   | 32:f:67:PHE:O     | 1.48                     | 1.14              |
| 23:V:885:C:N4     | 23:V:892:G:O6     | 1.81                     | 1.13              |
| 32:f:68:VAL:HG23  | 32:f:69:THR:N     | 1.45                     | 1.13              |
| 32:f:19:PRO:HA    | 32:f:22:PRO:CG    | 1.78                     | 1.12              |
| 8:G:222:U:H2'     | 8:G:223:U:C5      | 1.83                     | 1.12              |
| 8:G:474:G:C5'     | 22:U:75:ARG:HH21  | 1.62                     | 1.12              |
| 8:G:671:G:O2'     | 13:L:80:ARG:NH1   | 1.83                     | 1.12              |
| 20:S:29:ARG:HD3   | 20:S:42:ILE:HD11  | 1.19                     | 1.12              |
| 23:V:1106:G:H21   | 31:e:81:VAL:CB    | 1.61                     | 1.12              |
| 55:DD:48:U:O2'    | 55:DD:49:C:H5'    | 1.47                     | 1.12              |
| 51:y:14:THR:HG22  | 51:y:52:VAL:HB    | 1.21                     | 1.12              |
| 23:V:2196:C:H2'   | 23:V:2197:U:H6    | 1.12                     | 1.12              |
| 38:l:25:ARG:HB3   | 38:l:87:PHE:CE2   | 1.84                     | 1.12              |
| 23:V:153:C:H2'    | 23:V:154:G:C8     | 1.84                     | 1.12              |
| 23:V:1106:G:O2'   | 23:V:1107:G:C5'   | 1.97                     | 1.12              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:G:222:U:C2       | 8:G:223:U:C4      | 2.36                     | 1.11              |
| 23:V:1442:G:N1     | 23:V:1550:C:N3    | 1.96                     | 1.11              |
| 30:d:102:ALA:HA    | 30:d:123:PHE:HE2  | 0.99                     | 1.11              |
| 20:S:26:ARG:HD2    | 20:S:43:CYS:HB2   | 1.12                     | 1.11              |
| 23:V:1786:A:H2     | 23:V:1938:A:C8    | 1.69                     | 1.11              |
| 30:d:18:GLU:HB2    | 30:d:24:VAL:HG23  | 1.12                     | 1.11              |
| 23:V:270(X):G:H2'  | 23:V:270(Y):G:H5' | 1.32                     | 1.11              |
| 23:V:536:A:C6      | 23:V:558:G:C6     | 2.37                     | 1.11              |
| 23:V:1786:A:N3     | 23:V:1938:A:N7    | 1.99                     | 1.11              |
| 23:V:10:G:N2       | 23:V:2629:A:C4    | 2.18                     | 1.10              |
| 23:V:2630:G:N1     | 23:V:2790:A:H2    | 1.46                     | 1.10              |
| 23:V:2637:U:C4     | 23:V:2782:G:O6    | 2.04                     | 1.10              |
| 8:G:77:C:N4        | 8:G:92:G:O6       | 1.82                     | 1.10              |
| 23:V:1067:A:H4'    | 32:f:21:PRO:HG3   | 1.25                     | 1.10              |
| 25:Y:180:PHE:CD2   | 25:Y:185:LEU:HD12 | 1.87                     | 1.10              |
| 8:G:129(A):G:C2    | 8:G:191(A):G:N7   | 2.20                     | 1.10              |
| 23:V:972:G:H3'     | 23:V:973:A:H2'    | 1.23                     | 1.09              |
| 32:f:86:LYS:HB3    | 32:f:95:LYS:HB2   | 1.34                     | 1.09              |
| 23:V:1075:C:H1'    | 32:f:91:PRO:HG3   | 1.18                     | 1.09              |
| 30:d:101:ARG:O     | 30:d:123:PHE:HD2  | 1.19                     | 1.09              |
| 30:d:15:VAL:O      | 30:d:26:VAL:HG22  | 1.52                     | 1.09              |
| 23:V:137(A):G:O6   | 23:V:142:G:N1     | 1.86                     | 1.09              |
| 32:f:48:MET:HE3    | 32:f:69:THR:HG21  | 1.32                     | 1.09              |
| 32:f:52:ILE:HG13   | 32:f:76:TYR:CD2   | 1.87                     | 1.09              |
| 23:V:1067:A:H4'    | 32:f:21:PRO:HG2   | 1.29                     | 1.08              |
| 29:c:67:LYS:HZ3    | 29:c:90:LEU:CD1   | 1.56                     | 1.08              |
| 23:V:972:G:C3'     | 23:V:973:A:H2'    | 1.83                     | 1.08              |
| 32:f:22:PRO:HD2    | 32:f:23:VAL:H     | 1.08                     | 1.07              |
| 35:i:51:PHE:CB     | 35:i:57:THR:OG1   | 2.02                     | 1.07              |
| 23:V:536:A:N1      | 23:V:558:G:C2     | 2.20                     | 1.07              |
| 23:V:536:A:N6      | 23:V:558:G:O6     | 1.87                     | 1.07              |
| 23:V:2124:G:H21    | 25:Y:221:SER:N    | 1.51                     | 1.07              |
| 23:V:552:G:C2      | 23:V:553:U:O2     | 2.06                     | 1.07              |
| 23:V:1169:G:C6     | 23:V:1170:G:O6    | 2.08                     | 1.07              |
| 23:V:1444(A):A:H1' | 23:V:1732:A:H61   | 1.19                     | 1.07              |
| 23:V:2813:A:H2     | 23:V:2888:C:O2    | 1.35                     | 1.07              |
| 30:d:13:LYS:HE3    | 30:d:29:PRO:HD3   | 1.15                     | 1.07              |
| 30:d:18:GLU:HB2    | 30:d:24:VAL:CG2   | 1.84                     | 1.07              |
| 23:V:975:G:N2      | 23:V:990:A:C4     | 2.22                     | 1.06              |
| 29:c:47:LYS:HG3    | 29:c:80:PHE:CD2   | 1.90                     | 1.06              |
| 38:l:17:ARG:NH1    | 38:l:89:ARG:CD    | 2.18                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 32:f:48:MET:CE   | 32:f:69:THR:CB   | 2.27                     | 1.06              |
| 23:V:1169:G:C2'  | 23:V:1170:G:C8   | 2.37                     | 1.06              |
| 30:d:127:GLU:CB  | 30:d:128:PRO:CD  | 2.19                     | 1.06              |
| 23:V:96:G:C3'    | 47:u:43:HIS:CE1  | 2.38                     | 1.05              |
| 23:V:974:G:O6    | 23:V:1187:G:C2   | 2.09                     | 1.05              |
| 23:V:2209:C:C5   | 23:V:2212:A:C2   | 2.43                     | 1.05              |
| 25:Y:176:GLY:HA3 | 25:Y:180:PHE:CZ  | 1.91                     | 1.05              |
| 30:d:16:SER:O    | 30:d:17:VAL:HG23 | 0.87                     | 1.05              |
| 23:V:139:G:N2    | 23:V:1408:C:O2   | 1.87                     | 1.05              |
| 23:V:923:C:C5    | 23:V:924:C:N4    | 2.18                     | 1.05              |
| 23:V:2209:C:N3   | 23:V:2216:G:C2   | 2.23                     | 1.05              |
| 30:d:102:ALA:HA  | 30:d:123:PHE:CE2 | 1.90                     | 1.05              |
| 30:d:95:ARG:HB2  | 30:d:129:THR:OG1 | 1.52                     | 1.05              |
| 8:G:1306:A:N6    | 8:G:1331:G:C2    | 2.24                     | 1.05              |
| 23:V:1778:U:C5   | 23:V:1784:A:H2   | 1.49                     | 1.05              |
| 23:V:1445:C:C5   | 23:V:1446:C:N3   | 2.23                     | 1.04              |
| 8:G:69:G:N2      | 8:G:101:A:C5     | 2.26                     | 1.04              |
| 23:V:2226:C:C6   | 23:V:2227:A:C8   | 2.46                     | 1.04              |
| 8:G:129(A):G:C2  | 8:G:191(A):G:C5  | 2.45                     | 1.04              |
| 23:V:832:G:O2'   | 35:i:52:GLU:CG   | 2.04                     | 1.04              |
| 23:V:2124:G:C8   | 25:Y:217:THR:N   | 2.26                     | 1.04              |
| 20:S:29:ARG:HD2  | 20:S:42:ILE:HD11 | 1.07                     | 1.04              |
| 29:c:31:VAL:HG12 | 29:c:32:PRO:HD3  | 1.09                     | 1.04              |
| 29:c:31:VAL:CG1  | 29:c:32:PRO:CD   | 2.33                     | 1.03              |
| 20:S:29:ARG:CD   | 20:S:42:ILE:CD1  | 2.35                     | 1.03              |
| 29:c:31:VAL:HG12 | 29:c:32:PRO:CD   | 1.88                     | 1.03              |
| 8:G:69:G:C2      | 8:G:101:A:C6     | 2.45                     | 1.03              |
| 23:V:1173:G:C1'  | 23:V:1177:A:N6   | 2.20                     | 1.03              |
| 23:V:887:A:O2'   | 23:V:889:C:C6    | 2.11                     | 1.03              |
| 23:V:975:G:N2    | 23:V:990:A:C1'   | 2.21                     | 1.03              |
| 23:V:1742:C:C5   | 23:V:1743:G:O6   | 2.12                     | 1.03              |
| 20:S:29:ARG:HD3  | 20:S:42:ILE:CD1  | 1.88                     | 1.02              |
| 23:V:539:G:N3    | 23:V:556:G:N2    | 1.71                     | 1.02              |
| 32:f:48:MET:CB   | 32:f:69:THR:HG21 | 1.89                     | 1.02              |
| 32:f:48:MET:HB2  | 32:f:69:THR:HG21 | 1.34                     | 1.02              |
| 23:V:43:G:C6     | 23:V:438:G:N1    | 2.28                     | 1.02              |
| 23:V:1534:G:C2   | 23:V:1538:G:C6   | 2.47                     | 1.02              |
| 8:G:474:G:H5''   | 22:U:75:ARG:HH21 | 1.20                     | 1.02              |
| 23:V:2809:A:N6   | 27:a:60:ASN:ND2  | 2.03                     | 1.02              |
| 25:Y:180:PHE:CD2 | 25:Y:185:LEU:CD1 | 2.43                     | 1.02              |
| 32:f:19:PRO:CA   | 32:f:22:PRO:HG2  | 1.90                     | 1.02              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:G:82:U:O2        | 8:G:87:A:C2       | 2.12                     | 1.02              |
| 23:V:374:A:C2      | 23:V:401:A:C4     | 2.48                     | 1.02              |
| 23:V:972:G:O2'     | 23:V:973:A:OP1    | 1.78                     | 1.02              |
| 23:V:1063:G:OP1    | 32:f:52:ILE:HD11  | 1.57                     | 1.02              |
| 23:V:1084:A:C1'    | 23:V:1106:G:C5    | 2.41                     | 1.02              |
| 23:V:1300:U:C4     | 23:V:1627:G:OP2   | 2.12                     | 1.02              |
| 23:V:2124:G:C8     | 25:Y:217:THR:CA   | 2.43                     | 1.02              |
| 23:V:270(C):C:H2'  | 23:V:270(D):C:C6  | 1.94                     | 1.02              |
| 23:V:2092:U:O4'    | 23:V:2225:A:H2    | 1.40                     | 1.02              |
| 23:V:2637:U:N3     | 23:V:2782:G:C6    | 2.28                     | 1.02              |
| 8:G:222:U:H2'      | 8:G:223:U:C6      | 1.95                     | 1.01              |
| 23:V:2805:G:N2     | 23:V:2892:A:H62   | 1.58                     | 1.01              |
| 8:G:1203:C:H4'     | 20:S:27:CYS:CB    | 1.91                     | 1.01              |
| 23:V:1085:A:O3'    | 23:V:1104:C:O2'   | 1.79                     | 1.01              |
| 45:s:70:LEU:CD1    | 45:s:98:MET:CE    | 2.35                     | 1.01              |
| 23:V:270(M):U:H4'  | 23:V:270(N):G:H4' | 1.01                     | 1.01              |
| 23:V:270(O):U:H5'' | 23:V:270(P):C:H5  | 1.23                     | 1.01              |
| 23:V:1106:G:O2'    | 23:V:1107:G:H5'   | 1.57                     | 1.01              |
| 8:G:222:U:O2       | 8:G:223:U:C4      | 2.14                     | 1.00              |
| 23:V:2209:C:C6     | 23:V:2212:A:N1    | 2.29                     | 1.00              |
| 55:DD:47:7MG:O2'   | 55:DD:48:U:C4'    | 2.08                     | 1.00              |
| 23:V:270(M):U:C4'  | 23:V:270(N):G:H4' | 1.91                     | 1.00              |
| 29:c:86:MET:HB3    | 29:c:87:PRO:HD2   | 1.41                     | 1.00              |
| 35:i:47:ASP:C      | 35:i:49:ARG:H     | 1.68                     | 1.00              |
| 23:V:2124:G:C5'    | 25:Y:217:THR:OG1  | 2.10                     | 1.00              |
| 23:V:974:G:N2      | 23:V:1186:G:C5    | 2.28                     | 1.00              |
| 23:V:1544:C:H2'    | 23:V:1545:A:H5'   | 1.43                     | 1.00              |
| 8:G:222:U:C2       | 8:G:223:U:O4      | 2.14                     | 1.00              |
| 23:V:1534:G:N1     | 23:V:1538:G:O6    | 1.93                     | 1.00              |
| 38:l:12:PHE:HD1    | 38:l:13:ARG:N     | 1.60                     | 0.99              |
| 23:V:97:C:H4'      | 47:u:47:ASP:OD2   | 1.60                     | 0.99              |
| 23:V:270(Z):U:H5   | 23:V:370:G:N7     | 1.59                     | 0.99              |
| 23:V:10:G:N2       | 23:V:2629:A:C5    | 2.29                     | 0.99              |
| 23:V:2809:A:N1     | 27:a:60:ASN:CB    | 2.26                     | 0.99              |
| 38:l:25:ARG:CB     | 38:l:87:PHE:CZ    | 2.45                     | 0.99              |
| 25:Y:176:GLY:HA3   | 25:Y:180:PHE:CE1  | 1.97                     | 0.99              |
| 24:X:89:G:H2'      | 24:X:89(A):A:C8   | 1.97                     | 0.99              |
| 8:G:474:G:H5''     | 22:U:75:ARG:NH2   | 1.77                     | 0.98              |
| 23:V:10:G:O6       | 23:V:2628:C:OP1   | 1.79                     | 0.98              |
| 30:d:95:ARG:CB     | 30:d:129:THR:OG1  | 2.10                     | 0.98              |
| 29:c:47:LYS:HG3    | 29:c:80:PHE:HD2   | 1.19                     | 0.98              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:1067:A:C4'    | 32:f:21:PRO:HG3   | 1.93                     | 0.98              |
| 38:l:9:ARG:O       | 38:l:12:PHE:CD1   | 2.16                     | 0.98              |
| 23:V:1169:G:C6     | 23:V:1170:G:C6    | 2.49                     | 0.98              |
| 23:V:1482:U:O4     | 23:V:1510:A:N6    | 1.97                     | 0.98              |
| 23:V:2832:U:O2'    | 23:V:2879:C:N4    | 1.96                     | 0.98              |
| 8:G:86:U:OP2       | 8:G:87:A:N6       | 1.97                     | 0.98              |
| 8:G:222:U:C2       | 8:G:223:U:C5      | 2.51                     | 0.98              |
| 30:d:103:LEU:HD22  | 30:d:123:PHE:CZ   | 1.98                     | 0.98              |
| 23:V:96:G:C3'      | 47:u:43:HIS:HE1   | 1.75                     | 0.98              |
| 23:V:536:A:N6      | 23:V:558:G:C6     | 2.32                     | 0.98              |
| 23:V:1090:U:C4     | 23:V:1103:A:N6    | 2.32                     | 0.98              |
| 23:V:2809:A:N1     | 27:a:60:ASN:HB3   | 1.78                     | 0.98              |
| 32:f:37:PHE:CZ     | 32:f:62:ASP:CG    | 2.42                     | 0.98              |
| 35:i:47:ASP:OD2    | 35:i:50:ARG:HD2   | 1.63                     | 0.97              |
| 23:V:2813:A:C2     | 23:V:2888:C:O2    | 2.17                     | 0.97              |
| 55:DD:47:7MG:HO2'  | 55:DD:48:U:H4'    | 1.24                     | 0.97              |
| 23:V:1786:A:H2     | 23:V:1938:A:N7    | 1.39                     | 0.97              |
| 32:f:20:ALA:HB3    | 32:f:21:PRO:HD3   | 1.46                     | 0.97              |
| 32:f:86:LYS:HA     | 32:f:95:LYS:HD3   | 1.46                     | 0.97              |
| 23:V:2334:G:H1'    | 38:l:15:ARG:HE    | 1.30                     | 0.97              |
| 23:V:270(O):U:H5'' | 23:V:270(P):C:C5  | 1.97                     | 0.97              |
| 23:V:974(A):C:O2   | 23:V:989:G:N2     | 1.97                     | 0.97              |
| 32:f:37:PHE:HZ     | 32:f:62:ASP:CG    | 1.73                     | 0.96              |
| 32:f:48:MET:CE     | 32:f:69:THR:HG22  | 1.92                     | 0.96              |
| 51:y:34:LEU:HG     | 51:y:51:GLU:CD    | 1.87                     | 0.96              |
| 38:l:25:ARG:CB     | 38:l:87:PHE:CE2   | 2.47                     | 0.96              |
| 8:G:951:G:OP1      | 8:G:1362(A):C:N3  | 1.99                     | 0.96              |
| 23:V:270(X):G:C2'  | 23:V:270(Y):G:H5' | 1.96                     | 0.96              |
| 23:V:2124:G:OP2    | 25:Y:218:MET:CB   | 2.13                     | 0.96              |
| 23:V:87:C:C2       | 23:V:96:G:N2      | 2.34                     | 0.96              |
| 32:f:43:ALA:C      | 32:f:67:PHE:CD1   | 2.43                     | 0.95              |
| 23:V:270(M):U:H4'  | 23:V:270(N):G:C4' | 1.95                     | 0.95              |
| 23:V:1778:U:C2     | 23:V:1784:A:C2    | 2.55                     | 0.95              |
| 23:V:271(A):G:H4'  | 23:V:271(B):U:OP2 | 1.64                     | 0.95              |
| 23:V:134:C:N4      | 23:V:135:G:O6     | 1.99                     | 0.95              |
| 23:V:2196:C:H2'    | 23:V:2197:U:C6    | 2.00                     | 0.95              |
| 23:V:16:G:H1       | 23:V:525:U:H3     | 1.11                     | 0.95              |
| 8:G:1203:C:H5'     | 20:S:27:CYS:HB2   | 1.46                     | 0.95              |
| 23:V:2209:C:C6     | 23:V:2212:A:C2    | 2.54                     | 0.95              |
| 29:c:31:VAL:HB     | 29:c:32:PRO:HD2   | 0.95                     | 0.95              |
| 23:V:271(B):U:C4   | 23:V:404:C:N3     | 2.19                     | 0.94              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:V:2127:G:OP1  | 25:Y:36:LYS:HG2   | 1.67                     | 0.94              |
| 23:V:43:G:C6     | 23:V:438:G:C2     | 2.55                     | 0.94              |
| 23:V:1786:A:C2   | 23:V:1938:A:C8    | 2.49                     | 0.94              |
| 1:W:16:A:C2      | 1:W:17:U:N3       | 2.34                     | 0.94              |
| 23:V:1778:U:N3   | 23:V:1784:A:C2    | 2.19                     | 0.94              |
| 25:Y:176:GLY:CA  | 25:Y:180:PHE:CE1  | 2.50                     | 0.94              |
| 8:G:500:G:O6     | 8:G:546:G:C2      | 2.20                     | 0.93              |
| 23:V:975:G:N2    | 23:V:990:A:C8     | 2.35                     | 0.93              |
| 23:V:1173:G:H1'  | 23:V:1177:A:H62   | 1.17                     | 0.93              |
| 23:V:41:C:O2     | 23:V:439:G:C2     | 2.20                     | 0.93              |
| 30:d:102:ALA:CA  | 30:d:123:PHE:HE2  | 1.81                     | 0.93              |
| 23:V:536:A:C2    | 23:V:558:G:N3     | 2.36                     | 0.93              |
| 23:V:2226:C:C5   | 23:V:2227:A:N7    | 2.36                     | 0.93              |
| 23:V:2630:G:N1   | 23:V:2790:A:C2    | 2.35                     | 0.93              |
| 23:V:2791:C:H42  | 23:V:2893:G:N2    | 1.67                     | 0.93              |
| 23:V:1106:G:O2'  | 23:V:1107:G:P     | 2.25                     | 0.93              |
| 23:V:1778:U:C4   | 23:V:1784:A:N3    | 2.37                     | 0.93              |
| 23:V:153:C:C2'   | 23:V:154:G:C8     | 2.51                     | 0.93              |
| 23:V:2123:G:O2'  | 25:Y:217:THR:CA   | 2.17                     | 0.92              |
| 30:d:13:LYS:HE2  | 30:d:29:PRO:HD3   | 1.48                     | 0.92              |
| 23:V:1493:C:OP1  | 23:V:2210:G:N1    | 2.01                     | 0.92              |
| 23:V:2124:G:N7   | 25:Y:218:MET:N    | 2.12                     | 0.92              |
| 23:V:1478:G:N2   | 23:V:1515:C:O2    | 1.99                     | 0.92              |
| 23:V:1778:U:C2   | 23:V:1784:A:H2    | 1.86                     | 0.92              |
| 30:d:89:ILE:CG2  | 30:d:129:THR:HG22 | 1.98                     | 0.92              |
| 8:G:500:G:C6     | 8:G:546:G:C2      | 2.57                     | 0.92              |
| 23:V:43:G:N1     | 23:V:438:G:C2     | 2.38                     | 0.92              |
| 23:V:974:G:C5    | 23:V:1187:G:H1'   | 2.05                     | 0.92              |
| 23:V:134:C:C4    | 23:V:135:G:O6     | 2.23                     | 0.92              |
| 23:V:972:G:C2'   | 23:V:973:A:OP1    | 2.18                     | 0.92              |
| 23:V:1444:G:O6   | 23:V:1463:C:N4    | 2.02                     | 0.92              |
| 8:G:1306:A:H62   | 8:G:1331:G:H21    | 1.17                     | 0.91              |
| 23:V:1479:G:H2'  | 23:V:1480:G:C8    | 2.05                     | 0.91              |
| 25:Y:177:LYS:H   | 25:Y:180:PHE:HD1  | 1.05                     | 0.91              |
| 8:G:1306:A:N6    | 8:G:1331:G:N2     | 2.17                     | 0.91              |
| 23:V:280:C:C5    | 23:V:283:A:C6     | 2.59                     | 0.91              |
| 38:l:17:ARG:HH11 | 38:l:89:ARG:HD2   | 1.11                     | 0.91              |
| 23:V:265:A:N6    | 23:V:428:A:N7     | 2.18                     | 0.91              |
| 23:V:2226:C:C5   | 23:V:2227:A:C8    | 2.57                     | 0.91              |
| 8:G:1309:G:C2    | 8:G:1328:C:C4     | 2.58                     | 0.91              |
| 23:V:1718:G:N2   | 23:V:1741:C:O2    | 2.04                     | 0.91              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:G:69:G:N2      | 8:G:101:A:N1      | 2.18                     | 0.91              |
| 23:V:552:G:O2'   | 23:V:553:U:H5'    | 1.69                     | 0.91              |
| 32:f:19:PRO:C    | 32:f:22:PRO:CD    | 2.43                     | 0.91              |
| 23:V:1442:G:N2   | 23:V:1550:C:O2    | 2.03                     | 0.91              |
| 30:d:89:ILE:HG23 | 30:d:129:THR:HG22 | 1.52                     | 0.91              |
| 32:f:52:ILE:CG1  | 32:f:76:TYR:CG    | 2.53                     | 0.90              |
| 23:V:1169:G:H2'  | 23:V:1170:G:H8    | 1.34                     | 0.90              |
| 38:l:17:ARG:HH12 | 38:l:89:ARG:HD2   | 1.30                     | 0.90              |
| 8:G:500:G:O6     | 8:G:546:G:N2      | 2.04                     | 0.90              |
| 23:V:280:C:C5    | 23:V:283:A:C5     | 2.60                     | 0.90              |
| 23:V:852:G:H2'   | 23:V:853:G:H8     | 1.35                     | 0.90              |
| 23:V:975:G:H22   | 23:V:990:A:C1'    | 1.82                     | 0.90              |
| 23:V:1300:U:O4   | 23:V:1627:G:OP2   | 1.89                     | 0.90              |
| 23:V:1544:C:H2'  | 23:V:1545:A:C5'   | 2.02                     | 0.90              |
| 23:V:270(I):G:C2 | 23:V:270(J):G:H1' | 2.07                     | 0.90              |
| 23:V:2123:G:H2'  | 25:Y:217:THR:O    | 1.71                     | 0.90              |
| 23:V:2127:G:N2   | 23:V:2162:G:H2'   | 1.87                     | 0.90              |
| 25:Y:152:ILE:O   | 25:Y:156:ILE:HG13 | 1.72                     | 0.90              |
| 20:S:29:ARG:HD2  | 20:S:42:ILE:CD1   | 1.99                     | 0.89              |
| 23:V:879:G:N2    | 23:V:898:C:C2     | 2.40                     | 0.89              |
| 23:V:2123:G:O2'  | 25:Y:217:THR:C    | 2.15                     | 0.89              |
| 23:V:271(B):U:O4 | 23:V:404:C:C4     | 2.20                     | 0.89              |
| 23:V:527:C:O2    | 23:V:2779:U:H5    | 1.52                     | 0.89              |
| 23:V:1106:G:O2'  | 23:V:1107:G:O5'   | 1.90                     | 0.89              |
| 25:Y:66:HIS:N    | 25:Y:158:ALA:HB1  | 1.85                     | 0.89              |
| 23:V:2128:C:H5'' | 25:Y:6:ARG:HB3    | 1.55                     | 0.89              |
| 32:f:44:ALA:CB   | 32:f:67:PHE:O     | 2.21                     | 0.89              |
| 23:V:270(Z):U:C5 | 23:V:370:G:N7     | 2.41                     | 0.89              |
| 23:V:1075:C:C1'  | 32:f:91:PRO:HG3   | 2.01                     | 0.89              |
| 23:V:1542:G:O2'  | 23:V:1544:C:O4'   | 1.89                     | 0.89              |
| 23:V:14:A:H5'    | 23:V:14:A:N3      | 1.87                     | 0.89              |
| 8:G:440:A:H62    | 8:G:493:G:N2      | 1.70                     | 0.89              |
| 23:V:95:G:C4     | 23:V:96:G:H1'     | 2.08                     | 0.89              |
| 45:s:30:ASN:HD21 | 45:s:89:PHE:HE1   | 0.94                     | 0.88              |
| 23:V:2720:U:H2'  | 23:V:2721:A:C8    | 2.09                     | 0.88              |
| 30:d:18:GLU:CG   | 30:d:24:VAL:HB    | 2.03                     | 0.88              |
| 32:f:22:PRO:HD2  | 32:f:23:VAL:N     | 1.87                     | 0.88              |
| 45:s:30:ASN:ND2  | 45:s:89:PHE:CD1   | 2.33                     | 0.88              |
| 23:V:95:G:H2'    | 23:V:96:G:H1'     | 1.54                     | 0.88              |
| 23:V:2125:G:O2'  | 23:V:2126:A:O4'   | 1.89                     | 0.88              |
| 25:Y:176:GLY:CA  | 25:Y:180:PHE:CZ   | 2.56                     | 0.88              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:f:68:VAL:CG2  | 32:f:69:THR:N     | 2.18                     | 0.88              |
| 23:V:1067:A:C4'  | 32:f:21:PRO:CG    | 2.45                     | 0.88              |
| 23:V:2226:C:H2'  | 23:V:2227:A:O4'   | 1.72                     | 0.88              |
| 23:V:1869:G:H2'  | 23:V:1871:A:OP2   | 1.74                     | 0.87              |
| 38:l:35:ILE:HD11 | 38:l:97:ARG:HH12  | 1.34                     | 0.87              |
| 8:G:1203:C:C5'   | 20:S:27:CYS:HB2   | 2.04                     | 0.87              |
| 23:V:1864:U:O2'  | 23:V:1869:G:H5'   | 1.74                     | 0.87              |
| 38:l:17:ARG:HB3  | 38:l:17:ARG:HH21  | 1.39                     | 0.87              |
| 23:V:270(I):G:N3 | 23:V:270(J):G:H1' | 1.90                     | 0.87              |
| 23:V:1169:G:C5   | 23:V:1170:G:O6    | 2.27                     | 0.87              |
| 38:l:97:ARG:HG2  | 38:l:97:ARG:HH11  | 1.39                     | 0.87              |
| 50:x:30:LEU:HB2  | 50:x:39:MET:SD    | 2.12                     | 0.87              |
| 23:V:1532:C:C5   | 23:V:1539:G:N2    | 2.42                     | 0.87              |
| 29:c:71:THR:O    | 29:c:88:ILE:N     | 2.07                     | 0.87              |
| 51:y:14:THR:HG22 | 51:y:52:VAL:CB    | 2.05                     | 0.87              |
| 23:V:269:U:H3    | 23:V:270:A:H62    | 1.20                     | 0.87              |
| 23:V:2637:U:C4   | 23:V:2782:G:C6    | 2.63                     | 0.87              |
| 23:V:2720:U:H2'  | 23:V:2721:A:H8    | 1.37                     | 0.87              |
| 8:G:129(A):G:N1  | 8:G:191(A):G:C5   | 2.43                     | 0.86              |
| 23:V:265:A:N3    | 23:V:281:G:N2     | 2.21                     | 0.86              |
| 23:V:1442:G:C2   | 23:V:1550:C:C2    | 2.63                     | 0.86              |
| 23:V:2787:C:O2'  | 23:V:2809:A:N6    | 2.05                     | 0.86              |
| 23:V:974:G:O6    | 23:V:1187:G:N2    | 2.06                     | 0.86              |
| 23:V:87:C:N3     | 23:V:96:G:N2      | 2.22                     | 0.86              |
| 23:V:536:A:C2    | 23:V:558:G:N2     | 2.43                     | 0.86              |
| 23:V:265:A:C2    | 23:V:281:G:N3     | 2.43                     | 0.86              |
| 32:f:55:VAL:HG13 | 32:f:70:LYS:HG2   | 1.56                     | 0.86              |
| 23:V:1534:G:C2   | 23:V:1538:G:O6    | 2.29                     | 0.86              |
| 23:V:2128:C:H5'' | 25:Y:6:ARG:CB     | 2.05                     | 0.86              |
| 23:V:2124:G:H8   | 25:Y:218:MET:N    | 1.46                     | 0.86              |
| 25:Y:180:PHE:HD2 | 25:Y:185:LEU:HD12 | 1.35                     | 0.86              |
| 29:c:71:THR:HB   | 29:c:88:ILE:N     | 1.90                     | 0.86              |
| 23:V:280:C:H2'   | 23:V:283:A:C8     | 2.10                     | 0.86              |
| 24:X:57:A:H1'    | 29:c:30:GLU:CB    | 2.06                     | 0.86              |
| 29:c:71:THR:HB   | 29:c:87:PRO:CA    | 2.06                     | 0.86              |
| 23:V:95:G:H2'    | 23:V:96:G:O4'     | 1.75                     | 0.85              |
| 55:DD:9:G:O2'    | 55:DD:10:G:N7     | 2.08                     | 0.85              |
| 23:V:270(Z):U:N3 | 23:V:271(B):U:H1' | 1.91                     | 0.85              |
| 23:V:1106:G:N2   | 31:e:81:VAL:CB    | 2.37                     | 0.85              |
| 30:d:13:LYS:HE3  | 30:d:29:PRO:CD    | 2.04                     | 0.85              |
| 20:S:25:VAL:CG1  | 20:S:39:LEU:HD23  | 2.06                     | 0.85              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:832:G:O2'     | 35:i:52:GLU:CD    | 2.18                     | 0.85              |
| 8:G:474:G:H5'      | 22:U:75:ARG:HH21  | 1.40                     | 0.85              |
| 8:G:1359:C:O2'     | 8:G:1360:A:O5'    | 1.93                     | 0.85              |
| 23:V:2712:U:O2'    | 23:V:2713:A:H5'   | 1.77                     | 0.85              |
| 32:f:21:PRO:N      | 32:f:22:PRO:HD3   | 1.91                     | 0.85              |
| 32:f:44:ALA:CB     | 32:f:67:PHE:CA    | 2.14                     | 0.85              |
| 23:V:273(B):C:H2'  | 23:V:273(C):C:C6  | 2.11                     | 0.85              |
| 23:V:374:A:N1      | 23:V:401:A:C4     | 2.45                     | 0.85              |
| 23:V:552:G:C5      | 23:V:553:U:N3     | 2.44                     | 0.85              |
| 23:V:853:G:N2      | 23:V:925:C:O2     | 2.08                     | 0.85              |
| 32:f:20:ALA:HB3    | 32:f:21:PRO:CD    | 2.06                     | 0.85              |
| 23:V:269:U:H3      | 23:V:270:A:N6     | 1.74                     | 0.84              |
| 23:V:884:C:H5'     | 23:V:892:G:H22    | 1.41                     | 0.84              |
| 32:f:48:MET:HE3    | 32:f:69:THR:HG22  | 1.49                     | 0.84              |
| 23:V:2213:U:OP2    | 23:V:2213:U:H4'   | 1.78                     | 0.84              |
| 23:V:2710:C:H2'    | 23:V:2711:A:C8    | 2.12                     | 0.84              |
| 38:l:12:PHE:HD1    | 38:l:13:ARG:H     | 1.23                     | 0.84              |
| 1:W:19:U:O2'       | 1:W:20:U:OP1      | 1.94                     | 0.84              |
| 23:V:270(A):A:H5'  | 23:V:270(B):A:OP2 | 1.78                     | 0.84              |
| 23:V:270(B):A:H1'  | 23:V:270(C):C:C5  | 2.11                     | 0.84              |
| 8:G:1440:C:H2'     | 8:G:1441:G:H5'    | 1.58                     | 0.84              |
| 23:V:2124:G:N7     | 25:Y:218:MET:HA   | 1.93                     | 0.84              |
| 8:G:1203:C:H4'     | 20:S:27:CYS:SG    | 2.17                     | 0.84              |
| 23:V:153:C:C3'     | 23:V:154:G:C8     | 2.61                     | 0.84              |
| 23:V:974:G:C4      | 23:V:1187:G:H1'   | 2.12                     | 0.83              |
| 8:G:977:A:H62      | 8:G:1362(A):C:H5  | 1.22                     | 0.83              |
| 23:V:97:C:P        | 47:u:43:HIS:ND1   | 2.50                     | 0.83              |
| 8:G:68:G:O6        | 8:G:101:A:N6      | 2.11                     | 0.83              |
| 23:V:2124:G:N7     | 25:Y:217:THR:O    | 2.11                     | 0.83              |
| 23:V:2124:G:O5'    | 25:Y:218:MET:N    | 2.11                     | 0.83              |
| 38:l:12:PHE:CD1    | 38:l:13:ARG:N     | 2.45                     | 0.83              |
| 23:V:271(A):G:H5'' | 23:V:271(B):U:O4' | 1.77                     | 0.83              |
| 23:V:975:G:C2      | 23:V:990:A:C8     | 2.66                     | 0.83              |
| 23:V:2312:U:O2'    | 29:c:89:GLY:HA2   | 1.78                     | 0.83              |
| 32:f:44:ALA:HB2    | 32:f:67:PHE:C     | 2.03                     | 0.83              |
| 23:V:269:U:H5''    | 23:V:270(Y):G:C2' | 2.08                     | 0.83              |
| 23:V:2123:G:H22    | 23:V:2176:A:H61   | 1.27                     | 0.83              |
| 23:V:2124:G:C8     | 25:Y:218:MET:CA   | 2.61                     | 0.83              |
| 23:V:2809:A:N1     | 27:a:60:ASN:ND2   | 2.24                     | 0.83              |
| 8:G:977:A:N6       | 8:G:1362(A):C:H5  | 1.75                     | 0.83              |
| 23:V:1545(A):A:H3' | 23:V:1546:C:C4'   | 2.09                     | 0.82              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:489:G:C6      | 23:V:1284:A:N1    | 2.46                     | 0.82              |
| 32:f:23:VAL:O      | 32:f:23:VAL:HG12  | 1.78                     | 0.82              |
| 32:f:44:ALA:CB     | 32:f:67:PHE:C     | 2.51                     | 0.82              |
| 23:V:885:C:C5      | 23:V:889:C:O2'    | 2.30                     | 0.82              |
| 23:V:2636:U:H1'    | 23:V:2783:G:N2    | 1.93                     | 0.82              |
| 23:V:10:G:C6       | 23:V:2628:C:OP1   | 2.32                     | 0.82              |
| 23:V:362:U:C2'     | 23:V:363(A):A:OP1 | 2.26                     | 0.82              |
| 23:V:270(P):C:H2'  | 23:V:270(Q):C:C6  | 2.15                     | 0.82              |
| 23:V:1084:A:H1'    | 23:V:1106:G:O6    | 1.80                     | 0.82              |
| 20:S:23:ARG:HH11   | 20:S:30:ALA:HB2   | 1.45                     | 0.82              |
| 20:S:31:ARG:HB3    | 20:S:31:ARG:HH11  | 1.45                     | 0.82              |
| 23:V:885:C:N3      | 23:V:892:G:C5     | 2.48                     | 0.82              |
| 23:V:852:G:O2'     | 23:V:853:G:H5'    | 1.79                     | 0.81              |
| 23:V:2709:G:O2'    | 23:V:2710:C:H5'   | 1.80                     | 0.81              |
| 38:l:17:ARG:HH11   | 38:l:89:ARG:CD    | 1.85                     | 0.81              |
| 23:V:1545(A):A:H3' | 23:V:1546:C:H4'   | 1.61                     | 0.81              |
| 25:Y:177:LYS:N     | 25:Y:180:PHE:CE1  | 2.48                     | 0.81              |
| 38:l:25:ARG:HB3    | 38:l:87:PHE:HZ    | 1.42                     | 0.81              |
| 8:G:199:G:H2'      | 8:G:200:G:C8      | 2.15                     | 0.81              |
| 23:V:1040:C:O2     | 23:V:1116:C:O2    | 1.98                     | 0.81              |
| 20:S:23:ARG:NH1    | 20:S:30:ALA:HB2   | 1.96                     | 0.81              |
| 23:V:1055:G:N2     | 23:V:1105:U:O2    | 2.14                     | 0.81              |
| 23:V:1545:A:O2'    | 23:V:1546:C:OP2   | 1.97                     | 0.81              |
| 29:c:67:LYS:HZ2    | 29:c:90:LEU:CD1   | 1.89                     | 0.81              |
| 23:V:1550:C:OP1    | 23:V:1727:U:O2'   | 1.98                     | 0.81              |
| 23:V:972:G:H3'     | 23:V:973:A:O2'    | 1.81                     | 0.80              |
| 23:V:536:A:N3      | 23:V:558:G:N2     | 2.29                     | 0.80              |
| 23:V:972:G:C2'     | 23:V:973:A:H2'    | 2.11                     | 0.80              |
| 51:y:14:THR:CG2    | 51:y:52:VAL:HB    | 2.09                     | 0.80              |
| 23:V:2124:G:N7     | 25:Y:218:MET:CA   | 2.45                     | 0.80              |
| 32:f:44:ALA:HB2    | 32:f:67:PHE:N     | 1.96                     | 0.80              |
| 20:S:29:ARG:HD3    | 20:S:42:ILE:CG1   | 2.12                     | 0.80              |
| 23:V:280:C:H2'     | 23:V:283:A:H8     | 1.43                     | 0.80              |
| 45:s:30:ASN:ND2    | 45:s:89:PHE:HE1   | 1.57                     | 0.80              |
| 23:V:2198:A:H5''   | 23:V:2198:A:N3    | 1.96                     | 0.80              |
| 23:V:2630:G:C1'    | 23:V:2894:G:H1'   | 2.11                     | 0.80              |
| 29:c:28:VAL:O      | 29:c:31:VAL:HG23  | 1.81                     | 0.80              |
| 23:V:280:C:C6      | 23:V:283:A:C5     | 2.69                     | 0.80              |
| 23:V:2127:G:P      | 25:Y:36:LYS:HG2   | 2.21                     | 0.80              |
| 32:f:48:MET:CE     | 32:f:69:THR:HG21  | 1.96                     | 0.80              |
| 45:s:70:LEU:HD11   | 45:s:98:MET:HE3   | 1.61                     | 0.80              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:153:C:H3'     | 23:V:154:G:C8     | 2.16                     | 0.80              |
| 23:V:269:U:C5'     | 23:V:270(Y):G:H2' | 2.09                     | 0.80              |
| 23:V:2092:U:O4'    | 23:V:2225:A:C2    | 2.32                     | 0.79              |
| 32:f:67:PHE:O      | 32:f:68:VAL:C     | 2.24                     | 0.79              |
| 23:V:1938:A:C2     | 23:V:2590:A:O2'   | 2.35                     | 0.79              |
| 23:V:2126:A:N7     | 23:V:2164:C:OP1   | 2.14                     | 0.79              |
| 23:V:153:C:C3'     | 23:V:154:G:H8     | 1.94                     | 0.79              |
| 23:V:1169:G:C5     | 23:V:1170:G:C6    | 2.70                     | 0.79              |
| 23:V:1203:G:C6     | 23:V:1241:A:N7    | 2.51                     | 0.79              |
| 32:f:19:PRO:O      | 32:f:22:PRO:HD2   | 1.81                     | 0.79              |
| 23:V:2124:G:H8     | 25:Y:217:THR:CA   | 1.86                     | 0.79              |
| 38:l:17:ARG:HB3    | 38:l:17:ARG:NH2   | 1.96                     | 0.79              |
| 23:V:552:G:C6      | 23:V:553:U:N3     | 2.50                     | 0.79              |
| 32:f:37:PHE:CZ     | 32:f:62:ASP:OD1   | 2.36                     | 0.79              |
| 45:s:70:LEU:HD11   | 45:s:98:MET:HE1   | 0.79                     | 0.79              |
| 8:G:129(A):G:N2    | 8:G:191(A):G:C6   | 2.51                     | 0.79              |
| 29:c:86:MET:HB3    | 29:c:87:PRO:CD    | 2.13                     | 0.79              |
| 23:V:370:G:N3      | 23:V:370:G:H2'    | 1.98                     | 0.78              |
| 23:V:2123:G:C2'    | 25:Y:217:THR:C    | 2.57                     | 0.78              |
| 23:V:2630:G:C6     | 23:V:2790:A:H2    | 1.99                     | 0.78              |
| 23:V:12:U:O4       | 23:V:526:A:N7     | 2.16                     | 0.78              |
| 23:V:270:A:H2'     | 23:V:270(A):A:O4' | 1.84                     | 0.78              |
| 23:V:1169:G:H2'    | 23:V:1170:G:N7    | 1.97                     | 0.78              |
| 23:V:2791:C:N4     | 23:V:2892:A:H61   | 1.82                     | 0.78              |
| 30:d:98:LEU:HD11   | 30:d:125:VAL:HG23 | 1.62                     | 0.78              |
| 23:V:527:C:C2      | 23:V:2779:U:C5    | 2.72                     | 0.78              |
| 23:V:1533:C:O2     | 23:V:1538:G:N2    | 2.15                     | 0.78              |
| 23:V:1545(A):A:C3' | 23:V:1546:C:H4'   | 2.13                     | 0.78              |
| 25:Y:161:ILE:HG22  | 25:Y:174:PRO:HG2  | 1.66                     | 0.78              |
| 23:V:1443:G:O6     | 23:V:1549:C:N3    | 2.16                     | 0.78              |
| 23:V:2805:G:H21    | 23:V:2892:A:H62   | 1.32                     | 0.78              |
| 23:V:155:C:O2'     | 23:V:161:U:H3'    | 1.84                     | 0.78              |
| 23:V:270(P):C:H2'  | 23:V:270(Q):C:H6  | 1.49                     | 0.78              |
| 25:Y:22:ILE:O      | 25:Y:26:ALA:HB2   | 1.84                     | 0.78              |
| 8:G:1203:C:C4'     | 20:S:27:CYS:SG    | 2.72                     | 0.77              |
| 23:V:274:G:H3'     | 23:V:274:G:N3     | 1.98                     | 0.77              |
| 23:V:489:G:C5      | 23:V:1284:A:N1    | 2.52                     | 0.77              |
| 23:V:885:C:N3      | 23:V:892:G:C6     | 2.52                     | 0.77              |
| 23:V:1449(A):G:H2' | 23:V:1449(A):G:N3 | 1.99                     | 0.77              |
| 23:V:2096:U:O2'    | 23:V:2097:C:H5'   | 1.84                     | 0.77              |
| 32:f:22:PRO:CD     | 32:f:23:VAL:H     | 1.92                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:c:31:VAL:CB     | 29:c:32:PRO:HD3    | 2.01                     | 0.77              |
| 29:c:67:LYS:HZ2    | 29:c:90:LEU:HD13   | 1.39                     | 0.77              |
| 30:d:23:ARG:HG3    | 30:d:34:GLU:HB2    | 1.64                     | 0.77              |
| 23:V:374:A:C2      | 23:V:401:A:C5      | 2.73                     | 0.77              |
| 23:V:974:G:N7      | 23:V:1187:G:O2'    | 1.98                     | 0.77              |
| 23:V:1482:U:H2'    | 23:V:1483:G:H4'    | 1.66                     | 0.77              |
| 8:G:1308:U:O4      | 8:G:1330:U:O4      | 2.03                     | 0.77              |
| 29:c:71:THR:HB     | 29:c:87:PRO:HA     | 1.66                     | 0.77              |
| 29:c:47:LYS:HA     | 29:c:86:MET:CE     | 2.14                     | 0.77              |
| 32:f:43:ALA:C      | 32:f:67:PHE:HD1    | 1.89                     | 0.77              |
| 32:f:48:MET:SD     | 32:f:69:THR:HG21   | 2.24                     | 0.77              |
| 8:G:222:U:H2'      | 8:G:223:U:H5       | 1.46                     | 0.77              |
| 23:V:552:G:C2      | 23:V:553:U:C2      | 2.72                     | 0.77              |
| 23:V:13:A:N6       | 23:V:525:U:C6      | 2.53                     | 0.77              |
| 23:V:2811:G:N1     | 23:V:2891:G:N2     | 2.33                     | 0.77              |
| 23:V:134:C:H2'     | 23:V:135:G:C8      | 2.20                     | 0.77              |
| 23:V:270(X):G:N1   | 23:V:270(Y):G:H1'  | 2.00                     | 0.77              |
| 23:V:280:C:C6      | 23:V:283:A:N7      | 2.53                     | 0.77              |
| 23:V:1142(A):A:N3  | 23:V:1142(A):A:H2' | 2.00                     | 0.77              |
| 23:V:1742:C:C6     | 23:V:1743:G:C6     | 2.72                     | 0.77              |
| 8:G:1306:A:N6      | 8:G:1331:G:H21     | 1.82                     | 0.76              |
| 20:S:26:ARG:HD2    | 20:S:43:CYS:CB     | 2.05                     | 0.76              |
| 32:f:19:PRO:C      | 32:f:22:PRO:HD3    | 2.10                     | 0.76              |
| 55:DD:29:C:H2'     | 55:DD:30:G:H8      | 1.50                     | 0.76              |
| 8:G:69:G:C2        | 8:G:101:A:N6       | 2.54                     | 0.76              |
| 23:V:1786:A:H4'    | 23:V:1787:A:OP1    | 1.86                     | 0.76              |
| 23:V:2712(A):A:H4' | 37:k:13:HIS:CE1    | 2.20                     | 0.76              |
| 30:d:18:GLU:HG3    | 30:d:24:VAL:CB     | 2.10                     | 0.76              |
| 38:l:99:LYS:O      | 38:l:101:LEU:N     | 2.18                     | 0.76              |
| 38:l:99:LYS:O      | 38:l:102:ALA:N     | 2.19                     | 0.76              |
| 32:f:48:MET:SD     | 32:f:69:THR:CG2    | 2.74                     | 0.76              |
| 1:W:19:U:H1'       | 1:W:20:U:OP2       | 1.86                     | 0.76              |
| 23:V:2813:A:O2'    | 23:V:2814:C:H5'    | 1.85                     | 0.76              |
| 35:i:51:PHE:CG     | 35:i:57:THR:OG1    | 2.20                     | 0.76              |
| 23:V:95:G:C2'      | 23:V:96:G:O4'      | 2.33                     | 0.75              |
| 23:V:134:C:C4      | 23:V:135:G:C6      | 2.73                     | 0.75              |
| 8:G:77:C:C4        | 8:G:92:G:O6        | 2.38                     | 0.75              |
| 8:G:199:G:H2'      | 8:G:200:G:H8       | 1.49                     | 0.75              |
| 23:V:1441:G:O6     | 23:V:1442:G:O6     | 2.04                     | 0.75              |
| 30:d:13:LYS:CE     | 30:d:29:PRO:CD     | 2.55                     | 0.75              |
| 55:DD:29:C:H2'     | 55:DD:30:G:C8      | 2.21                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:671:G:O2'     | 13:L:80:ARG:CZ    | 2.35                     | 0.75              |
| 8:G:1442:G:H3'    | 8:G:1442:G:N3     | 2.00                     | 0.75              |
| 23:V:270(E):G:O2' | 23:V:270(F):U:H5' | 1.86                     | 0.75              |
| 23:V:371:A:N3     | 23:V:371:A:H2'    | 2.00                     | 0.75              |
| 32:f:48:MET:HB2   | 32:f:69:THR:CG2   | 2.16                     | 0.75              |
| 1:W:19:U:H1'      | 1:W:20:U:P        | 2.26                     | 0.75              |
| 23:V:852:G:H2'    | 23:V:853:G:C8     | 2.20                     | 0.75              |
| 23:V:1717:G:N3    | 23:V:1717:G:H5''  | 2.01                     | 0.75              |
| 23:V:1742:C:C5    | 23:V:1743:G:C6    | 2.75                     | 0.75              |
| 29:c:67:LYS:NZ    | 29:c:90:LEU:HD12  | 2.00                     | 0.75              |
| 23:V:95:G:C3'     | 23:V:96:G:O4'     | 2.35                     | 0.75              |
| 23:V:2097:C:O2'   | 23:V:2098:U:H5'   | 1.84                     | 0.75              |
| 23:V:2211:G:H3'   | 23:V:2211:G:N3    | 2.01                     | 0.75              |
| 29:c:86:MET:CB    | 29:c:87:PRO:HD2   | 2.17                     | 0.75              |
| 32:f:68:VAL:HG23  | 32:f:69:THR:H     | 0.64                     | 0.75              |
| 23:V:536:A:N1     | 23:V:558:G:C5     | 2.55                     | 0.75              |
| 23:V:43:G:O6      | 23:V:438:G:N1     | 2.18                     | 0.75              |
| 30:d:27:LYS:HE3   | 30:d:32:GLU:OE2   | 1.86                     | 0.75              |
| 23:V:856:C:C4     | 23:V:857:C:N4     | 2.55                     | 0.74              |
| 23:V:975:G:N2     | 23:V:990:A:H1'    | 2.01                     | 0.74              |
| 23:V:1106:G:O2'   | 23:V:1107:G:OP1   | 2.02                     | 0.74              |
| 20:S:31:ARG:HB3   | 20:S:31:ARG:NH1   | 2.02                     | 0.74              |
| 23:V:1169:G:N1    | 23:V:1170:G:C6    | 2.56                     | 0.74              |
| 23:V:1203:G:O6    | 23:V:1241:A:C5    | 2.40                     | 0.74              |
| 32:f:52:ILE:HG13  | 32:f:76:TYR:CD1   | 2.21                     | 0.74              |
| 45:s:4:ARG:HE     | 45:s:62:PRO:HB3   | 1.52                     | 0.74              |
| 8:G:1203:C:C4'    | 20:S:27:CYS:HG    | 1.99                     | 0.74              |
| 23:V:270(G):C:H2' | 23:V:270(H):C:C6  | 2.22                     | 0.74              |
| 23:V:270(Z):U:H4' | 23:V:270(Z):U:OP1 | 1.88                     | 0.74              |
| 23:V:270(Z):U:O2  | 23:V:270(Z):U:H2' | 1.85                     | 0.74              |
| 23:V:1728:G:H2'   | 23:V:1728:G:N3    | 2.02                     | 0.74              |
| 29:c:47:LYS:HA    | 29:c:86:MET:HE2   | 1.69                     | 0.74              |
| 38:l:94:TYR:OH    | 38:l:99:LYS:HG3   | 1.86                     | 0.74              |
| 23:V:2209:C:C5    | 23:V:2212:A:C6    | 2.75                     | 0.74              |
| 25:Y:152:ILE:HG23 | 25:Y:160:ARG:HD3  | 1.66                     | 0.74              |
| 1:W:16:A:N1       | 1:W:17:U:N3       | 2.34                     | 0.74              |
| 23:V:101:G:H4'    | 23:V:101:G:OP1    | 1.88                     | 0.74              |
| 23:V:138:G:H2'    | 23:V:138:G:N3     | 2.02                     | 0.74              |
| 23:V:1480:G:H2'   | 23:V:1480:G:N3    | 2.03                     | 0.74              |
| 23:V:1583:A:N7    | 23:V:1585:C:N4    | 2.31                     | 0.74              |
| 23:V:1084:A:O2'   | 23:V:1106:G:C8    | 2.40                     | 0.74              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:X:0:A:H5''      | 24:X:0:A:N3       | 2.03                     | 0.74              |
| 25:Y:64:LEU:HB2    | 25:Y:159:GLY:HA3  | 1.70                     | 0.74              |
| 23:V:2123:G:O2'    | 25:Y:217:THR:HA   | 1.87                     | 0.74              |
| 31:e:39:ALA:O      | 31:e:43:ALA:HB3   | 1.87                     | 0.74              |
| 23:V:270(C):C:O2'  | 23:V:270(D):C:H5' | 1.88                     | 0.73              |
| 23:V:1778:U:N1     | 23:V:1784:A:C2    | 2.56                     | 0.73              |
| 23:V:2123:G:C2'    | 25:Y:217:THR:O    | 2.35                     | 0.73              |
| 23:V:2335:A:OP1    | 38:l:12:PHE:CB    | 2.36                     | 0.73              |
| 30:d:16:SER:O      | 30:d:17:VAL:CB    | 2.35                     | 0.73              |
| 23:V:2630:G:C6     | 23:V:2790:A:C2    | 2.75                     | 0.73              |
| 32:f:44:ALA:CA     | 32:f:67:PHE:HA    | 2.17                     | 0.73              |
| 8:G:222:U:O2       | 8:G:223:U:C5      | 2.39                     | 0.73              |
| 29:c:86:MET:CB     | 29:c:87:PRO:CD    | 2.63                     | 0.73              |
| 23:V:2712(A):A:H4' | 37:k:13:HIS:HE1   | 1.51                     | 0.73              |
| 38:l:9:ARG:HB3     | 38:l:12:PHE:CZ    | 2.24                     | 0.73              |
| 23:V:11:G:H5''     | 23:V:11:G:N3      | 2.02                     | 0.73              |
| 23:V:2709:G:H2'    | 23:V:2710:C:C6    | 2.24                     | 0.73              |
| 25:Y:64:LEU:O      | 25:Y:159:GLY:HA3  | 1.88                     | 0.73              |
| 56:EE:96:GLN:CD    | 56:EE:96:GLN:H    | 1.96                     | 0.73              |
| 19:R:102:ARG:HG2   | 19:R:102:ARG:HH11 | 1.51                     | 0.73              |
| 23:V:270(H):C:H2'  | 23:V:270(I):G:H8  | 1.51                     | 0.73              |
| 23:V:2630:G:C4     | 23:V:2894:G:H8    | 2.06                     | 0.73              |
| 8:G:1166:G:H4'     | 8:G:1166:G:OP1    | 1.88                     | 0.73              |
| 23:V:2096:U:O2     | 23:V:2194:G:C2    | 2.42                     | 0.73              |
| 32:f:19:PRO:CA     | 32:f:22:PRO:CG    | 2.58                     | 0.73              |
| 8:G:199:G:O2'      | 8:G:200:G:H5'     | 1.88                     | 0.73              |
| 23:V:270(X):G:H2'  | 23:V:270(Y):G:C5' | 2.17                     | 0.73              |
| 23:V:271(A):G:H5'' | 23:V:271(B):U:C5' | 2.19                     | 0.73              |
| 23:V:1718:G:N2     | 23:V:1741:C:C2    | 2.57                     | 0.73              |
| 25:Y:180:PHE:CD2   | 25:Y:185:LEU:HD13 | 2.23                     | 0.73              |
| 8:G:465:A:N7       | 8:G:467:G:C2      | 2.57                     | 0.72              |
| 23:V:1075:C:H1'    | 32:f:91:PRO:CG    | 2.10                     | 0.72              |
| 23:V:97:C:P        | 47:u:43:HIS:CE1   | 2.81                     | 0.72              |
| 20:S:31:ARG:HH11   | 20:S:31:ARG:CB    | 2.02                     | 0.72              |
| 23:V:273(C):C:H2'  | 23:V:273(D):C:C6  | 2.24                     | 0.72              |
| 23:V:2226:C:O2'    | 23:V:2227:A:H5'   | 1.88                     | 0.72              |
| 38:l:35:ILE:HD11   | 38:l:97:ARG:NH1   | 2.04                     | 0.72              |
| 8:G:129(A):G:N2    | 8:G:191(A):G:C5   | 2.57                     | 0.72              |
| 23:V:2206:C:O2'    | 23:V:2207:C:H5'   | 1.88                     | 0.72              |
| 23:V:2213:U:O4     | 49:w:47:GLN:NE2   | 2.21                     | 0.72              |
| 23:V:270(J):G:H3'  | 23:V:270(K):C:C6  | 2.24                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:c:71:THR:HB    | 29:c:88:ILE:H     | 1.50                     | 0.72              |
| 25:Y:30:LYS:HG2   | 25:Y:179:SER:HA   | 1.72                     | 0.72              |
| 24:X:89:G:C8      | 24:X:89:G:OP2     | 2.43                     | 0.72              |
| 23:V:1174:A:N3    | 23:V:1174:A:H2'   | 2.05                     | 0.72              |
| 38:l:24:LEU:C     | 38:l:87:PHE:CE1   | 2.67                     | 0.72              |
| 55:DD:48:U:HO2'   | 55:DD:49:C:H5'    | 1.54                     | 0.72              |
| 23:V:140:A:H2'    | 23:V:140:A:N3     | 2.05                     | 0.72              |
| 23:V:2837:G:C2    | 23:V:2882:A:C2    | 2.78                     | 0.72              |
| 46:t:7:LEU:HD21   | 55:DD:3:C:OP1     | 1.90                     | 0.72              |
| 23:V:362:U:O2'    | 23:V:363(A):A:OP1 | 2.08                     | 0.71              |
| 23:V:885:C:C6     | 23:V:889:C:O2'    | 2.43                     | 0.71              |
| 23:V:374:A:N1     | 23:V:401:A:C5     | 2.58                     | 0.71              |
| 3:B:70:ILE:O      | 3:B:74:ARG:HB2    | 1.91                     | 0.71              |
| 23:V:972:G:O2'    | 23:V:973:A:P      | 2.48                     | 0.71              |
| 23:V:1782:C:H6    | 23:V:1782:C:C5'   | 2.02                     | 0.71              |
| 55:DD:30:G:O2'    | 55:DD:31:G:H5'    | 1.91                     | 0.71              |
| 55:DD:37:U:H2'    | 55:DD:38:A:H5'    | 1.72                     | 0.71              |
| 55:DD:37:U:O2'    | 55:DD:38:A:H5'    | 1.89                     | 0.71              |
| 8:G:465:A:N6      | 8:G:467:G:H21     | 1.88                     | 0.71              |
| 23:V:18:C:O2'     | 23:V:553:U:OP1    | 2.08                     | 0.71              |
| 23:V:1778:U:C5    | 23:V:1784:A:N1    | 2.46                     | 0.71              |
| 23:V:2813:A:H2'   | 23:V:2814:C:C6    | 2.25                     | 0.71              |
| 23:V:270(Q):C:O2' | 23:V:270(R):G:H5' | 1.91                     | 0.71              |
| 23:V:923:C:H2'    | 23:V:924:C:C6     | 2.25                     | 0.71              |
| 23:V:2124:G:N2    | 25:Y:221:SER:N    | 2.33                     | 0.71              |
| 30:d:127:GLU:CB   | 30:d:128:PRO:HD3  | 2.18                     | 0.71              |
| 23:V:270(Q):C:C2  | 23:V:270(R):G:C8  | 2.79                     | 0.71              |
| 32:f:86:LYS:CA    | 32:f:95:LYS:HD3   | 2.21                     | 0.71              |
| 8:G:1323:G:H4'    | 8:G:1362:C:C4     | 2.26                     | 0.71              |
| 23:V:96:G:H4'     | 47:u:43:HIS:NE2   | 2.03                     | 0.71              |
| 23:V:2335:A:OP1   | 38:l:12:PHE:HB2   | 1.90                     | 0.71              |
| 29:c:67:LYS:HZ3   | 29:c:90:LEU:HD13  | 0.66                     | 0.71              |
| 23:V:270(X):G:C6  | 23:V:270(Y):G:H1' | 2.26                     | 0.70              |
| 23:V:972:G:C3'    | 23:V:973:A:C2'    | 2.49                     | 0.70              |
| 23:V:2710:C:H2'   | 23:V:2711:A:H8    | 1.53                     | 0.70              |
| 32:f:93:ARG:CD    | 32:f:135:GLY:O    | 2.30                     | 0.70              |
| 45:s:94:GLU:H     | 45:s:95:PRO:CD    | 2.04                     | 0.70              |
| 23:V:2809:A:C2    | 27:a:60:ASN:HB3   | 2.25                     | 0.70              |
| 8:G:138:G:C4      | 8:G:226:G:N2      | 2.59                     | 0.70              |
| 23:V:374:A:C2     | 23:V:401:A:C2     | 2.79                     | 0.70              |
| 23:V:374:A:C2     | 23:V:401:A:N3     | 2.59                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:1103:A:H2'   | 23:V:1103:A:N3    | 2.05                     | 0.70              |
| 23:V:852:G:C4     | 23:V:853:G:N7     | 2.59                     | 0.70              |
| 29:c:71:THR:CA    | 29:c:88:ILE:H     | 2.04                     | 0.70              |
| 32:f:66:THR:O     | 32:f:68:VAL:HG13  | 1.92                     | 0.70              |
| 8:G:129(A):G:N2   | 8:G:191(A):G:O6   | 2.24                     | 0.70              |
| 23:V:1778:U:C6    | 23:V:1784:A:H2    | 1.85                     | 0.70              |
| 23:V:1862:G:O2'   | 23:V:1863:G:H5'   | 1.91                     | 0.70              |
| 29:c:165:THR:HG22 | 29:c:168:GLU:HG2  | 1.72                     | 0.70              |
| 23:V:278:A:C2     | 23:V:362:U:N3     | 2.57                     | 0.70              |
| 23:V:2782:G:H2'   | 23:V:2782:G:N3    | 2.06                     | 0.70              |
| 55:DD:7:G:H3'     | 55:DD:8:4SU:C5'   | 2.21                     | 0.70              |
| 23:V:374:A:C6     | 23:V:401:A:N7     | 2.60                     | 0.70              |
| 23:V:1479:G:O3'   | 23:V:1559:G:N7    | 2.12                     | 0.70              |
| 23:V:2627:G:N2    | 23:V:2777:G:C2    | 2.59                     | 0.70              |
| 25:Y:44:HIS:HA    | 25:Y:171:ILE:O    | 1.91                     | 0.70              |
| 30:d:18:GLU:CB    | 30:d:24:VAL:HG23  | 2.07                     | 0.70              |
| 20:S:25:VAL:HG11  | 20:S:39:LEU:HD23  | 1.73                     | 0.70              |
| 30:d:16:SER:OG    | 30:d:17:VAL:N     | 2.19                     | 0.70              |
| 38:l:97:ARG:HG2   | 38:l:97:ARG:NH1   | 1.98                     | 0.70              |
| 55:DD:37:U:C2'    | 55:DD:38:A:H5'    | 2.21                     | 0.70              |
| 23:V:374:A:C6     | 23:V:401:A:C5     | 2.80                     | 0.70              |
| 32:f:68:VAL:O     | 32:f:69:THR:CB    | 2.38                     | 0.70              |
| 45:s:100:VAL:HG12 | 45:s:133:ILE:HG13 | 1.73                     | 0.70              |
| 23:V:95:G:C2      | 23:V:96:G:N3      | 2.60                     | 0.69              |
| 23:V:1532:C:C4    | 23:V:1539:G:N2    | 2.58                     | 0.69              |
| 30:d:101:ARG:O    | 30:d:123:PHE:CE2  | 2.41                     | 0.69              |
| 23:V:270(E):G:H2' | 23:V:270(F):U:H6  | 1.57                     | 0.69              |
| 23:V:975:G:C2     | 23:V:990:A:C4     | 2.79                     | 0.69              |
| 23:V:2124:G:H5'   | 25:Y:217:THR:HG1  | 1.52                     | 0.69              |
| 30:d:27:LYS:HE3   | 30:d:32:GLU:CD    | 2.17                     | 0.69              |
| 35:i:51:PHE:HB3   | 35:i:57:THR:CB    | 2.23                     | 0.69              |
| 23:V:1418:G:H21   | 23:V:1579:A:H62   | 1.41                     | 0.69              |
| 23:V:923:C:N4     | 23:V:924:C:N4     | 2.40                     | 0.69              |
| 23:V:1938:A:N1    | 23:V:2590:A:O2'   | 2.24                     | 0.69              |
| 30:d:18:GLU:HB2   | 30:d:24:VAL:CB    | 2.22                     | 0.69              |
| 32:f:52:ILE:O     | 32:f:73:PRO:HD2   | 1.91                     | 0.69              |
| 23:V:1864:U:HO2'  | 23:V:1869:G:H5'   | 1.56                     | 0.69              |
| 23:V:2123:G:H2'   | 25:Y:217:THR:C    | 2.16                     | 0.69              |
| 29:c:31:VAL:CG1   | 29:c:32:PRO:HD2   | 2.10                     | 0.69              |
| 23:V:2209:C:H5    | 23:V:2212:A:C6    | 2.10                     | 0.69              |
| 29:c:71:THR:CB    | 29:c:88:ILE:H     | 2.04                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:V:270(K):C:H3' | 23:V:270(L):U:H6   | 1.57                     | 0.69              |
| 23:V:1450:C:OP2   | 23:V:1461:G:N1     | 2.25                     | 0.69              |
| 8:G:77:C:N3       | 8:G:92:G:C6        | 2.61                     | 0.69              |
| 8:G:267:C:H2'     | 8:G:268:C:C6       | 2.28                     | 0.69              |
| 23:V:12:U:N3      | 23:V:2626:C:O2'    | 2.20                     | 0.69              |
| 23:V:552:G:N2     | 23:V:553:U:O2      | 2.25                     | 0.69              |
| 31:e:11:ALA:C     | 31:e:13:LEU:H      | 2.00                     | 0.69              |
| 8:G:465:A:H62     | 8:G:467:G:N2       | 1.90                     | 0.68              |
| 8:G:977:A:N6      | 8:G:1362(A):C:C5   | 2.61                     | 0.68              |
| 23:V:1169:G:C4    | 23:V:1170:G:C5     | 2.81                     | 0.68              |
| 23:V:2098:U:H2'   | 23:V:2099:U:C6     | 2.28                     | 0.68              |
| 23:V:2198:A:N3    | 23:V:2198:A:H3'    | 2.08                     | 0.68              |
| 23:V:2209:C:C4    | 23:V:2216:G:N2     | 2.61                     | 0.68              |
| 29:c:83:ARG:O     | 29:c:84:LYS:C      | 2.37                     | 0.68              |
| 23:V:272:G:O2'    | 23:V:273:G:H5'     | 1.93                     | 0.68              |
| 23:V:972:G:O3'    | 23:V:973:A:H3'     | 1.94                     | 0.68              |
| 8:G:1309:G:N2     | 8:G:1328:C:C2      | 2.56                     | 0.68              |
| 23:V:2894:G:H3'   | 23:V:2894:G:N3     | 2.08                     | 0.68              |
| 25:Y:176:GLY:HA2  | 25:Y:185:LEU:HD13  | 1.76                     | 0.68              |
| 30:d:127:GLU:HB3  | 30:d:128:PRO:HD2   | 0.75                     | 0.68              |
| 23:V:974:G:N2     | 23:V:1186:G:C4     | 2.62                     | 0.68              |
| 23:V:1543:A:H2'   | 23:V:1544:C:H4'    | 1.76                     | 0.68              |
| 29:c:71:THR:C     | 29:c:88:ILE:H      | 2.02                     | 0.68              |
| 41:o:7:THR:O      | 41:o:21:ARG:NH1    | 2.27                     | 0.68              |
| 23:V:1449:A:H4'   | 23:V:1449(A):G:H5' | 1.73                     | 0.68              |
| 23:V:2123:G:O2'   | 25:Y:217:THR:CB    | 2.41                     | 0.68              |
| 28:b:168:ARG:HG2  | 28:b:169:ASN:HB2   | 1.75                     | 0.68              |
| 23:V:85:G:H1      | 23:V:98:G:H21      | 1.41                     | 0.68              |
| 23:V:270(Q):C:H2' | 23:V:270(R):G:H8   | 1.59                     | 0.68              |
| 23:V:275:G:H8     | 23:V:275:G:O5'     | 1.77                     | 0.68              |
| 23:V:373:U:C1'    | 23:V:400:G:H22     | 2.07                     | 0.68              |
| 23:V:1442:G:N1    | 23:V:1550:C:C2     | 2.60                     | 0.68              |
| 23:V:2127:G:H22   | 23:V:2162:G:H2'    | 1.57                     | 0.68              |
| 32:f:67:PHE:O     | 32:f:68:VAL:O      | 2.12                     | 0.68              |
| 20:S:26:ARG:CD    | 20:S:43:CYS:CB     | 2.61                     | 0.67              |
| 23:V:1138:G:C6    | 23:V:1139:G:C6     | 2.82                     | 0.67              |
| 24:X:89:G:OP2     | 24:X:89:G:H8       | 1.75                     | 0.67              |
| 25:Y:64:LEU:HD22  | 25:Y:188:ASN:HA    | 1.76                     | 0.67              |
| 8:G:1118:C:H42    | 8:G:1155:G:H1      | 1.42                     | 0.67              |
| 8:G:1161:C:H42    | 8:G:1176:A:H61     | 1.43                     | 0.67              |
| 23:V:1102:C:N3    | 23:V:1104:C:N4     | 2.42                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:1005:C:C6    | 23:V:1143:A:C8    | 2.82                     | 0.67              |
| 23:V:2450:A:H62   | 23:V:2501:C:H42   | 1.43                     | 0.67              |
| 23:V:2795:G:N3    | 23:V:2795:G:H2'   | 2.09                     | 0.67              |
| 32:f:55:VAL:HG13  | 32:f:70:LYS:CG    | 2.24                     | 0.67              |
| 23:V:270:A:H2'    | 23:V:270(A):A:C4' | 2.25                     | 0.67              |
| 23:V:362:U:H2'    | 23:V:363(A):A:OP1 | 1.94                     | 0.67              |
| 23:V:1778:U:N1    | 23:V:1784:A:N1    | 2.41                     | 0.67              |
| 25:Y:46:LYS:HA    | 25:Y:169:GLY:O    | 1.94                     | 0.67              |
| 38:l:9:ARG:O      | 38:l:12:PHE:CE1   | 2.47                     | 0.67              |
| 8:G:153:C:H42     | 8:G:169:C:H42     | 1.42                     | 0.67              |
| 23:V:2123:G:O2'   | 25:Y:217:THR:HB   | 1.95                     | 0.67              |
| 8:G:68:G:N1       | 8:G:102:G:N2      | 2.43                     | 0.67              |
| 23:V:1512:G:N7    | 23:V:1513:C:N4    | 2.43                     | 0.67              |
| 32:f:17:ALA:O     | 32:f:19:PRO:HD3   | 1.94                     | 0.67              |
| 32:f:37:PHE:HZ    | 32:f:62:ASP:OD2   | 1.76                     | 0.67              |
| 23:V:1450:C:OP2   | 23:V:1461:G:O6    | 2.12                     | 0.67              |
| 23:V:2217:G:H2'   | 23:V:2218:G:H5''  | 1.76                     | 0.67              |
| 28:b:18:ARG:HH12  | 28:b:201:VAL:HG21 | 1.59                     | 0.67              |
| 29:c:81:LYS:HG3   | 29:c:83:ARG:HH12  | 1.58                     | 0.67              |
| 32:f:21:PRO:N     | 32:f:22:PRO:CD    | 2.58                     | 0.67              |
| 20:S:9:LYS:CE     | 20:S:21:TYR:CE1   | 2.78                     | 0.67              |
| 20:S:26:ARG:HD3   | 20:S:43:CYS:HB2   | 1.72                     | 0.67              |
| 23:V:1041:C:C2    | 23:V:1115:G:O6    | 2.46                     | 0.67              |
| 23:V:2791:C:N4    | 23:V:2893:G:N2    | 2.43                     | 0.67              |
| 24:X:89:G:H8      | 24:X:89:G:P       | 2.17                     | 0.67              |
| 55:DD:33:OMC:O5'  | 55:DD:33:OMC:H6   | 1.78                     | 0.67              |
| 8:G:222:U:C2'     | 8:G:223:U:C5      | 2.71                     | 0.67              |
| 23:V:1441:G:N1    | 23:V:1442:G:C6    | 2.63                     | 0.67              |
| 8:G:1308:U:O4     | 8:G:1330:U:C4     | 2.48                     | 0.67              |
| 23:V:144:C:H6     | 23:V:144:C:O5'    | 1.78                     | 0.67              |
| 23:V:527:C:C2     | 23:V:2779:U:C6    | 2.83                     | 0.67              |
| 23:V:1102:C:C4    | 23:V:1104:C:N4    | 2.63                     | 0.67              |
| 23:V:1710:C:N3    | 23:V:1711:C:N3    | 2.42                     | 0.67              |
| 23:V:1864:U:C2'   | 23:V:1869:G:H5'   | 2.25                     | 0.67              |
| 23:V:1864:U:H5'   | 23:V:2410:G:O2'   | 1.95                     | 0.67              |
| 23:V:2098:U:O5'   | 23:V:2098:U:H6    | 1.78                     | 0.67              |
| 23:V:2829:C:O5'   | 23:V:2829:C:H6    | 1.78                     | 0.67              |
| 32:f:52:ILE:CG1   | 32:f:76:TYR:CD1   | 2.78                     | 0.67              |
| 29:c:71:THR:HB    | 29:c:87:PRO:C     | 2.19                     | 0.66              |
| 8:G:269:C:O5'     | 8:G:269:C:H6      | 1.78                     | 0.66              |
| 23:V:270(B):A:H1' | 23:V:270(C):C:C6  | 2.30                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:V:852:G:C6    | 23:V:926:A:N1     | 2.63                     | 0.66              |
| 23:V:988:A:H3'   | 48:v:12:PRO:HG3   | 1.77                     | 0.66              |
| 8:G:1203:C:H4'   | 20:S:27:CYS:HB3   | 1.75                     | 0.66              |
| 8:G:1359:C:O2'   | 8:G:1360:A:C5'    | 2.43                     | 0.66              |
| 23:V:270(J):G:C6 | 23:V:270(K):C:N3  | 2.64                     | 0.66              |
| 23:V:373:U:OP1   | 23:V:401:A:N7     | 2.28                     | 0.66              |
| 23:V:1751:C:O5'  | 23:V:1751:C:H6    | 1.79                     | 0.66              |
| 30:d:95:ARG:HB3  | 30:d:129:THR:OG1  | 1.92                     | 0.66              |
| 32:f:71:THR:HG21 | 32:f:113:PRO:HG2  | 1.77                     | 0.66              |
| 18:Q:76:ASN:HD21 | 18:Q:108:ALA:H    | 1.44                     | 0.66              |
| 23:V:1143:A:C5'  | 23:V:1143:A:H8    | 2.08                     | 0.66              |
| 32:f:93:ARG:NE   | 32:f:137:GLU:OE1  | 2.29                     | 0.66              |
| 8:G:129(A):G:N2  | 8:G:191(A):G:N7   | 2.42                     | 0.66              |
| 8:G:456:C:O5'    | 8:G:456:C:H6      | 1.78                     | 0.66              |
| 23:V:2637:U:C2   | 23:V:2782:G:N1    | 2.63                     | 0.66              |
| 38:l:26:LEU:HA   | 38:l:38:GLN:O     | 1.95                     | 0.66              |
| 55:DD:6:G:O2'    | 55:DD:7:G:O5'     | 2.13                     | 0.66              |
| 8:G:138:G:N3     | 8:G:226:G:N2      | 2.44                     | 0.66              |
| 8:G:200:G:N2     | 8:G:217:C:O2      | 2.26                     | 0.66              |
| 23:V:2633:G:O2'  | 27:a:61:ARG:NH2   | 2.28                     | 0.66              |
| 23:V:2099:U:H6   | 23:V:2099:U:O5'   | 1.79                     | 0.66              |
| 32:f:32:ALA:HA   | 32:f:59:ILE:CG2   | 2.25                     | 0.66              |
| 33:g:22:THR:O    | 33:g:26:LEU:CB    | 2.44                     | 0.66              |
| 8:G:93:U:O5'     | 8:G:93:U:H6       | 1.79                     | 0.65              |
| 50:x:32:PRO:HA   | 50:x:38:ALA:O     | 1.96                     | 0.65              |
| 8:G:99:C:H6      | 8:G:99:C:O5'      | 1.79                     | 0.65              |
| 23:V:375:C:O5'   | 23:V:375:C:H6     | 1.79                     | 0.65              |
| 23:V:1467:C:C4   | 23:V:1545(A):A:C8 | 2.84                     | 0.65              |
| 23:V:2828:C:O5'  | 23:V:2828:C:H6    | 1.80                     | 0.65              |
| 50:x:30:LEU:CD1  | 50:x:39:MET:SD    | 2.84                     | 0.65              |
| 8:G:82:U:C2      | 8:G:87:A:C2       | 2.84                     | 0.65              |
| 8:G:841:U:O5'    | 8:G:841:U:H6      | 1.78                     | 0.65              |
| 23:V:43:G:C2     | 23:V:438:G:C2     | 2.84                     | 0.65              |
| 23:V:1145:C:O5'  | 23:V:1145:C:H6    | 1.78                     | 0.65              |
| 44:r:23:ARG:NH1  | 44:r:38:ILE:O     | 2.29                     | 0.65              |
| 8:G:464:G:O5'    | 8:G:464:G:H8      | 1.80                     | 0.65              |
| 8:G:1165:C:O5'   | 8:G:1165:C:H6     | 1.79                     | 0.65              |
| 23:V:1445:C:H41  | 23:V:1446:C:H42   | 1.45                     | 0.65              |
| 8:G:268:C:O5'    | 8:G:268:C:H6      | 1.79                     | 0.65              |
| 8:G:1414:U:O5'   | 8:G:1414:U:H6     | 1.79                     | 0.65              |
| 17:P:40:ILE:HG22 | 17:P:41:THR:HG23  | 1.77                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:1063:G:OP1    | 32:f:52:ILE:CD1   | 2.39                     | 0.65              |
| 23:V:2878:U:O5'    | 23:V:2878:U:H6    | 1.78                     | 0.65              |
| 55:DD:5:G:O2'      | 55:DD:6:G:H5'     | 1.97                     | 0.65              |
| 8:G:192:U:O5'      | 8:G:192:U:H6      | 1.79                     | 0.65              |
| 8:G:1415:G:C6      | 8:G:1486:G:C6     | 2.85                     | 0.65              |
| 23:V:2197:U:C4     | 23:V:2224:G:C6    | 2.85                     | 0.65              |
| 23:V:2206:C:N3     | 23:V:2219:G:C2    | 2.65                     | 0.65              |
| 45:s:72:ARG:NH2    | 45:s:98:MET:SD    | 2.69                     | 0.65              |
| 8:G:442:C:O5'      | 8:G:442:C:H6      | 1.79                     | 0.65              |
| 23:V:539:G:O5'     | 23:V:539:G:H8     | 1.80                     | 0.65              |
| 23:V:2630:G:O4'    | 23:V:2894:G:H1'   | 1.96                     | 0.65              |
| 8:G:1162:C:H6      | 8:G:1162:C:O5'    | 1.80                     | 0.65              |
| 8:G:1415:G:N1      | 8:G:1486:G:C6     | 2.64                     | 0.65              |
| 23:V:374:A:C4      | 23:V:401:A:C6     | 2.85                     | 0.65              |
| 23:V:972:G:H2'     | 23:V:973:A:H2'    | 1.77                     | 0.65              |
| 23:V:1799:G:N2     | 23:V:1818:U:O2'   | 2.29                     | 0.65              |
| 23:V:1838:C:O2     | 23:V:1899:G:N2    | 2.29                     | 0.65              |
| 28:b:184:TYR:O     | 35:i:7:ARG:NH2    | 2.30                     | 0.65              |
| 23:V:274:G:C2'     | 23:V:275:G:H5'    | 2.27                     | 0.65              |
| 23:V:271(A):G:H5'' | 23:V:271(B):U:C4' | 2.27                     | 0.65              |
| 23:V:975:G:C2      | 23:V:990:A:C5     | 2.85                     | 0.65              |
| 55:DD:29:C:N4      | 55:DD:30:G:O6     | 2.30                     | 0.65              |
| 8:G:439:A:C8       | 8:G:496:A:N1      | 2.65                     | 0.64              |
| 8:G:670:G:H8       | 8:G:670:G:O5'     | 1.80                     | 0.64              |
| 23:V:363(F):G:O5'  | 23:V:363(F):G:H8  | 1.81                     | 0.64              |
| 23:V:1450:C:OP2    | 23:V:1461:G:C6    | 2.50                     | 0.64              |
| 23:V:2807:G:N2     | 23:V:2892:A:C2    | 2.65                     | 0.64              |
| 30:d:122:THR:HG21  | 30:d:133:VAL:HG23 | 1.78                     | 0.64              |
| 44:r:14:LEU:HD12   | 44:r:19:LYS:HB2   | 1.80                     | 0.64              |
| 23:V:1480:G:H5''   | 23:V:1482:U:OP2   | 1.98                     | 0.64              |
| 30:d:89:ILE:HG23   | 30:d:129:THR:CG2  | 2.26                     | 0.64              |
| 50:x:30:LEU:HD13   | 50:x:39:MET:SD    | 2.37                     | 0.64              |
| 8:G:225:C:O5'      | 8:G:225:C:H6      | 1.81                     | 0.64              |
| 8:G:1306:A:H8      | 8:G:1306:A:O5'    | 1.80                     | 0.64              |
| 23:V:1102:C:C2     | 23:V:1104:C:N4    | 2.65                     | 0.64              |
| 23:V:1422:G:H22    | 23:V:1576:U:H1'   | 1.62                     | 0.64              |
| 23:V:1442:G:C2     | 23:V:1550:C:O2    | 2.48                     | 0.64              |
| 8:G:186(B):C:H2'   | 8:G:186(C):G:H8   | 1.61                     | 0.64              |
| 23:V:552:G:C4      | 23:V:553:U:N3     | 2.65                     | 0.64              |
| 23:V:1041:C:O2     | 23:V:1115:G:C6    | 2.48                     | 0.64              |
| 30:d:89:ILE:HG21   | 30:d:129:THR:HG22 | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:DD:38:A:O2'    | 55:DD:39:A:H5'    | 1.97                     | 0.64              |
| 8:G:1116:C:O5'    | 8:G:1116:C:H6     | 1.81                     | 0.64              |
| 23:V:1863:G:N2    | 23:V:1880:C:O2    | 2.29                     | 0.64              |
| 23:V:1872:A:H8    | 23:V:1872:A:O5'   | 1.81                     | 0.64              |
| 23:V:2128:C:OP1   | 25:Y:6:ARG:HD2    | 1.98                     | 0.64              |
| 23:V:2710:C:O5'   | 23:V:2710:C:H6    | 1.79                     | 0.64              |
| 32:f:86:LYS:HE3   | 32:f:93:ARG:HA    | 1.79                     | 0.64              |
| 41:o:34:GLU:HA    | 41:o:62:LEU:O     | 1.97                     | 0.64              |
| 23:V:489:G:C5     | 23:V:1284:A:C6    | 2.86                     | 0.64              |
| 23:V:1057:A:OP2   | 23:V:1084:A:N6    | 2.30                     | 0.64              |
| 29:c:47:LYS:CG    | 29:c:80:PHE:CD2   | 2.76                     | 0.64              |
| 32:f:48:MET:CG    | 32:f:69:THR:HG21  | 2.27                     | 0.64              |
| 8:G:77:C:N3       | 8:G:92:G:O6       | 2.30                     | 0.64              |
| 8:G:84:U:H6       | 8:G:84:U:O5'      | 1.81                     | 0.64              |
| 23:V:43:G:N1      | 23:V:438:G:N1     | 2.45                     | 0.64              |
| 23:V:2124:G:H1'   | 25:Y:216:THR:OG1  | 1.98                     | 0.64              |
| 23:V:2794:C:C2    | 23:V:2799:A:N6    | 2.66                     | 0.64              |
| 23:V:43:G:C2      | 23:V:438:G:N3     | 2.65                     | 0.64              |
| 23:V:972:G:OP1    | 23:V:974:G:OP2    | 2.16                     | 0.64              |
| 23:V:2814:C:O2'   | 50:x:29:THR:OG1   | 2.03                     | 0.64              |
| 23:V:374:A:H8     | 23:V:374:A:O5'    | 1.80                     | 0.64              |
| 23:V:573:G:N1     | 23:V:2031:A:OP2   | 2.29                     | 0.64              |
| 23:V:852:G:C2     | 23:V:853:G:C5     | 2.86                     | 0.64              |
| 30:d:25:LYS:HG3   | 30:d:34:GLU:HA    | 1.80                     | 0.64              |
| 8:G:1310:G:H1     | 8:G:1327:C:H42    | 1.46                     | 0.63              |
| 23:V:270(W):G:C5  | 23:V:270(X):G:C8  | 2.85                     | 0.63              |
| 23:V:1869:G:N2    | 23:V:1872:A:OP2   | 2.30                     | 0.63              |
| 55:DD:33:OMC:H3'  | 55:DD:34:A:H5''   | 1.80                     | 0.63              |
| 8:G:474:G:OP2     | 22:U:75:ARG:NE    | 2.31                     | 0.63              |
| 23:V:270(S):G:C2  | 23:V:270(T):G:N7  | 2.66                     | 0.63              |
| 23:V:270(U):C:H2' | 23:V:270(V):G:C1' | 2.29                     | 0.63              |
| 23:V:402:A:H8     | 23:V:402:A:O5'    | 1.82                     | 0.63              |
| 23:V:923:C:N4     | 23:V:924:C:H42    | 1.95                     | 0.63              |
| 23:V:1106:G:C2'   | 23:V:1107:G:O5'   | 2.46                     | 0.63              |
| 23:V:1106:G:H2'   | 23:V:1107:G:O4'   | 1.98                     | 0.63              |
| 23:V:2127:G:C2    | 23:V:2163:C:O4'   | 2.51                     | 0.63              |
| 23:V:2224:G:H8    | 23:V:2224:G:O5'   | 1.80                     | 0.63              |
| 23:V:2626:C:H6    | 23:V:2626:C:O5'   | 1.81                     | 0.63              |
| 23:V:489:G:N7     | 23:V:1284:A:C2    | 2.66                     | 0.63              |
| 25:Y:74:VAL:HA    | 25:Y:112:ALA:O    | 1.97                     | 0.63              |
| 27:a:45:THR:HG21  | 27:a:79:ARG:HG3   | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:1129:C:N3     | 8:G:1143:G:N2     | 2.46                     | 0.63              |
| 23:V:10:G:H2'     | 23:V:11:G:N3      | 2.14                     | 0.63              |
| 30:d:25:LYS:HE3   | 30:d:34:GLU:HB3   | 1.79                     | 0.63              |
| 32:f:20:ALA:CB    | 32:f:21:PRO:HD3   | 2.25                     | 0.63              |
| 23:V:2197:U:O4    | 23:V:2224:G:C5    | 2.52                     | 0.63              |
| 23:V:2637:U:O4    | 23:V:2782:G:O6    | 2.17                     | 0.63              |
| 38:l:24:LEU:O     | 38:l:87:PHE:CE1   | 2.51                     | 0.63              |
| 19:R:24:GLY:O     | 19:R:29:ARG:NH1   | 2.32                     | 0.63              |
| 23:V:271(B):U:O4  | 23:V:404:C:C2     | 2.52                     | 0.63              |
| 23:V:1479:G:H2'   | 23:V:1480:G:N7    | 2.13                     | 0.63              |
| 23:V:1534:G:N2    | 23:V:1538:G:C6    | 2.66                     | 0.63              |
| 23:V:2064:C:H42   | 23:V:2446:G:H1    | 1.46                     | 0.63              |
| 32:f:44:ALA:N     | 32:f:67:PHE:HD1   | 1.97                     | 0.63              |
| 54:BB:16:VAL:HG22 | 54:BB:25:VAL:HG22 | 1.81                     | 0.63              |
| 12:K:76:ILE:HG13  | 12:K:142:LEU:HD11 | 1.78                     | 0.63              |
| 23:V:97:C:H4'     | 47:u:47:ASP:CG    | 2.22                     | 0.63              |
| 32:f:93:ARG:NH2   | 32:f:137:GLU:OE2  | 2.32                     | 0.63              |
| 38:l:9:ARG:O      | 38:l:12:PHE:HD1   | 1.80                     | 0.63              |
| 23:V:701:G:H1     | 23:V:731:C:H42    | 1.46                     | 0.63              |
| 23:V:2813:A:H2    | 23:V:2888:C:C2    | 2.14                     | 0.63              |
| 25:Y:163:PHE:HB3  | 25:Y:171:ILE:HD11 | 1.80                     | 0.63              |
| 11:J:11:LEU:HD13  | 11:J:66:ARG:HD2   | 1.81                     | 0.63              |
| 23:V:1660:C:O3'   | 23:V:2712:U:O4    | 2.17                     | 0.63              |
| 24:X:88:C:H3'     | 24:X:89:G:N7      | 2.14                     | 0.63              |
| 1:W:19:U:C1'      | 1:W:20:U:P        | 2.85                     | 0.62              |
| 3:B:34:TYR:HB2    | 3:B:73:ALA:HB2    | 1.81                     | 0.62              |
| 8:G:69:G:N2       | 8:G:101:A:C4      | 2.66                     | 0.62              |
| 23:V:270(E):G:H2' | 23:V:270(F):U:C6  | 2.34                     | 0.62              |
| 23:V:489:G:C5     | 23:V:1284:A:C2    | 2.87                     | 0.62              |
| 23:V:1173:G:H3'   | 23:V:1173:G:N3    | 2.14                     | 0.62              |
| 43:q:73:ARG:HH12  | 43:q:76:ARG:HH21  | 1.45                     | 0.62              |
| 23:V:138:G:O6     | 43:q:41:ASN:OD1   | 2.17                     | 0.62              |
| 23:V:270(L):U:H2' | 23:V:270(L):U:O2  | 1.98                     | 0.62              |
| 23:V:1782:C:H6    | 23:V:1782:C:H5''  | 1.63                     | 0.62              |
| 32:f:68:VAL:O     | 32:f:69:THR:HB    | 1.99                     | 0.62              |
| 32:f:86:LYS:NZ    | 32:f:134:MET:SD   | 2.71                     | 0.62              |
| 35:i:49:ARG:O     | 35:i:49:ARG:HG3   | 1.98                     | 0.62              |
| 8:G:69:G:N2       | 8:G:101:A:C2      | 2.58                     | 0.62              |
| 8:G:500:G:C5      | 8:G:546:G:N2      | 2.66                     | 0.62              |
| 23:V:96:G:C5'     | 47:u:43:HIS:HE1   | 2.10                     | 0.62              |
| 23:V:1791:A:N6    | 23:V:1828:G:O2'   | 2.32                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:464:G:N1      | 8:G:466:C:H4'     | 2.14                     | 0.62              |
| 23:V:95:G:C2'     | 23:V:96:G:C1'     | 2.67                     | 0.62              |
| 23:V:269:U:H3'    | 23:V:270(Y):G:O2' | 2.00                     | 0.62              |
| 23:V:1726:G:H2'   | 23:V:1726:G:N3    | 2.13                     | 0.62              |
| 23:V:2096:U:O5'   | 23:V:2096:U:H6    | 1.81                     | 0.62              |
| 29:c:82:LEU:O     | 29:c:83:ARG:HB2   | 1.98                     | 0.62              |
| 8:G:1203:C:C4'    | 20:S:27:CYS:CB    | 2.72                     | 0.62              |
| 23:V:270(I):G:H2' | 23:V:270(J):G:O4' | 2.00                     | 0.62              |
| 24:X:89(A):A:O5'  | 24:X:89(A):A:H8   | 1.81                     | 0.62              |
| 25:Y:153:ILE:HA   | 25:Y:156:ILE:HG13 | 1.82                     | 0.62              |
| 8:G:69:G:C2       | 8:G:101:A:N1      | 2.64                     | 0.62              |
| 23:V:270(X):G:H4' | 23:V:272:G:O3'    | 1.99                     | 0.62              |
| 23:V:1857:G:H21   | 23:V:1885:A:H62   | 1.47                     | 0.62              |
| 51:y:45:LYS:HD2   | 51:y:47:THR:HG22  | 1.80                     | 0.62              |
| 15:N:113:SER:HB3  | 15:N:132:GLU:HB3  | 1.80                     | 0.62              |
| 23:V:1090:U:O4    | 23:V:1103:A:N6    | 2.32                     | 0.62              |
| 23:V:1614:A:N6    | 42:p:91:GLY:O     | 2.33                     | 0.62              |
| 23:V:2637:U:N3    | 23:V:2782:G:N1    | 2.47                     | 0.62              |
| 23:V:2710:C:O2'   | 23:V:2711:A:H5'   | 1.99                     | 0.62              |
| 30:d:23:ARG:HB3   | 30:d:36:PRO:HA    | 1.79                     | 0.62              |
| 30:d:27:LYS:HE3   | 30:d:32:GLU:OE1   | 1.98                     | 0.62              |
| 8:G:662:G:N2      | 8:G:663:A:N1      | 2.47                     | 0.62              |
| 23:V:139:G:H8     | 23:V:139:G:O5'    | 1.81                     | 0.62              |
| 23:V:2794:C:O2    | 23:V:2799:A:C6    | 2.52                     | 0.62              |
| 41:o:2:PHE:HB2    | 41:o:43:GLU:HB3   | 1.82                     | 0.62              |
| 8:G:837:G:H8      | 8:G:837:G:O5'     | 1.81                     | 0.62              |
| 23:V:95:G:N1      | 23:V:96:G:N3      | 2.47                     | 0.62              |
| 23:V:2123:G:H2'   | 25:Y:218:MET:HG2  | 1.81                     | 0.62              |
| 23:V:2123:G:O3'   | 25:Y:217:THR:HB   | 2.00                     | 0.62              |
| 23:V:2226:C:H5    | 23:V:2227:A:N7    | 1.95                     | 0.62              |
| 23:V:2787:C:OP1   | 27:a:64:LYS:NZ    | 2.33                     | 0.62              |
| 30:d:26:VAL:O     | 30:d:26:VAL:HG12  | 1.99                     | 0.62              |
| 23:V:1203:G:O6    | 23:V:1241:A:N7    | 2.32                     | 0.62              |
| 23:V:2805:G:N2    | 23:V:2892:A:N6    | 2.40                     | 0.62              |
| 8:G:546:G:HO2'    | 8:G:548:G:HO2'    | 1.46                     | 0.61              |
| 23:V:1049:C:N3    | 23:V:1050:A:N6    | 2.48                     | 0.61              |
| 23:V:1627:G:H2'   | 23:V:1628:G:H5'   | 1.82                     | 0.61              |
| 45:s:30:ASN:CG    | 45:s:89:PHE:CD1   | 2.77                     | 0.61              |
| 23:V:280:C:C2     | 23:V:283:A:C8     | 2.87                     | 0.61              |
| 23:V:1565:C:N4    | 26:Z:84:TYR:OH    | 2.30                     | 0.61              |
| 23:V:1731:G:H8    | 23:V:1731:G:OP1   | 1.83                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:f:86:LYS:HD2    | 32:f:94:GLU:O     | 2.00                     | 0.61              |
| 23:V:854:G:H8      | 23:V:854:G:O5'    | 1.84                     | 0.61              |
| 23:V:1169:G:C2'    | 23:V:1170:G:H8    | 1.99                     | 0.61              |
| 23:V:1807:G:H21    | 23:V:1810:A:H2    | 1.47                     | 0.61              |
| 23:V:2197:U:N3     | 23:V:2224:G:C2    | 2.69                     | 0.61              |
| 8:G:1170:A:H8      | 8:G:1170:A:O5'    | 1.83                     | 0.61              |
| 23:V:274:G:H2'     | 23:V:275:G:H5'    | 1.82                     | 0.61              |
| 23:V:2887:U:O5'    | 23:V:2887:U:H6    | 1.82                     | 0.61              |
| 27:a:47:VAL:HG21   | 27:a:79:ARG:HH11  | 1.65                     | 0.61              |
| 38:l:97:ARG:HH11   | 38:l:97:ARG:CG    | 2.13                     | 0.61              |
| 44:r:84:ARG:HD2    | 44:r:86:ARG:HB3   | 1.83                     | 0.61              |
| 8:G:474:G:C5'      | 22:U:75:ARG:NH2   | 2.42                     | 0.61              |
| 8:G:1448:C:C5      | 8:G:1449:C:C5     | 2.88                     | 0.61              |
| 8:G:1137:C:O2'     | 8:G:1138:G:N2     | 2.34                     | 0.61              |
| 23:V:95:G:N1       | 23:V:96:G:C2      | 2.69                     | 0.61              |
| 23:V:151:C:O2      | 23:V:176:G:N2     | 2.33                     | 0.61              |
| 23:V:931:G:N7      | 23:V:932:G:O2'    | 2.32                     | 0.61              |
| 23:V:1056:G:H4'    | 31:e:31:GLY:HA2   | 1.82                     | 0.61              |
| 23:V:1173:G:C1'    | 23:V:1177:A:H62   | 1.93                     | 0.61              |
| 23:V:1786:A:H1'    | 23:V:1938:A:N6    | 2.16                     | 0.61              |
| 23:V:2466:C:H5''   | 54:BB:5:ALA:HB3   | 1.83                     | 0.61              |
| 23:V:2837:G:H8     | 23:V:2837:G:O5'   | 1.83                     | 0.61              |
| 29:c:71:THR:O      | 29:c:87:PRO:HA    | 1.99                     | 0.61              |
| 45:s:89:PHE:CE2    | 45:s:95:PRO:HG3   | 2.35                     | 0.61              |
| 23:V:270(U):C:H2'  | 23:V:270(V):G:H1' | 1.82                     | 0.61              |
| 23:V:273:G:H2'     | 23:V:273(A):G:H8  | 1.66                     | 0.61              |
| 23:V:2098:U:H2'    | 23:V:2099:U:C5    | 2.36                     | 0.61              |
| 8:G:1413:A:O5'     | 8:G:1413:A:H8     | 1.82                     | 0.61              |
| 23:V:270(B):A:H1'  | 23:V:270(C):C:H5  | 1.62                     | 0.61              |
| 23:V:270(B):A:HO2' | 23:V:270(C):C:H6  | 1.47                     | 0.61              |
| 23:V:2124:G:H8     | 25:Y:217:THR:C    | 1.61                     | 0.61              |
| 23:V:1786:A:H1'    | 23:V:1938:A:H62   | 1.66                     | 0.61              |
| 23:V:2719:G:O5'    | 23:V:2719:G:H8    | 1.83                     | 0.61              |
| 24:X:43:C:O2       | 29:c:95:ARG:NH1   | 2.33                     | 0.61              |
| 43:q:25:LYS:HA     | 43:q:81:VAL:O     | 2.00                     | 0.61              |
| 8:G:273:A:H8       | 8:G:273:A:O5'     | 1.84                     | 0.61              |
| 8:G:1483:A:OP2     | 8:G:1484:C:N4     | 2.34                     | 0.61              |
| 23:V:1081:U:O2     | 32:f:116:ASN:ND2  | 2.34                     | 0.61              |
| 23:V:2123:G:N2     | 23:V:2176:A:H61   | 1.97                     | 0.61              |
| 29:c:44:GLY:HA2    | 29:c:88:ILE:HD13  | 1.83                     | 0.61              |
| 29:c:44:GLY:CA     | 29:c:88:ILE:CD1   | 2.79                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:I:153:VAL:HG12 | 10:I:198:VAL:HG12  | 1.82                     | 0.60              |
| 23:V:95:G:H3'     | 23:V:96:G:O4'      | 2.00                     | 0.60              |
| 23:V:265:A:C2     | 23:V:281:G:N2      | 2.66                     | 0.60              |
| 23:V:1467:C:N4    | 23:V:1545(A):A:C8  | 2.69                     | 0.60              |
| 23:V:1870:C:H2'   | 23:V:1871:A:C8     | 2.36                     | 0.60              |
| 23:V:1871:A:H8    | 23:V:1871:A:O5'    | 1.84                     | 0.60              |
| 24:X:57:A:O2'     | 29:c:30:GLU:CB     | 2.48                     | 0.60              |
| 25:Y:27:HIS:HA    | 25:Y:30:LYS:HD3    | 1.84                     | 0.60              |
| 25:Y:56:GLN:NE2   | 25:Y:203:GLY:O     | 2.33                     | 0.60              |
| 4:C:79:ARG:NH2    | 8:G:263:A:OP2      | 2.33                     | 0.60              |
| 8:G:1448:C:C4     | 8:G:1449:C:C5      | 2.89                     | 0.60              |
| 23:V:1545:A:C2'   | 23:V:1545(A):A:H4' | 2.31                     | 0.60              |
| 36:j:63:LYS:NZ    | 45:s:173:ALA:O     | 2.33                     | 0.60              |
| 8:G:500:G:N1      | 8:G:546:G:N3       | 2.49                     | 0.60              |
| 23:V:1467:C:C4    | 23:V:1545(A):A:N7  | 2.69                     | 0.60              |
| 23:V:1710:C:C2    | 23:V:1711:C:N3     | 2.69                     | 0.60              |
| 23:V:2123:G:O2'   | 25:Y:217:THR:O     | 2.18                     | 0.60              |
| 2:A:66:SER:H      | 8:G:265:G:H4'      | 1.67                     | 0.60              |
| 8:G:226:G:H4'     | 8:G:226:G:OP1      | 2.02                     | 0.60              |
| 8:G:538:G:OP2     | 18:Q:115:LYS:NZ    | 2.35                     | 0.60              |
| 8:G:1202:G:H1'    | 20:S:42:ILE:HD12   | 1.83                     | 0.60              |
| 23:V:741:G:N1     | 23:V:757:U:O2      | 2.33                     | 0.60              |
| 23:V:924:C:H6     | 23:V:924:C:O5'     | 1.83                     | 0.60              |
| 23:V:2128:C:C5'   | 25:Y:6:ARG:HB3     | 2.30                     | 0.60              |
| 33:g:22:THR:O     | 33:g:26:LEU:HB3    | 2.01                     | 0.60              |
| 38:l:24:LEU:O     | 38:l:87:PHE:CD1    | 2.54                     | 0.60              |
| 3:B:45:SER:H      | 3:B:51:LEU:HD11    | 1.67                     | 0.60              |
| 8:G:465:A:H62     | 8:G:467:G:H21      | 1.47                     | 0.60              |
| 8:G:542:G:OP1     | 11:J:10:ARG:NH2    | 2.34                     | 0.60              |
| 23:V:295:G:H1     | 23:V:343:C:H42     | 1.49                     | 0.60              |
| 23:V:1171:G:C2    | 23:V:1178:C:N3     | 2.46                     | 0.60              |
| 23:V:2128:C:O5'   | 23:V:2128:C:H6     | 1.85                     | 0.60              |
| 27:a:12:THR:HA    | 27:a:22:PRO:HD2    | 1.83                     | 0.60              |
| 38:l:9:ARG:HA     | 38:l:12:PHE:CD1    | 2.36                     | 0.60              |
| 23:V:676:A:H8     | 23:V:2069:G:H21    | 1.50                     | 0.60              |
| 23:V:884:C:C5'    | 23:V:892:G:H22     | 2.13                     | 0.60              |
| 23:V:904:C:O2     | 45:s:122:ARG:NH2   | 2.33                     | 0.60              |
| 23:V:1128:A:N7    | 23:V:2518:A:N6     | 2.48                     | 0.60              |
| 32:f:52:ILE:HG13  | 32:f:76:TYR:CE2    | 2.36                     | 0.60              |
| 1:W:17:U:H6       | 1:W:17:U:O5'       | 1.84                     | 0.60              |
| 8:G:138:G:C4      | 8:G:226:G:C2       | 2.90                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:1710:C:C4     | 23:V:1711:C:N4    | 2.70                     | 0.60              |
| 23:V:1782:C:C5'    | 23:V:1782:C:C6    | 2.84                     | 0.60              |
| 32:f:22:PRO:CD     | 32:f:23:VAL:N     | 2.56                     | 0.60              |
| 55:DD:32:G:H5'     | 55:DD:33:OMC:OP2  | 2.01                     | 0.60              |
| 55:DD:37:U:H2'     | 55:DD:38:A:C5'    | 2.32                     | 0.60              |
| 8:G:1349:A:H62     | 8:G:1373:G:H21    | 1.50                     | 0.60              |
| 23:V:540:G:H2'     | 23:V:541:C:H6     | 1.66                     | 0.60              |
| 23:V:552:G:N3      | 23:V:553:U:C2     | 2.70                     | 0.60              |
| 23:V:660:G:H21     | 35:i:15:ARG:HH21  | 1.50                     | 0.60              |
| 39:m:54:ARG:HG3    | 39:m:64:ARG:HG3   | 1.83                     | 0.60              |
| 23:V:2630:G:C2     | 23:V:2790:A:H2    | 2.17                     | 0.60              |
| 32:f:105:LEU:O     | 32:f:108:ALA:C    | 2.45                     | 0.60              |
| 41:o:37:VAL:HB     | 41:o:60:GLU:HB3   | 1.83                     | 0.60              |
| 8:G:1308:U:OP2     | 19:R:98:VAL:HB    | 2.02                     | 0.59              |
| 23:V:832:G:C2'     | 35:i:52:GLU:HG3   | 2.31                     | 0.59              |
| 23:V:2631:G:H8     | 23:V:2631:G:O5'   | 1.84                     | 0.59              |
| 32:f:23:VAL:CG1    | 32:f:35:MET:HB2   | 2.31                     | 0.59              |
| 23:V:270(X):G:C3'  | 23:V:270(Y):G:H5' | 2.31                     | 0.59              |
| 23:V:1449(A):G:O2' | 23:V:1450:C:O5'   | 2.20                     | 0.59              |
| 23:V:1543:A:C8     | 23:V:1544:C:H1'   | 2.37                     | 0.59              |
| 23:V:2128:C:H5''   | 25:Y:6:ARG:HB2    | 1.81                     | 0.59              |
| 45:s:89:PHE:HE2    | 45:s:95:PRO:HG3   | 1.66                     | 0.59              |
| 23:V:879:G:C2      | 23:V:898:C:C2     | 2.90                     | 0.59              |
| 23:V:1543:A:N7     | 23:V:1544:C:H1'   | 2.17                     | 0.59              |
| 30:d:16:SER:C      | 30:d:17:VAL:CG2   | 2.46                     | 0.59              |
| 45:s:30:ASN:OD1    | 45:s:89:PHE:CD1   | 2.55                     | 0.59              |
| 8:G:714:G:H21      | 8:G:777:A:H1'     | 1.67                     | 0.59              |
| 23:V:270(Z):U:C4   | 23:V:271(B):U:H1' | 2.37                     | 0.59              |
| 8:G:1252:A:H61     | 8:G:1285:A:H61    | 1.50                     | 0.59              |
| 19:R:102:ARG:HG2   | 19:R:102:ARG:NH1  | 2.12                     | 0.59              |
| 24:X:88:C:H6       | 24:X:88:C:OP1     | 1.85                     | 0.59              |
| 45:s:96:VAL:O      | 45:s:98:MET:HG2   | 2.03                     | 0.59              |
| 6:E:3:LYS:N        | 6:E:74:ILE:O      | 2.34                     | 0.59              |
| 8:G:465:A:N6       | 8:G:467:G:N2      | 2.50                     | 0.59              |
| 8:G:1359:C:HO2'    | 8:G:1360:A:P      | 2.25                     | 0.59              |
| 23:V:95:G:H2'      | 23:V:96:G:C2'     | 2.33                     | 0.59              |
| 23:V:273(B):C:H2'  | 23:V:273(C):C:H6  | 1.67                     | 0.59              |
| 23:V:536:A:N3      | 23:V:558:G:C2     | 2.61                     | 0.59              |
| 23:V:2129:C:O5'    | 23:V:2129:C:H6    | 1.86                     | 0.59              |
| 10:I:177:THR:HG23  | 10:I:180:ALA:HB2  | 1.83                     | 0.59              |
| 23:V:1539:G:H8     | 23:V:1539:G:O5'   | 1.86                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:X:88:C:H3'     | 24:X:89:G:C8       | 2.36                     | 0.59              |
| 32:f:71:THR:HG21  | 32:f:113:PRO:CG    | 2.33                     | 0.59              |
| 33:g:22:THR:O     | 33:g:26:LEU:HB2    | 2.02                     | 0.59              |
| 45:s:69:THR:HG23  | 45:s:89:PHE:H      | 1.66                     | 0.59              |
| 2:A:67:LYS:NZ     | 8:G:253:U:OP1      | 2.36                     | 0.59              |
| 8:G:1447:G:H8     | 8:G:1447:G:OP1     | 1.85                     | 0.59              |
| 14:M:54:THR:OG1   | 14:M:56:GLN:NE2    | 2.36                     | 0.59              |
| 23:V:373:U:O4'    | 23:V:400:G:N2      | 2.36                     | 0.59              |
| 23:V:1398:C:O3'   | 43:q:25:LYS:NZ     | 2.35                     | 0.59              |
| 23:V:1864:U:H2'   | 23:V:1869:G:C8     | 2.37                     | 0.59              |
| 23:V:2126:A:H4'   | 23:V:2127:G:OP1    | 2.02                     | 0.59              |
| 8:G:828:A:H62     | 8:G:858:G:H21      | 1.48                     | 0.59              |
| 23:V:552:G:C5     | 23:V:553:U:C4      | 2.90                     | 0.59              |
| 23:V:1252:G:N7    | 40:n:36:ARG:NH1    | 2.51                     | 0.59              |
| 23:V:2809:A:N1    | 27:a:60:ASN:CG     | 2.61                     | 0.59              |
| 29:c:80:PHE:O     | 29:c:82:LEU:N      | 2.35                     | 0.59              |
| 32:f:23:VAL:HG12  | 32:f:35:MET:HB2    | 1.84                     | 0.59              |
| 38:l:25:ARG:CA    | 38:l:87:PHE:CZ     | 2.85                     | 0.59              |
| 55:DD:35:C:H2'    | 55:DD:36:A:C8      | 2.37                     | 0.59              |
| 8:G:1454:G:H2'    | 8:G:1455:G:C8      | 2.38                     | 0.59              |
| 17:P:33:THR:HA    | 17:P:39:PRO:HA     | 1.85                     | 0.59              |
| 20:S:25:VAL:HG13  | 20:S:25:VAL:O      | 2.02                     | 0.59              |
| 23:V:972:G:H2'    | 23:V:973:A:OP1     | 2.02                     | 0.59              |
| 23:V:2334:G:H1'   | 38:l:15:ARG:NE     | 2.10                     | 0.59              |
| 23:V:2126:A:N6    | 23:V:2164:C:OP2    | 2.35                     | 0.58              |
| 32:f:105:LEU:O    | 32:f:108:ALA:O     | 2.21                     | 0.58              |
| 45:s:94:GLU:O     | 45:s:96:VAL:HG23   | 2.03                     | 0.58              |
| 8:G:129(A):G:N3   | 8:G:191(A):G:N7    | 2.49                     | 0.58              |
| 8:G:1135:U:H2'    | 8:G:1137:C:H1'     | 1.86                     | 0.58              |
| 19:R:20:THR:HG23  | 19:R:26:GLY:HA2    | 1.85                     | 0.58              |
| 23:V:153:C:H2'    | 23:V:154:G:N9      | 2.16                     | 0.58              |
| 23:V:265:A:C2     | 23:V:281:G:C2      | 2.91                     | 0.58              |
| 23:V:270(E):G:OP2 | 23:V:270(E):G:H8   | 1.86                     | 0.58              |
| 23:V:270(X):G:N2  | 23:V:270(Y):G:HO2' | 2.02                     | 0.58              |
| 23:V:2821:A:OP2   | 37:k:2:ARG:NH2     | 2.36                     | 0.58              |
| 25:Y:15:ASP:OD2   | 25:Y:17:ASN:ND2    | 2.36                     | 0.58              |
| 29:c:84:LYS:HG3   | 29:c:84:LYS:O      | 2.03                     | 0.58              |
| 8:G:467:G:H8      | 8:G:467:G:O5'      | 1.85                     | 0.58              |
| 8:G:511:C:O2'     | 11:J:43:HIS:NE2    | 2.36                     | 0.58              |
| 18:Q:86:ARG:HH21  | 18:Q:99:HIS:HE1    | 1.51                     | 0.58              |
| 23:V:270(C):C:N4  | 23:V:270(D):C:N4   | 2.51                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:1169:G:C2    | 23:V:1170:G:C6    | 2.91                     | 0.58              |
| 23:V:270(V):G:H2' | 23:V:270(W):G:C8  | 2.38                     | 0.58              |
| 1:W:17:U:C2'      | 1:W:18:G:H5'      | 2.34                     | 0.58              |
| 20:S:25:VAL:HG12  | 20:S:39:LEU:HD23  | 1.86                     | 0.58              |
| 23:V:293:U:H3     | 23:V:346:A:H61    | 1.52                     | 0.58              |
| 23:V:1466:G:H2'   | 23:V:1547:C:N4    | 2.18                     | 0.58              |
| 23:V:1470:G:N2    | 23:V:1520:U:O2    | 2.36                     | 0.58              |
| 39:m:55:ASN:HA    | 39:m:64:ARG:HG2   | 1.85                     | 0.58              |
| 55:DD:7:G:H3'     | 55:DD:8:4SU:H5'   | 1.85                     | 0.58              |
| 8:G:1441:G:H8     | 8:G:1441:G:O5'    | 1.87                     | 0.58              |
| 23:V:1446:C:H6    | 23:V:1447:G:C8    | 2.22                     | 0.58              |
| 23:V:2122:U:H2'   | 23:V:2123:G:O4'   | 2.03                     | 0.58              |
| 27:a:49:LEU:HG    | 27:a:74:PRO:HB3   | 1.84                     | 0.58              |
| 29:c:44:GLY:CA    | 29:c:88:ILE:HD13  | 2.33                     | 0.58              |
| 30:d:31:GLY:HA3   | 30:d:79:VAL:HB    | 1.86                     | 0.58              |
| 8:G:191(E):G:H8   | 8:G:191(E):G:O5'  | 1.87                     | 0.58              |
| 11:J:63:LYS:HE2   | 11:J:198:VAL:HG12 | 1.85                     | 0.58              |
| 23:V:270(X):G:H4' | 23:V:273:G:H5'    | 1.85                     | 0.58              |
| 23:V:1173:G:O4'   | 23:V:1177:A:N6    | 2.37                     | 0.58              |
| 23:V:1534:G:N2    | 23:V:1538:G:C5    | 2.71                     | 0.58              |
| 23:V:2127:G:N2    | 23:V:2162:G:C2'   | 2.64                     | 0.58              |
| 23:V:2807:G:C8    | 23:V:2891:G:N2    | 2.71                     | 0.58              |
| 25:Y:176:GLY:HA2  | 25:Y:180:PHE:CZ   | 2.38                     | 0.58              |
| 38:l:25:ARG:HB2   | 38:l:87:PHE:CE2   | 2.36                     | 0.58              |
| 23:V:404:C:OP1    | 23:V:406:G:O4'    | 2.22                     | 0.58              |
| 23:V:2785:C:H2'   | 23:V:2786:U:C6    | 2.38                     | 0.58              |
| 32:f:20:ALA:N     | 32:f:22:PRO:HD3   | 2.18                     | 0.58              |
| 20:S:24:CYS:HB3   | 20:S:28:GLY:O     | 2.04                     | 0.58              |
| 23:V:270(B):A:O2' | 23:V:270(C):C:H6  | 1.86                     | 0.58              |
| 23:V:535:C:H6     | 23:V:535:C:O5'    | 1.87                     | 0.58              |
| 23:V:1785:A:H2    | 23:V:2588:G:H21   | 1.52                     | 0.58              |
| 23:V:2124:G:P     | 25:Y:218:MET:N    | 2.77                     | 0.58              |
| 23:V:2335:A:OP1   | 38:l:12:PHE:HB3   | 2.03                     | 0.58              |
| 35:i:58:THR:O     | 53:AA:13:ARG:NH1  | 2.37                     | 0.58              |
| 1:W:16:A:H2       | 1:W:17:U:O2       | 1.82                     | 0.58              |
| 8:G:129(A):G:C2   | 8:G:191(A):G:C8   | 2.91                     | 0.58              |
| 10:I:150:LYS:HB3  | 10:I:201:TYR:HB2  | 1.84                     | 0.58              |
| 23:V:552:G:N3     | 23:V:553:U:O2     | 2.36                     | 0.58              |
| 23:V:1441:G:C6    | 23:V:1442:G:C6    | 2.91                     | 0.58              |
| 23:V:1939:U:H3'   | 23:V:1940:U:C5'   | 2.33                     | 0.58              |
| 23:V:2076:U:OP1   | 26:Z:244:ARG:NH2  | 2.37                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:2127:G:H21   | 23:V:2162:G:H2'   | 1.69                     | 0.58              |
| 23:V:2636:U:H4'   | 27:a:79:ARG:HD2   | 1.86                     | 0.58              |
| 25:Y:89:ALA:HB2   | 25:Y:154:ARG:HG3  | 1.85                     | 0.58              |
| 32:f:48:MET:SD    | 32:f:69:THR:HG22  | 2.41                     | 0.58              |
| 35:i:65:ARG:HD2   | 53:AA:11:LYS:HA   | 1.84                     | 0.58              |
| 38:l:15:ARG:HG2   | 38:l:15:ARG:HH21  | 1.69                     | 0.58              |
| 8:G:448:A:OP2     | 8:G:485:G:N2      | 2.37                     | 0.57              |
| 8:G:1309:G:N2     | 8:G:1328:C:N1     | 2.51                     | 0.57              |
| 23:V:270(V):G:C6  | 23:V:270(W):G:O6  | 2.57                     | 0.57              |
| 23:V:1093:G:H21   | 23:V:1098:A:N6    | 2.00                     | 0.57              |
| 23:V:1748:G:H2'   | 23:V:1749:A:H8    | 1.67                     | 0.57              |
| 23:V:2197:U:O4    | 23:V:2224:G:C6    | 2.57                     | 0.57              |
| 8:G:778:G:O2'     | 17:P:119:CYS:SG   | 2.60                     | 0.57              |
| 8:G:1415:G:C6     | 8:G:1486:G:O6     | 2.57                     | 0.57              |
| 11:J:15:GLU:OE2   | 11:J:66:ARG:NH2   | 2.36                     | 0.57              |
| 16:O:10:ARG:NE    | 16:O:75:ASP:OD2   | 2.37                     | 0.57              |
| 23:V:856:C:N4     | 23:V:857:C:N4     | 2.52                     | 0.57              |
| 23:V:1192:G:C4    | 23:V:1193:G:H1'   | 2.40                     | 0.57              |
| 23:V:1467:C:N3    | 23:V:1545(A):A:N7 | 2.51                     | 0.57              |
| 44:r:73:ARG:NH2   | 44:r:74:PRO:O     | 2.35                     | 0.57              |
| 49:w:57:GLU:OE1   | 49:w:57:GLU:N     | 2.35                     | 0.57              |
| 15:N:48:TYR:HA    | 15:N:60:ARG:O     | 2.05                     | 0.57              |
| 20:S:9:LYS:NZ     | 20:S:21:TYR:CE1   | 2.72                     | 0.57              |
| 23:V:270(J):G:H2' | 23:V:270(J):G:N3  | 2.18                     | 0.57              |
| 23:V:366:C:OP2    | 23:V:366:C:H6     | 1.87                     | 0.57              |
| 23:V:532:A:N6     | 40:n:45:TYR:OH    | 2.38                     | 0.57              |
| 23:V:552:G:C2'    | 23:V:553:U:H5'    | 2.33                     | 0.57              |
| 23:V:1441:G:C6    | 23:V:1442:G:O6    | 2.57                     | 0.57              |
| 23:V:1493:C:P     | 23:V:2210:G:H1    | 2.27                     | 0.57              |
| 23:V:1859:A:N6    | 23:V:1883:G:O2'   | 2.38                     | 0.57              |
| 29:c:20:ILE:HG23  | 29:c:21:ARG:HE    | 1.70                     | 0.57              |
| 55:DD:22:A:N6     | 55:DD:48:U:H1'    | 2.19                     | 0.57              |
| 6:E:57:LYS:O      | 6:E:60:ARG:NH2    | 2.38                     | 0.57              |
| 8:G:1455:G:O5'    | 8:G:1455:G:H8     | 1.88                     | 0.57              |
| 19:R:87:TYR:OH    | 19:R:91:ARG:NH2   | 2.37                     | 0.57              |
| 23:V:95:G:N3      | 23:V:96:G:H1'     | 2.18                     | 0.57              |
| 23:V:99:U:H3'     | 23:V:99:U:H6      | 1.68                     | 0.57              |
| 23:V:373:U:O4     | 49:w:59:PHE:CE1   | 2.58                     | 0.57              |
| 23:V:852:G:N3     | 23:V:853:G:C8     | 2.71                     | 0.57              |
| 32:f:82:ALA:HB2   | 32:f:99:ILE:HG23  | 1.86                     | 0.57              |
| 23:V:269:U:C5     | 23:V:270(Z):U:OP2 | 2.58                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:V:570:G:OP1   | 23:V:973:A:OP2    | 2.23                     | 0.57              |
| 23:V:885:C:N4    | 23:V:892:G:C6     | 2.67                     | 0.57              |
| 23:V:1106:G:HO2' | 23:V:1107:G:P     | 2.14                     | 0.57              |
| 23:V:1537:C:H3'  | 23:V:1538:G:H8    | 1.70                     | 0.57              |
| 23:V:1630:G:H2'  | 23:V:1630(A):C:O2 | 2.04                     | 0.57              |
| 23:V:2226:C:H3'  | 23:V:2226:C:H6    | 1.69                     | 0.57              |
| 25:Y:28:LEU:O    | 25:Y:32:LEU:HB2   | 2.03                     | 0.57              |
| 29:c:71:THR:CB   | 29:c:88:ILE:N     | 2.64                     | 0.57              |
| 5:D:39:THR:HB    | 5:D:70:LYS:HG2    | 1.87                     | 0.57              |
| 23:V:2124:G:H1'  | 25:Y:216:THR:CB   | 2.34                     | 0.57              |
| 25:Y:39:GLU:H    | 25:Y:178:ALA:HB2  | 1.68                     | 0.57              |
| 29:c:28:VAL:C    | 29:c:30:GLU:H     | 2.12                     | 0.57              |
| 32:f:86:LYS:HB3  | 32:f:95:LYS:CB    | 2.23                     | 0.57              |
| 38:l:9:ARG:HA    | 38:l:12:PHE:CE1   | 2.39                     | 0.57              |
| 47:u:48:LEU:HA   | 47:u:51:GLN:HG2   | 1.86                     | 0.57              |
| 23:V:270(R):G:N2 | 23:V:270(S):G:N3  | 2.52                     | 0.57              |
| 23:V:270(X):G:N2 | 23:V:270(Y):G:O2' | 2.38                     | 0.57              |
| 23:V:1548:C:H6   | 23:V:1548:C:O5'   | 1.88                     | 0.57              |
| 32:f:66:THR:OG1  | 32:f:67:PHE:N     | 2.37                     | 0.57              |
| 8:G:186(A):C:N4  | 8:G:191:G:N1      | 2.52                     | 0.57              |
| 8:G:191(C):G:O5' | 8:G:191(C):G:H8   | 1.88                     | 0.57              |
| 17:P:67:ASP:O    | 17:P:71:LYS:NZ    | 2.37                     | 0.57              |
| 23:V:404:C:H3'   | 23:V:404:C:OP2    | 2.05                     | 0.57              |
| 37:k:86:ARG:NH2  | 37:k:118:GLU:OE1  | 2.38                     | 0.57              |
| 38:l:14:VAL:HG22 | 38:l:89:ARG:HD2   | 1.87                     | 0.57              |
| 47:u:51:GLN:HA   | 47:u:54:ARG:HG2   | 1.87                     | 0.57              |
| 55:DD:30:G:H2'   | 55:DD:31:G:C8     | 2.40                     | 0.57              |
| 55:DD:37:U:H2'   | 55:DD:38:A:H8     | 1.69                     | 0.57              |
| 55:DD:38:A:H2'   | 55:DD:39:A:C8     | 2.40                     | 0.57              |
| 16:O:42:ARG:NH1  | 16:O:71:SER:OG    | 2.37                     | 0.57              |
| 18:Q:53:ARG:NH1  | 18:Q:92:ASP:OD2   | 2.38                     | 0.57              |
| 18:Q:73:GLU:OE2  | 18:Q:113:ARG:NH1  | 2.38                     | 0.57              |
| 23:V:270(J):G:C6 | 23:V:270(K):C:C4  | 2.93                     | 0.57              |
| 23:V:888:C:H4'   | 23:V:889:C:C4'    | 2.35                     | 0.57              |
| 23:V:972:G:H3'   | 23:V:973:A:C3'    | 2.30                     | 0.57              |
| 23:V:2094:G:N2   | 23:V:2095:C:C2    | 2.73                     | 0.57              |
| 25:Y:176:GLY:HA2 | 25:Y:180:PHE:CE2  | 2.40                     | 0.57              |
| 31:e:11:ALA:C    | 31:e:13:LEU:N     | 2.63                     | 0.57              |
| 32:f:19:PRO:C    | 32:f:22:PRO:HD2   | 2.20                     | 0.57              |
| 34:h:47:ILE:O    | 34:h:53:LYS:NZ    | 2.38                     | 0.57              |
| 45:s:96:VAL:O    | 45:s:98:MET:N     | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 56:EE:96:GLN:OE1 | 56:EE:96:GLN:N   | 2.36                     | 0.57              |
| 7:F:7:ARG:NH1    | 8:G:1328:C:OP2   | 2.38                     | 0.57              |
| 8:G:272:C:H6     | 8:G:272:C:O5'    | 1.88                     | 0.57              |
| 9:H:56:ARG:NH1   | 9:H:60:ASP:OD2   | 2.38                     | 0.57              |
| 17:P:22:HIS:HB3  | 17:P:85:ARG:HB2  | 1.87                     | 0.57              |
| 23:V:1056:G:O2'  | 23:V:1084:A:N1   | 2.37                     | 0.57              |
| 23:V:1543:A:C8   | 23:V:1544:C:C1'  | 2.87                     | 0.57              |
| 23:V:2061:G:O2'  | 23:V:2063:C:N4   | 2.38                     | 0.57              |
| 34:h:20:MET:HE2  | 34:h:44:LYS:HE3  | 1.87                     | 0.57              |
| 6:E:47:PHE:CE2   | 20:S:37:PHE:HZ   | 2.24                     | 0.56              |
| 8:G:464:G:C2     | 8:G:466:C:H5'    | 2.40                     | 0.56              |
| 23:V:374:A:C6    | 23:V:401:A:C8    | 2.93                     | 0.56              |
| 23:V:923:C:H2'   | 23:V:924:C:C5    | 2.40                     | 0.56              |
| 23:V:1541:U:O5'  | 23:V:1541:U:H6   | 1.88                     | 0.56              |
| 23:V:2295:C:C6   | 38:l:9:ARG:NH2   | 2.73                     | 0.56              |
| 25:Y:130:ILE:O   | 25:Y:134:ARG:NH1 | 2.39                     | 0.56              |
| 30:d:18:GLU:CG   | 30:d:24:VAL:CB   | 2.79                     | 0.56              |
| 52:z:35:ARG:O    | 52:z:39:ARG:NH1  | 2.38                     | 0.56              |
| 8:G:439:A:C8     | 8:G:496:A:C6     | 2.93                     | 0.56              |
| 23:V:77:C:OP1    | 47:u:54:ARG:NH2  | 2.33                     | 0.56              |
| 23:V:1582:C:H6   | 23:V:1582:C:O5'  | 1.87                     | 0.56              |
| 23:V:1787:A:O5'  | 23:V:1787:A:H8   | 1.87                     | 0.56              |
| 32:f:19:PRO:HB2  | 32:f:23:VAL:CG2  | 2.35                     | 0.56              |
| 5:D:46:GLY:H     | 5:D:62:ILE:HG23  | 1.70                     | 0.56              |
| 8:G:1202:G:H1'   | 20:S:42:ILE:CD1  | 2.34                     | 0.56              |
| 14:M:71:PRO:O    | 14:M:96:GLN:NE2  | 2.39                     | 0.56              |
| 21:T:5:LYS:HE2   | 21:T:9:GLN:HG3   | 1.88                     | 0.56              |
| 23:V:1042:G:N3   | 23:V:1114:G:O6   | 2.39                     | 0.56              |
| 23:V:1447:G:H3'  | 23:V:1448:G:H5'' | 1.87                     | 0.56              |
| 23:V:1550:C:H5'' | 23:V:1727:U:H1'  | 1.87                     | 0.56              |
| 23:V:2127:G:C6   | 23:V:2163:C:H1'  | 2.39                     | 0.56              |
| 23:V:2127:G:N1   | 23:V:2163:C:H1'  | 2.20                     | 0.56              |
| 23:V:2226:C:C6   | 23:V:2227:A:H8   | 2.19                     | 0.56              |
| 23:V:2813:A:C2   | 23:V:2888:C:C2   | 2.90                     | 0.56              |
| 45:s:7:ALA:HB3   | 45:s:36:LYS:O    | 2.05                     | 0.56              |
| 3:B:16:PRO:HB3   | 3:B:54:ARG:HB2   | 1.87                     | 0.56              |
| 8:G:1203:C:H5'   | 20:S:27:CYS:CB   | 2.28                     | 0.56              |
| 18:Q:71:PRO:O    | 18:Q:102:ARG:NH1 | 2.39                     | 0.56              |
| 20:S:9:LYS:NZ    | 20:S:21:TYR:CD1  | 2.69                     | 0.56              |
| 23:V:928:G:O5'   | 23:V:928:G:H8    | 1.88                     | 0.56              |
| 23:V:1143:A:C8   | 23:V:1143:A:C5'  | 2.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:1451:C:H5'   | 23:V:1452:A:H4'   | 1.88                     | 0.56              |
| 23:V:2839:G:H8    | 23:V:2839:G:O5'   | 1.89                     | 0.56              |
| 25:Y:176:GLY:C    | 25:Y:180:PHE:CE1  | 2.83                     | 0.56              |
| 32:f:37:PHE:CZ    | 32:f:62:ASP:OD2   | 2.54                     | 0.56              |
| 1:W:16:A:H2'      | 1:W:16:A:N3       | 2.21                     | 0.56              |
| 8:G:440:A:N6      | 8:G:493:G:N2      | 2.45                     | 0.56              |
| 23:V:270(J):G:H3' | 23:V:270(K):C:H6  | 1.68                     | 0.56              |
| 28:b:11:VAL:HG22  | 28:b:124:LEU:HD23 | 1.87                     | 0.56              |
| 45:s:15:PRO:O     | 45:s:19:ARG:NH1   | 2.39                     | 0.56              |
| 23:V:270(U):C:H2' | 23:V:270(V):G:O4' | 2.06                     | 0.56              |
| 23:V:2124:G:H21   | 25:Y:220:PRO:C    | 2.10                     | 0.56              |
| 23:V:2127:G:N1    | 23:V:2163:C:C1'   | 2.69                     | 0.56              |
| 23:V:2837:G:H2'   | 23:V:2838:G:H8    | 1.70                     | 0.56              |
| 26:Z:54:ARG:O     | 26:Z:218:ARG:NH1  | 2.39                     | 0.56              |
| 27:a:5:LEU:HB3    | 27:a:196:VAL:O    | 2.06                     | 0.56              |
| 6:E:88:LEU:HD12   | 6:E:90:LEU:HD13   | 1.86                     | 0.56              |
| 8:G:1510:U:O2     | 8:G:1526:G:N2     | 2.38                     | 0.56              |
| 12:K:76:ILE:HG23  | 12:K:93:PRO:HB3   | 1.88                     | 0.56              |
| 23:V:707:G:O6     | 23:V:725:G:N2     | 2.38                     | 0.56              |
| 25:Y:22:ILE:O     | 25:Y:26:ALA:CB    | 2.54                     | 0.56              |
| 16:O:28:VAL:HG22  | 16:O:63:ILE:HD11  | 1.88                     | 0.56              |
| 17:P:48:ILE:HD12  | 17:P:63:LEU:HD22  | 1.87                     | 0.56              |
| 23:V:270(K):C:H3' | 23:V:270(L):U:O4' | 2.06                     | 0.56              |
| 23:V:645:C:OP2    | 23:V:2367:G:N2    | 2.39                     | 0.56              |
| 23:V:805:G:N2     | 23:V:829:A:OP1    | 2.39                     | 0.56              |
| 23:V:2206:C:C2    | 23:V:2219:G:N2    | 2.74                     | 0.56              |
| 23:V:2711:A:H8    | 23:V:2711:A:O5'   | 1.88                     | 0.56              |
| 23:V:2805:G:N1    | 23:V:2892:A:N7    | 2.52                     | 0.56              |
| 25:Y:182:PRO:O    | 25:Y:186:ALA:CB   | 2.54                     | 0.56              |
| 30:d:27:LYS:CE    | 30:d:32:GLU:OE2   | 2.54                     | 0.56              |
| 32:f:19:PRO:O     | 32:f:22:PRO:CD    | 2.50                     | 0.56              |
| 23:V:270(X):G:C2  | 23:V:270(Y):G:H1' | 2.41                     | 0.56              |
| 23:V:536:A:N1     | 23:V:558:G:C4     | 2.74                     | 0.56              |
| 23:V:852:G:C2'    | 23:V:853:G:H5'    | 2.36                     | 0.56              |
| 23:V:1175:U:H2'   | 23:V:1176:G:C8    | 2.41                     | 0.56              |
| 23:V:2127:G:H21   | 23:V:2162:G:C2'   | 2.19                     | 0.56              |
| 26:Z:34:VAL:HG13  | 26:Z:35:LYS:HG2   | 1.86                     | 0.56              |
| 36:j:63:LYS:HE2   | 45:s:175:VAL:H    | 1.71                     | 0.56              |
| 55:DD:48:U:O2'    | 55:DD:49:C:C5'    | 2.38                     | 0.56              |
| 11:J:175:SER:HB2  | 11:J:184:LYS:HB3  | 1.87                     | 0.56              |
| 23:V:536:A:C4     | 23:V:558:G:N2     | 2.74                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:2807:G:H8     | 23:V:2891:G:N2    | 2.03                     | 0.56              |
| 23:V:2837:G:N1     | 23:V:2882:A:C2    | 2.74                     | 0.56              |
| 24:X:89:G:H8       | 24:X:89:G:O5'     | 1.89                     | 0.56              |
| 31:e:11:ALA:O      | 31:e:13:LEU:N     | 2.39                     | 0.56              |
| 23:V:16:G:N1       | 23:V:525:U:N3     | 2.35                     | 0.55              |
| 23:V:43:G:C5       | 23:V:438:G:N2     | 2.74                     | 0.55              |
| 23:V:286:C:O2      | 23:V:356:G:N2     | 2.33                     | 0.55              |
| 23:V:863:A:OP1     | 36:j:22:LYS:NZ    | 2.39                     | 0.55              |
| 23:V:1452:A:H5'    | 23:V:1453:A:H4'   | 1.88                     | 0.55              |
| 23:V:2633:G:H8     | 23:V:2633:G:O5'   | 1.88                     | 0.55              |
| 23:V:2785:C:H2'    | 23:V:2786:U:H6    | 1.71                     | 0.55              |
| 23:V:2837:G:N1     | 23:V:2882:A:N1    | 2.54                     | 0.55              |
| 29:c:76:SER:OG     | 29:c:84:LYS:HB3   | 2.06                     | 0.55              |
| 32:f:71:THR:HG23   | 32:f:71:THR:O     | 2.06                     | 0.55              |
| 55:DD:33:OMC:HM23  | 55:DD:33:OMC:O2   | 2.06                     | 0.55              |
| 9:H:168:THR:OG1    | 9:H:191:ASP:O     | 2.24                     | 0.55              |
| 23:V:270(K):C:H5'' | 23:V:270(L):U:C6  | 2.41                     | 0.55              |
| 23:V:280:C:N1      | 23:V:283:A:N7     | 2.54                     | 0.55              |
| 23:V:2226:C:H2'    | 23:V:2227:A:C5'   | 2.37                     | 0.55              |
| 29:c:111:LEU:HD11  | 29:c:120:LEU:HD21 | 1.88                     | 0.55              |
| 35:i:47:ASP:OD2    | 35:i:50:ARG:CD    | 2.47                     | 0.55              |
| 36:j:68:ILE:HG13   | 36:j:103:MET:HG3  | 1.89                     | 0.55              |
| 38:l:17:ARG:HH11   | 38:l:89:ARG:CG    | 2.19                     | 0.55              |
| 8:G:465:A:C5       | 8:G:467:G:N3      | 2.74                     | 0.55              |
| 8:G:591:U:H3       | 8:G:648:A:H61     | 1.55                     | 0.55              |
| 23:V:269:U:O2      | 23:V:269:U:H2'    | 2.06                     | 0.55              |
| 23:V:1106:G:H2'    | 23:V:1107:G:H8    | 1.71                     | 0.55              |
| 23:V:2251:G:OP2    | 36:j:82:ARG:NH2   | 2.40                     | 0.55              |
| 49:w:48:ARG:NH2    | 49:w:65:ASP:OD2   | 2.39                     | 0.55              |
| 4:C:74:LYS:O       | 4:C:76:ALA:N      | 2.35                     | 0.55              |
| 18:Q:69:TYR:HB3    | 18:Q:99:HIS:HB3   | 1.87                     | 0.55              |
| 23:V:270(F):U:C4   | 23:V:270(G):C:C5  | 2.94                     | 0.55              |
| 23:V:2197:U:O2     | 23:V:2197:U:H2'   | 2.06                     | 0.55              |
| 30:d:89:ILE:CG2    | 30:d:129:THR:CG2  | 2.80                     | 0.55              |
| 36:j:16:ARG:HD3    | 36:j:73:PRO:HD2   | 1.88                     | 0.55              |
| 37:k:28:LEU:HD23   | 37:k:48:VAL:HG11  | 1.89                     | 0.55              |
| 44:r:23:ARG:HH12   | 44:r:38:ILE:HB    | 1.71                     | 0.55              |
| 3:B:74:ARG:HH12    | 8:G:719:C:H42     | 1.55                     | 0.55              |
| 23:V:74:A:N1       | 47:u:46:ARG:NH2   | 2.51                     | 0.55              |
| 23:V:569:U:OP2     | 23:V:945:A:N6     | 2.39                     | 0.55              |
| 29:c:71:THR:HA     | 29:c:88:ILE:O     | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B:46:GLU:HB3     | 3:B:85:LEU:HD11    | 1.89                     | 0.55              |
| 8:G:547:A:OP2      | 11:J:2:GLY:N       | 2.39                     | 0.55              |
| 11:J:208:SER:O     | 11:J:209:ARG:NH1   | 2.40                     | 0.55              |
| 23:V:13:A:C2       | 23:V:526:A:N7      | 2.75                     | 0.55              |
| 23:V:884:C:H5'     | 23:V:892:G:N2      | 2.17                     | 0.55              |
| 23:V:1169:G:C4     | 23:V:1170:G:N7     | 2.75                     | 0.55              |
| 23:V:1545:A:H2'    | 23:V:1545(A):A:C4' | 2.36                     | 0.55              |
| 23:V:2097:C:HO2'   | 23:V:2098:U:H5'    | 1.71                     | 0.55              |
| 23:V:2295:C:H6     | 38:l:9:ARG:NH2     | 2.04                     | 0.55              |
| 23:V:2807:G:C8     | 23:V:2891:G:C2     | 2.94                     | 0.55              |
| 32:f:20:ALA:C      | 32:f:22:PRO:HD3    | 2.31                     | 0.55              |
| 8:G:1128:C:O2'     | 8:G:1130:A:N7      | 2.39                     | 0.55              |
| 10:I:20:SER:HA     | 10:I:57:ILE:O      | 2.06                     | 0.55              |
| 27:a:12:THR:OG1    | 27:a:19:ARG:NH1    | 2.40                     | 0.55              |
| 39:m:53:ARG:HH21   | 39:m:54:ARG:HD2    | 1.72                     | 0.55              |
| 55:DD:48:U:H3'     | 55:DD:48:U:H6      | 1.72                     | 0.55              |
| 8:G:537:G:OP1      | 18:Q:113:ARG:NH2   | 2.38                     | 0.55              |
| 23:V:270(E):G:OP2  | 23:V:270(E):G:C8   | 2.60                     | 0.55              |
| 23:V:274:G:N3      | 23:V:274:G:O5'     | 2.40                     | 0.55              |
| 23:V:771:G:HO2'    | 23:V:1355:G:HO2'   | 1.55                     | 0.55              |
| 23:V:975:G:H8      | 23:V:975:G:O5'     | 1.89                     | 0.55              |
| 23:V:1447:G:H2'    | 23:V:1447:G:N3     | 2.22                     | 0.55              |
| 23:V:1589:C:H2'    | 23:V:1590:U:H6     | 1.71                     | 0.55              |
| 23:V:1711:C:H3'    | 23:V:1711:C:H6     | 1.72                     | 0.55              |
| 23:V:1716:U:H6     | 23:V:1716:U:H3'    | 1.72                     | 0.55              |
| 23:V:2757:A:H8     | 23:V:2758:A:H5'    | 1.72                     | 0.55              |
| 25:Y:114:VAL:HG11  | 25:Y:152:ILE:HG21  | 1.89                     | 0.55              |
| 34:h:70:LYS:HG3    | 34:h:72:PRO:HD2    | 1.87                     | 0.55              |
| 11:J:125:HIS:HA    | 11:J:149:ALA:HB3   | 1.89                     | 0.55              |
| 23:V:137(A):G:O6   | 23:V:142:G:C6      | 2.56                     | 0.55              |
| 23:V:270(Y):G:H5'' | 23:V:270(Z):U:OP1  | 2.06                     | 0.55              |
| 23:V:271(C):G:N3   | 23:V:272:G:C8      | 2.75                     | 0.55              |
| 23:V:1084:A:O2'    | 23:V:1105:U:H2'    | 2.07                     | 0.55              |
| 23:V:2096:U:O2     | 23:V:2194:G:N2     | 2.40                     | 0.55              |
| 23:V:2802:G:H8     | 23:V:2802:G:O5'    | 1.90                     | 0.55              |
| 23:V:2893:G:H4'    | 23:V:2893:G:OP1    | 2.07                     | 0.55              |
| 8:G:497:U:O2       | 8:G:497:U:H2'      | 2.06                     | 0.55              |
| 8:G:1440:C:C2'     | 8:G:1441:G:H5'     | 2.31                     | 0.55              |
| 23:V:926:A:H8      | 23:V:926:A:O5'     | 1.89                     | 0.55              |
| 23:V:1093:G:H21    | 23:V:1098:A:H62    | 1.55                     | 0.55              |
| 23:V:1155:A:H5'    | 40:n:55:ARG:HD3    | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:2108:C:O2'   | 23:V:2181:G:N2    | 2.40                     | 0.55              |
| 30:d:13:LYS:HE2   | 30:d:28:GLY:HA3   | 1.88                     | 0.55              |
| 35:i:41:ARG:NH2   | 35:i:45:LEU:HD13  | 2.22                     | 0.55              |
| 23:V:536:A:C2     | 23:V:558:G:C4     | 2.95                     | 0.54              |
| 23:V:552:G:C4     | 23:V:553:U:C2     | 2.94                     | 0.54              |
| 23:V:905:U:O2     | 45:s:121:HIS:NE2  | 2.40                     | 0.54              |
| 23:V:1646:C:H5''  | 23:V:1647:G:H5''  | 1.89                     | 0.54              |
| 23:V:1864:U:H2'   | 23:V:1869:G:H8    | 1.72                     | 0.54              |
| 23:V:2210:G:H5'   | 23:V:2211:G:OP2   | 2.07                     | 0.54              |
| 23:V:2827:C:H6    | 23:V:2827:C:O5'   | 1.90                     | 0.54              |
| 25:Y:176:GLY:CA   | 25:Y:180:PHE:CD1  | 2.89                     | 0.54              |
| 28:b:192:LEU:HD21 | 28:b:194:MET:HE3  | 1.90                     | 0.54              |
| 49:w:5:ILE:HG22   | 49:w:7:PRO:HD2    | 1.90                     | 0.54              |
| 23:V:270(L):U:C6  | 23:V:270(L):U:OP2 | 2.61                     | 0.54              |
| 23:V:2832:U:C2'   | 23:V:2879:C:H42   | 2.19                     | 0.54              |
| 25:Y:100:ILE:HD11 | 25:Y:123:VAL:HG12 | 1.87                     | 0.54              |
| 25:Y:178:ALA:O    | 25:Y:179:SER:HB3  | 2.07                     | 0.54              |
| 29:c:67:LYS:HZ1   | 29:c:90:LEU:CD1   | 2.11                     | 0.54              |
| 8:G:808:C:OP2     | 21:T:48:LYS:NZ    | 2.38                     | 0.54              |
| 23:V:20:C:O2      | 23:V:521:G:N2     | 2.41                     | 0.54              |
| 23:V:84:A:N1      | 23:V:99:U:O2      | 2.39                     | 0.54              |
| 23:V:134:C:N4     | 23:V:135:G:C6     | 2.76                     | 0.54              |
| 23:V:270(W):G:C4  | 23:V:270(X):G:C8  | 2.94                     | 0.54              |
| 23:V:270(Z):U:O2' | 23:V:271:C:OP1    | 2.23                     | 0.54              |
| 23:V:1493:C:OP1   | 23:V:2210:G:C2    | 2.60                     | 0.54              |
| 23:V:2124:G:C1'   | 25:Y:216:THR:HB   | 2.38                     | 0.54              |
| 27:a:17:ASP:O     | 34:h:71:ARG:NH1   | 2.40                     | 0.54              |
| 35:i:23:PRO:HG3   | 35:i:33:ARG:HD2   | 1.89                     | 0.54              |
| 36:j:63:LYS:HE3   | 45:s:117:LEU:HB2  | 1.88                     | 0.54              |
| 38:l:9:ARG:CA     | 38:l:12:PHE:CE1   | 2.90                     | 0.54              |
| 55:DD:9:G:O2'     | 55:DD:10:G:C8     | 2.61                     | 0.54              |
| 8:G:40:C:H42      | 8:G:403:C:H42     | 1.53                     | 0.54              |
| 13:L:35:ALA:HB1   | 13:L:65:VAL:HG13  | 1.89                     | 0.54              |
| 15:N:135:CYS:SG   | 15:N:136:GLU:N    | 2.80                     | 0.54              |
| 23:V:95:G:O3'     | 23:V:96:G:H4'     | 2.07                     | 0.54              |
| 23:V:161:U:O2     | 23:V:161:U:H2'    | 2.06                     | 0.54              |
| 23:V:478:A:C6     | 23:V:480:A:N6     | 2.76                     | 0.54              |
| 23:V:2115:G:H21   | 23:V:2119:A:H62   | 1.56                     | 0.54              |
| 23:V:2197:U:C4    | 23:V:2224:G:N1    | 2.76                     | 0.54              |
| 23:V:2630:G:H1'   | 23:V:2894:G:H1'   | 1.87                     | 0.54              |
| 25:Y:60:GLY:H     | 25:Y:163:PHE:HB2  | 1.72                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 32:f:54:PRO:HD2   | 32:f:73:PRO:HD3  | 1.88                     | 0.54              |
| 50:x:39:MET:O     | 50:x:40:LYS:HB2  | 2.07                     | 0.54              |
| 8:G:82:U:O2       | 8:G:87:A:H2      | 1.79                     | 0.54              |
| 8:G:881:G:OP2     | 18:Q:9:GLN:NE2   | 2.37                     | 0.54              |
| 16:O:75:ASP:OD1   | 16:O:75:ASP:N    | 2.39                     | 0.54              |
| 20:S:44:LEU:HD23  | 20:S:44:LEU:C    | 2.32                     | 0.54              |
| 23:V:324:A:N6     | 23:V:339:U:O2'   | 2.41                     | 0.54              |
| 23:V:370:G:N1     | 23:V:404:C:H5    | 2.06                     | 0.54              |
| 23:V:631:A:OP1    | 23:V:640:C:O2'   | 2.23                     | 0.54              |
| 23:V:1169:G:N1    | 23:V:1170:G:N1   | 2.55                     | 0.54              |
| 23:V:1826:G:O3'   | 26:Z:242:ARG:NH2 | 2.41                     | 0.54              |
| 23:V:2840:C:O5'   | 23:V:2840:C:H6   | 1.89                     | 0.54              |
| 30:d:27:LYS:HG2   | 30:d:32:GLU:OE1  | 2.08                     | 0.54              |
| 36:j:32:TYR:HE2   | 36:j:110:THR:HA  | 1.71                     | 0.54              |
| 41:o:57:VAL:HG13  | 41:o:58:VAL:HG23 | 1.89                     | 0.54              |
| 7:F:2:GLY:N       | 8:G:1305:G:OP1   | 2.41                     | 0.54              |
| 8:G:222:U:C2'     | 8:G:223:U:C6     | 2.83                     | 0.54              |
| 19:R:79:LYS:HA    | 19:R:82:MET:HG2  | 1.90                     | 0.54              |
| 20:S:9:LYS:HE3    | 20:S:21:TYR:CZ   | 2.43                     | 0.54              |
| 23:V:690:G:H21    | 26:Z:43:ARG:HH22 | 1.56                     | 0.54              |
| 23:V:884:C:C5'    | 23:V:892:G:N2    | 2.70                     | 0.54              |
| 23:V:892:G:O2'    | 23:V:893:C:C1'   | 2.56                     | 0.54              |
| 23:V:1090:U:C4    | 23:V:1103:A:C6   | 2.96                     | 0.54              |
| 23:V:1106:G:O5'   | 23:V:1106:G:H8   | 1.90                     | 0.54              |
| 23:V:2304:G:O6    | 23:V:2307:G:N2   | 2.40                     | 0.54              |
| 25:Y:43:VAL:HG22  | 25:Y:214:VAL:HB  | 1.90                     | 0.54              |
| 35:i:63:PRO:HB3   | 53:AA:12:LYS:HA  | 1.90                     | 0.54              |
| 49:w:61:ARG:NH1   | 49:w:66:SER:OG   | 2.40                     | 0.54              |
| 23:V:1694:C:O2    | 23:V:1695:G:N2   | 2.40                     | 0.54              |
| 23:V:1803:A:OP1   | 26:Z:261:LYS:NZ  | 2.40                     | 0.54              |
| 23:V:2627:G:H2'   | 23:V:2781:A:N1   | 2.23                     | 0.54              |
| 30:d:13:LYS:HE2   | 30:d:29:PRO:CD   | 2.29                     | 0.54              |
| 8:G:1359:C:O2'    | 8:G:1360:A:H5''  | 2.08                     | 0.54              |
| 23:V:270(X):G:O3' | 23:V:272:G:H4'   | 2.08                     | 0.54              |
| 23:V:1093:G:N2    | 23:V:1098:A:H62  | 2.06                     | 0.54              |
| 29:c:130:ASN:ND2  | 29:c:161:THR:O   | 2.41                     | 0.54              |
| 43:q:90:GLU:HA    | 43:q:93:GLU:HG2  | 1.90                     | 0.54              |
| 51:y:34:LEU:CD2   | 51:y:51:GLU:HG3  | 2.38                     | 0.54              |
| 55:DD:38:A:H2'    | 55:DD:39:A:H8    | 1.72                     | 0.54              |
| 8:G:342:C:H42     | 8:G:347:G:H1     | 1.56                     | 0.54              |
| 8:G:475:G:O5'     | 8:G:475:G:H8     | 1.91                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:V:975:G:H21   | 23:V:990:A:H1'    | 1.69                     | 0.54              |
| 23:V:1778:U:H3'  | 23:V:1784:A:H61   | 1.72                     | 0.54              |
| 23:V:1863:G:C2   | 23:V:1880:C:O2    | 2.61                     | 0.54              |
| 23:V:2825:C:H2'  | 23:V:2826:A:H5'   | 1.90                     | 0.54              |
| 2:A:6:LEU:HD23   | 2:A:23:VAL:HG21   | 1.90                     | 0.54              |
| 8:G:85:U:H6      | 8:G:85:U:O5'      | 1.91                     | 0.54              |
| 8:G:1097:C:O2'   | 8:G:1169:A:H1'    | 2.08                     | 0.54              |
| 12:K:117:ASP:N   | 12:K:117:ASP:OD1  | 2.40                     | 0.54              |
| 23:V:280:C:C6    | 23:V:283:A:C6     | 2.95                     | 0.54              |
| 23:V:536:A:H2    | 23:V:558:G:N3     | 1.99                     | 0.54              |
| 23:V:2473:U:OP1  | 23:V:2529:G:N2    | 2.40                     | 0.54              |
| 31:e:39:ALA:O    | 31:e:43:ALA:CB    | 2.55                     | 0.54              |
| 34:h:14:THR:OG1  | 34:h:16:ALA:O     | 2.25                     | 0.54              |
| 17:P:80:VAL:HG22 | 17:P:105:VAL:HA   | 1.90                     | 0.53              |
| 23:V:1078:U:H5'  | 32:f:132:ARG:HD2  | 1.90                     | 0.53              |
| 23:V:1143:A:H8   | 23:V:1143:A:H5'   | 1.73                     | 0.53              |
| 23:V:1493:C:O5'  | 23:V:2210:G:N2    | 2.41                     | 0.53              |
| 23:V:2627:G:N2   | 23:V:2777:G:N3    | 2.56                     | 0.53              |
| 25:Y:180:PHE:CG  | 25:Y:185:LEU:HD12 | 2.42                     | 0.53              |
| 32:f:32:ALA:HA   | 32:f:59:ILE:HG21  | 1.88                     | 0.53              |
| 33:g:46:VAL:HB   | 33:g:48:MET:HE1   | 1.91                     | 0.53              |
| 55:DD:6:G:C2'    | 55:DD:7:G:O5'     | 2.56                     | 0.53              |
| 55:DD:35:C:H2'   | 55:DD:35:C:O2     | 2.08                     | 0.53              |
| 8:G:187:C:H1'    | 8:G:191(A):G:H22  | 1.71                     | 0.53              |
| 9:H:96:ARG:NH2   | 9:H:148:TYR:OH    | 2.41                     | 0.53              |
| 23:V:2787:C:H3'  | 23:V:2787:C:H6    | 1.71                     | 0.53              |
| 28:b:78:ILE:HA   | 28:b:83:PHE:HZ    | 1.72                     | 0.53              |
| 29:c:137:GLU:HA  | 29:c:154:GLY:HA2  | 1.90                     | 0.53              |
| 32:f:79:ARG:HD2  | 32:f:134:MET:HB2  | 1.90                     | 0.53              |
| 46:t:31:VAL:HB   | 46:t:35:ASN:HD22  | 1.73                     | 0.53              |
| 34:h:14:THR:OG1  | 34:h:15:GLY:N     | 2.42                     | 0.53              |
| 4:C:105:SER:OG   | 8:G:186(A):C:N3   | 2.42                     | 0.53              |
| 23:V:180:G:O2'   | 23:V:181:A:N7     | 2.38                     | 0.53              |
| 23:V:832:G:O2'   | 35:i:52:GLU:OE1   | 2.26                     | 0.53              |
| 30:d:9:ILE:HB    | 30:d:50:VAL:HB    | 1.90                     | 0.53              |
| 42:p:35:ILE:O    | 42:p:39:THR:OG1   | 2.27                     | 0.53              |
| 44:r:66:PRO:HB2  | 44:r:68:HIS:HB2   | 1.90                     | 0.53              |
| 45:s:99:TYR:HE1  | 45:s:124:ILE:HG23 | 1.74                     | 0.53              |
| 4:C:89:ARG:NH2   | 8:G:186(A):C:O2   | 2.41                     | 0.53              |
| 24:X:88:C:H2'    | 24:X:88:C:O2      | 2.08                     | 0.53              |
| 25:Y:184:LYS:O   | 25:Y:187:ASP:N    | 2.40                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:l:23:ARG:NH1   | 38:l:86:ALA:O     | 2.40                     | 0.53              |
| 51:y:34:LEU:CG    | 51:y:51:GLU:CD    | 2.72                     | 0.53              |
| 51:y:53:LYS:O     | 51:y:53:LYS:HD3   | 2.08                     | 0.53              |
| 8:G:1160:G:OP2    | 8:G:1161:C:OP2    | 2.27                     | 0.53              |
| 8:G:1431:C:H5'    | 39:m:110:ILE:HD12 | 1.90                     | 0.53              |
| 18:Q:57:LYS:HG2   | 18:Q:67:THR:HG22  | 1.91                     | 0.53              |
| 20:S:36:PHE:O     | 20:S:36:PHE:HD1   | 1.91                     | 0.53              |
| 23:V:41:C:H2'     | 23:V:43:G:C8      | 2.43                     | 0.53              |
| 23:V:270(F):U:H2' | 23:V:270(G):C:O4' | 2.08                     | 0.53              |
| 23:V:270(J):G:C2  | 23:V:270(K):C:C2  | 2.97                     | 0.53              |
| 23:V:814:C:O2'    | 23:V:1224:G:N2    | 2.40                     | 0.53              |
| 23:V:1128:A:H62   | 23:V:2518:A:H61   | 1.55                     | 0.53              |
| 23:V:2331:G:O2'   | 23:V:2336:A:N6    | 2.42                     | 0.53              |
| 23:V:2811:G:C6    | 23:V:2891:G:N2    | 2.76                     | 0.53              |
| 13:L:18:GLN:HA    | 13:L:21:LEU:HG    | 1.91                     | 0.53              |
| 23:V:541:C:H2'    | 23:V:541:C:O2     | 2.08                     | 0.53              |
| 23:V:1021:A:H5'   | 23:V:1123:C:H5''  | 1.90                     | 0.53              |
| 23:V:2124:G:H3'   | 25:Y:218:MET:O    | 2.08                     | 0.53              |
| 23:V:2789:C:H3'   | 23:V:2789:C:H6    | 1.72                     | 0.53              |
| 23:V:2791:C:N4    | 23:V:2892:A:N6    | 2.56                     | 0.53              |
| 55:DD:5:G:C2'     | 55:DD:6:G:H5'     | 2.39                     | 0.53              |
| 19:R:34:LEU:HA    | 19:R:37:THR:HG22  | 1.90                     | 0.53              |
| 23:V:270(W):G:N2  | 23:V:273:G:H4'    | 2.23                     | 0.53              |
| 23:V:271(A):G:C5' | 23:V:271(B):U:O4' | 2.53                     | 0.53              |
| 23:V:374:A:N1     | 23:V:401:A:C8     | 2.77                     | 0.53              |
| 23:V:2141:G:H1    | 23:V:2150:U:H3    | 1.55                     | 0.53              |
| 25:Y:190:ARG:HA   | 25:Y:193:ILE:HD12 | 1.90                     | 0.53              |
| 37:k:60:LEU:HA    | 37:k:63:ARG:HG2   | 1.88                     | 0.53              |
| 38:l:12:PHE:CD1   | 38:l:12:PHE:C     | 2.84                     | 0.53              |
| 8:G:439:A:C8      | 8:G:496:A:C2      | 2.97                     | 0.53              |
| 8:G:1360:A:H8     | 8:G:1360:A:OP1    | 1.90                     | 0.53              |
| 8:G:1522:U:H2'    | 8:G:1523:G:H8     | 1.74                     | 0.53              |
| 23:V:139:G:O6     | 23:V:1595:G:O2'   | 2.20                     | 0.53              |
| 23:V:796:C:OP1    | 28:b:62:ARG:NH1   | 2.42                     | 0.53              |
| 23:V:833:U:O4'    | 35:i:52:GLU:HB3   | 2.09                     | 0.53              |
| 23:V:833:U:H5'    | 35:i:52:GLU:HG2   | 1.90                     | 0.53              |
| 23:V:1300:U:C5    | 23:V:1627:G:OP2   | 2.62                     | 0.53              |
| 30:d:104:GLU:HA   | 30:d:113:VAL:O    | 2.09                     | 0.53              |
| 36:j:59:ARG:HH12  | 36:j:109:VAL:HG11 | 1.73                     | 0.53              |
| 39:m:50:ILE:HG13  | 39:m:68:TYR:HB3   | 1.91                     | 0.53              |
| 8:G:1163:C:H2'    | 8:G:1164:G:H8     | 1.74                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:G:1203:C:C4'     | 20:S:27:CYS:HB2   | 2.39                     | 0.53              |
| 11:J:57:ARG:NH1    | 11:J:205:GLU:OE1  | 2.41                     | 0.53              |
| 23:V:172:C:H3'     | 23:V:172:C:H6     | 1.73                     | 0.53              |
| 23:V:274:G:N3      | 23:V:274:G:C3'    | 2.70                     | 0.53              |
| 23:V:536:A:C2      | 23:V:558:G:N1     | 2.45                     | 0.53              |
| 23:V:904:C:O2'     | 45:s:122:ARG:NH1  | 2.31                     | 0.53              |
| 23:V:1817:G:OP1    | 26:Z:88:ARG:NH2   | 2.42                     | 0.53              |
| 24:X:85:G:H2'      | 24:X:86:G:H5'     | 1.91                     | 0.53              |
| 25:Y:182:PRO:HD2   | 25:Y:183:GLU:H    | 1.73                     | 0.53              |
| 30:d:80:SER:OG     | 30:d:81:GLU:OE1   | 2.25                     | 0.53              |
| 38:l:17:ARG:HH11   | 38:l:89:ARG:HB3   | 1.74                     | 0.53              |
| 23:V:95:G:C2'      | 23:V:96:G:H1'     | 2.33                     | 0.52              |
| 23:V:97:C:H5''     | 47:u:43:HIS:ND1   | 2.24                     | 0.52              |
| 23:V:500:G:N1      | 23:V:503:A:OP2    | 2.39                     | 0.52              |
| 23:V:1667:G:O2'    | 23:V:1991:U:O4    | 2.27                     | 0.52              |
| 23:V:2124:G:C8     | 25:Y:216:THR:C    | 2.86                     | 0.52              |
| 23:V:2628:C:O2     | 23:V:2781:A:H2'   | 2.09                     | 0.52              |
| 23:V:2773:C:OP1    | 27:a:164:ARG:NH2  | 2.42                     | 0.52              |
| 23:V:2785:C:O5'    | 23:V:2785:C:H6    | 1.91                     | 0.52              |
| 25:Y:13:LYS:HD3    | 25:Y:32:LEU:HD23  | 1.92                     | 0.52              |
| 26:Z:230:ASP:OD1   | 26:Z:230:ASP:N    | 2.41                     | 0.52              |
| 8:G:201:C:O2       | 8:G:201:C:H2'     | 2.08                     | 0.52              |
| 23:V:10:G:N2       | 23:V:2629:A:N9    | 2.56                     | 0.52              |
| 23:V:853:G:C2      | 23:V:925:C:O2     | 2.61                     | 0.52              |
| 23:V:1424:G:N1     | 23:V:1573:G:O6    | 2.42                     | 0.52              |
| 23:V:2791:C:O2     | 23:V:2791:C:H2'   | 2.08                     | 0.52              |
| 28:b:3:GLU:HG2     | 28:b:22:ALA:HA    | 1.91                     | 0.52              |
| 32:f:65:PHE:N      | 32:f:65:PHE:CD1   | 2.76                     | 0.52              |
| 38:l:15:ARG:HH21   | 38:l:15:ARG:CG    | 2.22                     | 0.52              |
| 40:n:45:TYR:O      | 40:n:49:HIS:ND1   | 2.41                     | 0.52              |
| 45:s:30:ASN:OD1    | 45:s:90:VAL:HG22  | 2.08                     | 0.52              |
| 45:s:92:SER:OG     | 45:s:93:ASP:N     | 2.42                     | 0.52              |
| 7:F:10:ARG:HH12    | 8:G:1289:A:H5''   | 1.73                     | 0.52              |
| 8:G:1169:A:O5'     | 8:G:1169:A:H8     | 1.92                     | 0.52              |
| 23:V:43:G:O6       | 23:V:438:G:C6     | 2.63                     | 0.52              |
| 23:V:540:G:H2'     | 23:V:541:C:C6     | 2.45                     | 0.52              |
| 23:V:557:U:H2'     | 23:V:558:G:C8     | 2.44                     | 0.52              |
| 23:V:892:G:HO2'    | 23:V:893:C:C1'    | 2.22                     | 0.52              |
| 23:V:1057:A:H2'    | 31:e:34:ALA:HA    | 1.90                     | 0.52              |
| 23:V:1444(A):A:O5' | 23:V:1444(A):A:H8 | 1.91                     | 0.52              |
| 23:V:1943:U:H4'    | 23:V:1944:U:H5'   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:f:21:PRO:CD    | 32:f:22:PRO:HD3   | 2.38                     | 0.52              |
| 8:G:1309:G:C8     | 8:G:1329:A:N7     | 2.78                     | 0.52              |
| 13:L:3:ARG:HG3    | 13:L:93:SER:HB2   | 1.92                     | 0.52              |
| 13:L:5:GLU:HB2    | 13:L:62:TRP:HE1   | 1.74                     | 0.52              |
| 23:V:366:C:O2     | 23:V:366:C:H2'    | 2.08                     | 0.52              |
| 23:V:879:G:C2     | 23:V:898:C:O2     | 2.62                     | 0.52              |
| 23:V:1424:G:H22   | 23:V:1573:G:H1    | 1.57                     | 0.52              |
| 29:c:63:ILE:HG22  | 29:c:64:THR:HG23  | 1.91                     | 0.52              |
| 3:B:82:THR:HG21   | 8:G:675:A:H5'     | 1.90                     | 0.52              |
| 8:G:440:A:N6      | 8:G:493:G:H21     | 2.07                     | 0.52              |
| 8:G:1355:G:H2'    | 8:G:1356:G:H8     | 1.75                     | 0.52              |
| 23:V:49:A:N6      | 23:V:177:G:N7     | 2.57                     | 0.52              |
| 23:V:1044:G:O2'   | 23:V:1047:G:OP1   | 2.27                     | 0.52              |
| 23:V:1417:C:O5'   | 23:V:1417:C:H6    | 1.93                     | 0.52              |
| 23:V:2791:C:H42   | 23:V:2893:G:H21   | 1.54                     | 0.52              |
| 23:V:2837:G:H2'   | 23:V:2838:G:C8    | 2.44                     | 0.52              |
| 23:V:2880:C:O2    | 23:V:2880:C:H2'   | 2.08                     | 0.52              |
| 23:V:2896:C:O2    | 23:V:2896:C:H2'   | 2.08                     | 0.52              |
| 29:c:44:GLY:HA2   | 29:c:88:ILE:CD1   | 2.39                     | 0.52              |
| 30:d:109:PHE:HD2  | 30:d:112:PRO:HD2  | 1.74                     | 0.52              |
| 34:h:94:ARG:HG3   | 34:h:96:THR:H     | 1.75                     | 0.52              |
| 35:i:128:HIS:HB3  | 35:i:147:LEU:HD12 | 1.92                     | 0.52              |
| 41:o:43:GLU:HG2   | 41:o:46:VAL:HA    | 1.92                     | 0.52              |
| 1:W:19:U:O2'      | 1:W:19:U:O2       | 2.28                     | 0.52              |
| 8:G:439:A:H3'     | 8:G:440:A:H8      | 1.73                     | 0.52              |
| 8:G:1311:G:C5     | 8:G:1312:G:C8     | 2.97                     | 0.52              |
| 23:V:274:G:N2     | 23:V:274:G:OP2    | 2.43                     | 0.52              |
| 23:V:2634:G:N2    | 23:V:2785:C:N3    | 2.57                     | 0.52              |
| 36:j:36:ALA:HB2   | 36:j:103:MET:HE1  | 1.91                     | 0.52              |
| 44:r:26:LYS:HG2   | 44:r:27:VAL:HG23  | 1.91                     | 0.52              |
| 8:G:1118:C:O2     | 8:G:1118:C:H2'    | 2.08                     | 0.52              |
| 16:O:96:LEU:HA    | 16:O:100:GLY:HA2  | 1.92                     | 0.52              |
| 23:V:271(A):G:OP1 | 23:V:271(B):U:O4' | 2.28                     | 0.52              |
| 23:V:1173:G:N3    | 23:V:1173:G:C5'   | 2.73                     | 0.52              |
| 23:V:1446:C:H2'   | 23:V:1447:G:C8    | 2.44                     | 0.52              |
| 23:V:2334:G:C8    | 38:l:15:ARG:CD    | 2.93                     | 0.52              |
| 26:Z:8:PRO:HB3    | 26:Z:14:ARG:HB3   | 1.91                     | 0.52              |
| 32:f:19:PRO:CB    | 32:f:22:PRO:HG2   | 2.39                     | 0.52              |
| 8:G:1261:A:N6     | 8:G:1274:G:O2'    | 2.42                     | 0.52              |
| 13:L:21:LEU:HD12  | 13:L:22:GLU:HG3   | 1.92                     | 0.52              |
| 15:N:96:GLY:H     | 15:N:99:GLU:HB2   | 1.74                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:O:26:VAL:HG12 | 16:O:61:ALA:HB3   | 1.92                     | 0.52              |
| 23:V:478:A:C6    | 23:V:480:A:C6     | 2.97                     | 0.52              |
| 23:V:527:C:H2'   | 23:V:2779:U:H6    | 1.75                     | 0.52              |
| 23:V:2258:C:O2'  | 23:V:2427:C:OP2   | 2.27                     | 0.52              |
| 25:Y:68:LEU:HD23 | 25:Y:69:GLY:H     | 1.75                     | 0.52              |
| 25:Y:161:ILE:O   | 25:Y:162:GLU:HB2  | 2.09                     | 0.52              |
| 32:f:57:ILE:HG23 | 32:f:57:ILE:O     | 2.09                     | 0.52              |
| 1:W:19:U:C1'     | 1:W:20:U:OP2      | 2.55                     | 0.52              |
| 8:G:390:C:O3'    | 22:U:28:ARG:NH2   | 2.43                     | 0.52              |
| 23:V:612:G:N1    | 23:V:613:U:O4     | 2.43                     | 0.52              |
| 23:V:2809:A:N1   | 27:a:60:ASN:HB2   | 2.22                     | 0.52              |
| 28:b:131:GLY:HA3 | 28:b:138:GLU:HG3  | 1.91                     | 0.52              |
| 7:F:10:ARG:HA    | 7:F:13:ILE:HG22   | 1.91                     | 0.52              |
| 9:H:7:VAL:HG23   | 9:H:8:LYS:HG3     | 1.92                     | 0.52              |
| 20:S:11:LYS:NZ   | 20:S:13:THR:OG1   | 2.33                     | 0.52              |
| 23:V:442:G:H21   | 28:b:48:THR:HG1   | 1.58                     | 0.52              |
| 24:X:0:A:N3      | 24:X:0:A:C5'      | 2.73                     | 0.52              |
| 29:c:71:THR:CB   | 29:c:87:PRO:HA    | 2.39                     | 0.52              |
| 6:E:4:ILE:HB     | 6:E:74:ILE:HB     | 1.91                     | 0.51              |
| 16:O:10:ARG:NH1  | 16:O:105:ASP:OD2  | 2.43                     | 0.51              |
| 23:V:833:U:H5'   | 35:i:52:GLU:CB    | 2.40                     | 0.51              |
| 23:V:1103:A:N3   | 23:V:1103:A:C2'   | 2.73                     | 0.51              |
| 23:V:1445:C:C4   | 23:V:1446:C:N3    | 2.77                     | 0.51              |
| 23:V:1455:G:O6   | 23:V:2705:A:C2    | 2.64                     | 0.51              |
| 23:V:2894:G:N3   | 23:V:2894:G:C3'   | 2.73                     | 0.51              |
| 29:c:83:ARG:HG3  | 55:DD:57:C:H5''   | 1.92                     | 0.51              |
| 38:l:99:LYS:C    | 38:l:101:LEU:N    | 2.67                     | 0.51              |
| 44:r:73:ARG:HG2  | 44:r:77:PRO:HB3   | 1.92                     | 0.51              |
| 8:G:138:G:H1'    | 8:G:226:G:N2      | 2.25                     | 0.51              |
| 9:H:178:ARG:HH21 | 15:N:74:PRO:HD3   | 1.75                     | 0.51              |
| 11:J:98:GLU:HA   | 11:J:103:ASN:HD22 | 1.75                     | 0.51              |
| 23:V:885:C:C4    | 23:V:892:G:C6     | 2.98                     | 0.51              |
| 23:V:1247:A:OP2  | 35:i:18:ARG:NH2   | 2.43                     | 0.51              |
| 23:V:2198:A:N3   | 23:V:2198:A:C3'   | 2.73                     | 0.51              |
| 25:Y:66:HIS:H    | 25:Y:158:ALA:HB1  | 1.68                     | 0.51              |
| 25:Y:176:GLY:HA2 | 25:Y:180:PHE:CE1  | 2.43                     | 0.51              |
| 30:d:168:PRO:HB2 | 30:d:170:ARG:HH12 | 1.74                     | 0.51              |
| 39:m:67:SER:HB3  | 39:m:75:ILE:HD12  | 1.91                     | 0.51              |
| 41:o:72:VAL:HG13 | 41:o:88:ARG:HD2   | 1.90                     | 0.51              |
| 1:W:16:A:C2      | 1:W:17:U:C4       | 2.98                     | 0.51              |
| 8:G:138:G:N3     | 8:G:226:G:C2      | 2.78                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:95:G:O3'     | 23:V:96:G:C4'     | 2.58                     | 0.51              |
| 23:V:2117:A:O3'   | 23:V:2147:G:N2    | 2.43                     | 0.51              |
| 35:i:50:ARG:HB3   | 35:i:51:PHE:CD1   | 2.45                     | 0.51              |
| 8:G:129(A):G:C4   | 8:G:191(A):G:C8   | 2.99                     | 0.51              |
| 13:L:10:LEU:HB2   | 13:L:59:TYR:HB3   | 1.91                     | 0.51              |
| 21:T:15:PHE:HB2   | 21:T:27:VAL:HG23  | 1.92                     | 0.51              |
| 23:V:265:A:N6     | 23:V:428:A:C5     | 2.78                     | 0.51              |
| 23:V:363(A):A:N3  | 23:V:363(A):A:H2' | 2.25                     | 0.51              |
| 23:V:892:G:H2'    | 23:V:893:C:C6     | 2.46                     | 0.51              |
| 23:V:1479:G:H8    | 23:V:1479:G:O5'   | 1.92                     | 0.51              |
| 23:V:2064:C:O2'   | 23:V:2251:G:N2    | 2.43                     | 0.51              |
| 23:V:2894:G:N3    | 23:V:2894:G:C2'   | 2.73                     | 0.51              |
| 25:Y:58:VAL:HG11  | 25:Y:201:PRO:HD3  | 1.91                     | 0.51              |
| 29:c:113:ARG:NH1  | 49:CC:23:GLU:O    | 2.43                     | 0.51              |
| 38:l:28:VAL:HG22  | 38:l:90:GLY:HA2   | 1.92                     | 0.51              |
| 38:l:50:SER:O     | 38:l:76:LYS:NZ    | 2.33                     | 0.51              |
| 39:m:79:HIS:HB2   | 39:m:82:LEU:HD22  | 1.92                     | 0.51              |
| 8:G:476:G:H2'     | 8:G:477:G:C8      | 2.44                     | 0.51              |
| 8:G:1311:G:C6     | 8:G:1312:G:C4     | 2.99                     | 0.51              |
| 23:V:11:G:N3      | 23:V:11:G:C5'     | 2.73                     | 0.51              |
| 23:V:531:C:O2'    | 23:V:2035:G:N2    | 2.43                     | 0.51              |
| 29:c:4:ASP:HA     | 29:c:7:LEU:HD12   | 1.92                     | 0.51              |
| 7:F:12:LYS:NZ     | 8:G:1326:C:OP1    | 2.40                     | 0.51              |
| 8:G:191(F):U:O5'  | 8:G:191(F):U:H6   | 1.92                     | 0.51              |
| 8:G:476:G:H2'     | 8:G:477:G:H8      | 1.76                     | 0.51              |
| 8:G:876:G:O5'     | 15:N:14:ARG:NH2   | 2.42                     | 0.51              |
| 8:G:1028(B):C:H3' | 8:G:1029:G:H4'    | 1.92                     | 0.51              |
| 9:H:166:ASP:O     | 9:H:170:GLU:HB2   | 2.11                     | 0.51              |
| 13:L:48:LEU:HD13  | 13:L:52:ILE:HD12  | 1.92                     | 0.51              |
| 20:S:44:LEU:HD23  | 20:S:44:LEU:O     | 2.10                     | 0.51              |
| 23:V:991:C:O2     | 23:V:1164:G:N2    | 2.43                     | 0.51              |
| 23:V:1085:A:OP1   | 23:V:1106:G:OP2   | 2.29                     | 0.51              |
| 26:Z:124:PRO:O    | 26:Z:129:ASN:ND2  | 2.44                     | 0.51              |
| 27:a:59:VAL:HG23  | 27:a:62:PRO:HD2   | 1.91                     | 0.51              |
| 38:l:99:LYS:O     | 38:l:100:ALA:C    | 2.51                     | 0.51              |
| 51:y:37:ARG:O     | 51:y:48:VAL:HG23  | 2.09                     | 0.51              |
| 5:D:3:ARG:NH2     | 8:G:1312:G:O6     | 2.44                     | 0.51              |
| 8:G:1055:A:O2'    | 10:I:156:ARG:NH1  | 2.41                     | 0.51              |
| 8:G:1362(A):C:O2  | 8:G:1362(A):C:O2' | 2.20                     | 0.51              |
| 23:V:374:A:N1     | 23:V:401:A:N9     | 2.58                     | 0.51              |
| 23:V:670:A:H4'    | 23:V:671:C:H5'    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:2124:G:P     | 25:Y:218:MET:H    | 2.28                     | 0.51              |
| 11:J:148:VAL:HB   | 11:J:181:MET:HE3  | 1.93                     | 0.51              |
| 21:T:7:GLU:HA     | 21:T:10:LYS:HG2   | 1.93                     | 0.51              |
| 23:V:1203:G:O6    | 23:V:1241:A:C6    | 2.64                     | 0.51              |
| 23:V:2217:G:O5'   | 23:V:2217:G:H8    | 1.94                     | 0.51              |
| 25:Y:164:ARG:NH1  | 25:Y:165:ASN:O    | 2.44                     | 0.51              |
| 39:m:29:ARG:HG2   | 39:m:91:ARG:HB2   | 1.92                     | 0.51              |
| 8:G:126:G:OP1     | 8:G:605:U:O2'     | 2.29                     | 0.51              |
| 23:V:1102:C:H2'   | 23:V:1103:A:H5''  | 1.92                     | 0.51              |
| 23:V:1445:C:H5'   | 23:V:1446:C:OP2   | 2.11                     | 0.51              |
| 23:V:2127:G:N1    | 23:V:2163:C:O4'   | 2.44                     | 0.51              |
| 45:s:29:TYR:HE1   | 45:s:87:ASP:HB2   | 1.75                     | 0.51              |
| 4:C:86:ARG:HG3    | 8:G:186(A):C:H5'' | 1.93                     | 0.51              |
| 6:E:47:PHE:CE2    | 20:S:37:PHE:CZ    | 2.99                     | 0.51              |
| 8:G:1163:C:H2'    | 8:G:1164:G:C8     | 2.46                     | 0.51              |
| 23:V:478:A:C5     | 23:V:480:A:N6     | 2.79                     | 0.51              |
| 23:V:853:G:H2'    | 23:V:854:G:C8     | 2.46                     | 0.51              |
| 23:V:1143:A:H8    | 23:V:1143:A:H5''  | 1.74                     | 0.51              |
| 8:G:159:G:N2      | 8:G:162:A:OP2     | 2.43                     | 0.50              |
| 10:I:55:VAL:HG22  | 10:I:68:VAL:HG12  | 1.93                     | 0.50              |
| 23:V:270(H):C:H2' | 23:V:270(I):G:C8  | 2.40                     | 0.50              |
| 23:V:271(C):G:C2  | 23:V:272:G:C8     | 2.99                     | 0.50              |
| 27:a:104:VAL:HG11 | 27:a:188:VAL:HG13 | 1.93                     | 0.50              |
| 36:j:43:THR:HA    | 36:j:94:VAL:HG12  | 1.92                     | 0.50              |
| 53:AA:14:VAL:HG12 | 53:AA:24:ALA:HB2  | 1.93                     | 0.50              |
| 23:V:270(N):G:H3' | 23:V:270(O):U:C6  | 2.45                     | 0.50              |
| 23:V:511:U:O2'    | 23:V:1215:G:N2    | 2.44                     | 0.50              |
| 23:V:602:G:O2'    | 23:V:655:A:N6     | 2.44                     | 0.50              |
| 8:G:1372:U:H5'    | 16:O:71:SER:HB3   | 1.94                     | 0.50              |
| 23:V:1544:C:N4    | 23:V:1545:A:H62   | 2.10                     | 0.50              |
| 23:V:2211:G:N3    | 23:V:2211:G:C3'   | 2.73                     | 0.50              |
| 30:d:18:GLU:CB    | 30:d:24:VAL:CB    | 2.90                     | 0.50              |
| 8:G:1309:G:N3     | 8:G:1328:C:C4     | 2.79                     | 0.50              |
| 23:V:41:C:H2'     | 23:V:43:G:H8      | 1.76                     | 0.50              |
| 23:V:270(X):G:O6  | 23:V:270(Y):G:N3  | 2.43                     | 0.50              |
| 23:V:1493:C:P     | 23:V:2210:G:N1    | 2.84                     | 0.50              |
| 23:V:2392:A:H2    | 23:V:2424:C:H42   | 1.59                     | 0.50              |
| 23:V:2832:U:O2    | 23:V:2832:U:H2'   | 2.11                     | 0.50              |
| 27:a:81:ILE:HG22  | 27:a:82:ARG:HG2   | 1.93                     | 0.50              |
| 29:c:57:ALA:HA    | 29:c:67:LYS:HD3   | 1.92                     | 0.50              |
| 29:c:167:GLU:HA   | 29:c:170:ARG:HB3  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:j:17:LEU:O     | 36:j:72:LYS:NZ     | 2.34                     | 0.50              |
| 3:B:59:SER:OG     | 3:B:62:GLU:OE1     | 2.26                     | 0.50              |
| 8:G:464:G:H1      | 8:G:466:C:H4'      | 1.75                     | 0.50              |
| 8:G:718:G:H1'     | 17:P:116:HIS:HA    | 1.93                     | 0.50              |
| 23:V:13:A:N9      | 23:V:15:G:O6       | 2.44                     | 0.50              |
| 23:V:553:U:H3'    | 23:V:553:U:H6      | 1.76                     | 0.50              |
| 23:V:974:G:N2     | 23:V:1186:G:C6     | 2.64                     | 0.50              |
| 23:V:1275:A:N6    | 23:V:1295:C:O2'    | 2.44                     | 0.50              |
| 35:i:49:ARG:HH12  | 53:AA:3:LYS:HD2    | 1.76                     | 0.50              |
| 6:E:5:ARG:NH2     | 8:G:1125:U:O4      | 2.45                     | 0.50              |
| 8:G:129(A):G:N1   | 8:G:191(A):G:C6    | 2.80                     | 0.50              |
| 8:G:217:C:O5'     | 8:G:217:C:H6       | 1.94                     | 0.50              |
| 8:G:266:G:H4'     | 8:G:268:C:H41      | 1.77                     | 0.50              |
| 20:S:21:TYR:CD1   | 20:S:21:TYR:N      | 2.79                     | 0.50              |
| 23:V:270(A):A:OP2 | 23:V:270(B):A:C2   | 2.64                     | 0.50              |
| 23:V:280:C:C4     | 23:V:283:A:C4      | 2.99                     | 0.50              |
| 23:V:974(A):C:H4' | 23:V:975:G:H5'     | 1.92                     | 0.50              |
| 23:V:1031:G:H21   | 54:BB:36:GLN:HE22  | 1.60                     | 0.50              |
| 23:V:1143:A:C8    | 23:V:1143:A:H5'    | 2.45                     | 0.50              |
| 23:V:1449(A):G:N3 | 23:V:1449(A):G:C2' | 2.73                     | 0.50              |
| 23:V:1717:G:N3    | 23:V:1717:G:C5'    | 2.73                     | 0.50              |
| 23:V:2213:U:O4    | 49:w:47:GLN:CD     | 2.54                     | 0.50              |
| 25:Y:46:LYS:HG2   | 25:Y:210:ARG:HH21  | 1.77                     | 0.50              |
| 38:l:17:ARG:HH12  | 38:l:89:ARG:CD     | 2.04                     | 0.50              |
| 41:o:19:LYS:HE3   | 41:o:21:ARG:HH21   | 1.77                     | 0.50              |
| 51:y:28:ARG:O     | 51:y:32:ASN:ND2    | 2.45                     | 0.50              |
| 8:G:439:A:N7      | 8:G:496:A:C6       | 2.80                     | 0.50              |
| 8:G:1415:G:H8     | 8:G:1415:G:O5'     | 1.95                     | 0.50              |
| 23:V:993:G:OP1    | 40:n:50:ARG:NH1    | 2.40                     | 0.50              |
| 23:V:1169:G:C4    | 23:V:1170:G:C6     | 2.99                     | 0.50              |
| 23:V:1545:A:H2'   | 23:V:1545(A):A:H4' | 1.92                     | 0.50              |
| 23:V:2584:U:O2'   | 23:V:2602:A:N1     | 2.45                     | 0.50              |
| 23:V:2720:U:O5'   | 23:V:2720:U:H6     | 1.95                     | 0.50              |
| 25:Y:159:GLY:O    | 25:Y:160:ARG:HB2   | 2.11                     | 0.50              |
| 28:b:200:GLU:OE2  | 28:b:204:ASN:ND2   | 2.45                     | 0.50              |
| 38:l:17:ARG:NH2   | 38:l:17:ARG:CB     | 2.73                     | 0.50              |
| 45:s:151:HIS:HB3  | 45:s:171:ILE:HG22  | 1.94                     | 0.50              |
| 51:y:14:THR:CG2   | 51:y:52:VAL:CB     | 2.79                     | 0.50              |
| 55:DD:59:A:O2'    | 55:DD:61:U:OP2     | 2.25                     | 0.50              |
| 8:G:35:G:N2       | 18:Q:118:SER:OG    | 2.39                     | 0.50              |
| 16:O:3:GLN:HE21   | 16:O:18:PHE:HB3    | 1.77                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:T:24:SER:H     | 21:T:27:VAL:HG12   | 1.76                     | 0.50              |
| 23:V:270(H):C:O2' | 23:V:270(I):G:H5'  | 2.12                     | 0.50              |
| 23:V:1005:C:C5    | 23:V:1143:A:O4'    | 2.65                     | 0.50              |
| 23:V:1112:G:O2'   | 23:V:1113:U:O5'    | 2.21                     | 0.50              |
| 23:V:1142(A):A:N3 | 23:V:1142(A):A:C2' | 2.73                     | 0.50              |
| 38:l:9:ARG:C      | 38:l:12:PHE:CD1    | 2.88                     | 0.50              |
| 43:q:75:ASP:OD1   | 43:q:75:ASP:N      | 2.44                     | 0.50              |
| 8:G:138:G:H1'     | 8:G:226:G:H22      | 1.76                     | 0.50              |
| 8:G:464:G:N2      | 8:G:474:G:C6       | 2.80                     | 0.50              |
| 8:G:1256:A:N6     | 8:G:1278:U:O2'     | 2.45                     | 0.50              |
| 13:L:74:ASP:OD1   | 13:L:77:ARG:NH1    | 2.45                     | 0.50              |
| 23:V:270(L):U:O2' | 23:V:270(M):U:P    | 2.69                     | 0.50              |
| 23:V:2748:A:N1    | 23:V:2757:A:N6     | 2.59                     | 0.50              |
| 25:Y:175:VAL:O    | 25:Y:180:PHE:CE2   | 2.65                     | 0.50              |
| 28:b:32:LEU:HD11  | 28:b:105:VAL:HG13  | 1.94                     | 0.50              |
| 29:c:71:THR:O     | 29:c:88:ILE:HG22   | 2.12                     | 0.50              |
| 35:i:15:ARG:HH12  | 35:i:16:ARG:HD2    | 1.76                     | 0.50              |
| 45:s:94:GLU:N     | 45:s:95:PRO:CD     | 2.73                     | 0.50              |
| 55:DD:31:G:O5'    | 55:DD:31:G:H8      | 1.95                     | 0.50              |
| 8:G:643:C:H2'     | 8:G:644:G:H8       | 1.76                     | 0.49              |
| 8:G:778:G:H21     | 17:P:120:ARG:HD3   | 1.77                     | 0.49              |
| 8:G:1203:C:H4'    | 20:S:27:CYS:HB2    | 1.82                     | 0.49              |
| 19:R:42:ALA:O     | 19:R:44:ARG:NH1    | 2.45                     | 0.49              |
| 20:S:9:LYS:NZ     | 20:S:21:TYR:CZ     | 2.80                     | 0.49              |
| 23:V:833:U:H5'    | 35:i:52:GLU:CG     | 2.42                     | 0.49              |
| 23:V:1139:G:O5'   | 23:V:1139:G:H8     | 1.94                     | 0.49              |
| 23:V:2624:G:H8    | 23:V:2624:G:O5'    | 1.94                     | 0.49              |
| 32:f:19:PRO:HA    | 32:f:22:PRO:HG3    | 1.82                     | 0.49              |
| 8:G:1355:G:H1     | 8:G:1367:C:H42     | 1.60                     | 0.49              |
| 23:V:43:G:C6      | 23:V:438:G:C6      | 3.00                     | 0.49              |
| 23:V:122:G:H1     | 23:V:129:C:H42     | 1.60                     | 0.49              |
| 23:V:537:C:H2'    | 23:V:539:G:C8      | 2.47                     | 0.49              |
| 24:X:14:U:O2'     | 24:X:106:G:N2      | 2.43                     | 0.49              |
| 29:c:113:ARG:HG2  | 29:c:141:PHE:HB3   | 1.94                     | 0.49              |
| 55:DD:29:C:C2     | 55:DD:30:G:N7      | 2.81                     | 0.49              |
| 8:G:272:C:H2'     | 8:G:273:A:C8       | 2.48                     | 0.49              |
| 8:G:1485:U:H2'    | 8:G:1486:G:C8      | 2.47                     | 0.49              |
| 23:V:83:G:O2'     | 23:V:84:A:O4'      | 2.31                     | 0.49              |
| 23:V:265:A:N6     | 23:V:428:A:C8      | 2.79                     | 0.49              |
| 23:V:270(X):G:N3  | 23:V:270(Y):G:H4'  | 2.26                     | 0.49              |
| 23:V:545:G:N1     | 23:V:548:A:OP2     | 2.41                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:547:A:H2'    | 23:V:548:A:H8     | 1.77                     | 0.49              |
| 23:V:641:C:H42    | 23:V:644:A:H62    | 1.60                     | 0.49              |
| 23:V:879:G:N1     | 23:V:898:C:C2     | 2.80                     | 0.49              |
| 23:V:1445:C:H5    | 23:V:1446:C:N3    | 2.00                     | 0.49              |
| 23:V:1586:A:O5'   | 23:V:1586:A:H8    | 1.96                     | 0.49              |
| 23:V:1728:G:N3    | 23:V:1728:G:C2'   | 2.73                     | 0.49              |
| 23:V:1944:U:H1'   | 23:V:1955:U:H1'   | 1.94                     | 0.49              |
| 38:l:94:TYR:CD2   | 38:l:98:VAL:CG1   | 2.96                     | 0.49              |
| 8:G:439:A:N7      | 8:G:496:A:C5      | 2.80                     | 0.49              |
| 22:U:33:ILE:HG22  | 22:U:34:GLU:HG3   | 1.94                     | 0.49              |
| 23:V:30:G:O2'     | 23:V:1214:A:N3    | 2.37                     | 0.49              |
| 23:V:87:C:O2      | 23:V:96:G:N2      | 2.43                     | 0.49              |
| 23:V:374:A:N3     | 23:V:401:A:C6     | 2.81                     | 0.49              |
| 23:V:1312:U:H5'   | 43:q:63:LYS:HD2   | 1.93                     | 0.49              |
| 25:Y:182:PRO:O    | 25:Y:186:ALA:HB2  | 2.11                     | 0.49              |
| 27:a:14:ILE:HG13  | 27:a:19:ARG:HB3   | 1.94                     | 0.49              |
| 8:G:976:G:C2      | 8:G:1363:A:C6     | 3.00                     | 0.49              |
| 23:V:138:G:N3     | 23:V:138:G:C2'    | 2.74                     | 0.49              |
| 23:V:144:C:H2'    | 23:V:145:G:H8     | 1.78                     | 0.49              |
| 25:Y:177:LYS:CA   | 25:Y:180:PHE:HD1  | 2.25                     | 0.49              |
| 5:D:1:MET:HE3     | 8:G:1311:G:P      | 2.53                     | 0.49              |
| 14:M:26:PHE:HA    | 14:M:101:LEU:HD21 | 1.94                     | 0.49              |
| 23:V:102:G:H8     | 23:V:102:G:OP2    | 1.95                     | 0.49              |
| 23:V:1541:U:H5''  | 23:V:1542:G:OP2   | 2.11                     | 0.49              |
| 23:V:2630:G:H1'   | 23:V:2894:G:C1'   | 2.42                     | 0.49              |
| 23:V:2828:C:H2'   | 23:V:2829:C:C6    | 2.48                     | 0.49              |
| 25:Y:182:PRO:CD   | 25:Y:183:GLU:H    | 2.25                     | 0.49              |
| 29:c:47:LYS:HA    | 29:c:86:MET:HE1   | 1.91                     | 0.49              |
| 32:f:11:GLN:NE2   | 32:f:12:LEU:O     | 2.46                     | 0.49              |
| 32:f:52:ILE:O     | 32:f:73:PRO:CD    | 2.61                     | 0.49              |
| 8:G:1100:C:N4     | 8:G:1103:C:OP1    | 2.45                     | 0.49              |
| 23:V:1480:G:N3    | 23:V:1480:G:C2'   | 2.75                     | 0.49              |
| 23:V:2631:G:H2'   | 23:V:2632:A:H5''  | 1.94                     | 0.49              |
| 23:V:2831:G:H8    | 23:V:2831:G:O5'   | 1.94                     | 0.49              |
| 25:Y:56:GLN:HE21  | 25:Y:208:PHE:HE1  | 1.60                     | 0.49              |
| 30:d:125:VAL:HG13 | 30:d:130:ARG:O    | 2.13                     | 0.49              |
| 8:G:439:A:OP2     | 8:G:493:G:N1      | 2.36                     | 0.49              |
| 8:G:592:G:H2'     | 8:G:593:G:H8      | 1.78                     | 0.49              |
| 8:G:1459:C:O5'    | 8:G:1459:C:H6     | 1.95                     | 0.49              |
| 23:V:1058:G:N2    | 23:V:1059:G:N7    | 2.60                     | 0.49              |
| 23:V:1137:G:N2    | 33:g:106:MET:SD   | 2.74                     | 0.49              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 23:V:1169:G:C3'  | 23:V:1170:G:C8     | 2.96                     | 0.49              |
| 23:V:1285:G:N2   | 23:V:1329:U:OP1    | 2.45                     | 0.49              |
| 23:V:1418:G:H21  | 23:V:1579:A:N6     | 2.08                     | 0.49              |
| 23:V:1589:C:H2'  | 23:V:1590:U:C6     | 2.47                     | 0.49              |
| 23:V:2126:A:N7   | 23:V:2164:C:P      | 2.85                     | 0.49              |
| 23:V:2230:G:H1'  | 49:w:58:ARG:HH12   | 1.78                     | 0.49              |
| 23:V:2636:U:C2   | 23:V:2783:G:N1     | 2.54                     | 0.49              |
| 25:Y:36:LYS:HG3  | 25:Y:37:PHE:HD1    | 1.77                     | 0.49              |
| 25:Y:138:PRO:HA  | 25:Y:144:THR:HG21  | 1.94                     | 0.49              |
| 2:A:62:SER:OG    | 2:A:72:ARG:NE      | 2.46                     | 0.49              |
| 6:E:37:PRO:HB2   | 6:E:70:ARG:HH11    | 1.77                     | 0.49              |
| 8:G:362:G:N2     | 8:G:365:U:OP2      | 2.45                     | 0.49              |
| 8:G:1117:G:O3'   | 16:O:104:ARG:HD2   | 2.13                     | 0.49              |
| 20:S:40:CYS:SG   | 20:S:41:ARG:N      | 2.85                     | 0.49              |
| 23:V:526:A:C2    | 23:V:2625:G:N2     | 2.65                     | 0.49              |
| 23:V:975:G:N3    | 23:V:990:A:C5      | 2.81                     | 0.49              |
| 23:V:1418:G:N2   | 23:V:1579:A:H62    | 2.10                     | 0.49              |
| 23:V:1862:G:N2   | 23:V:1863:G:C5     | 2.81                     | 0.49              |
| 23:V:2632:A:H2'  | 23:V:2633:G:C8     | 2.47                     | 0.49              |
| 25:Y:176:GLY:C   | 25:Y:180:PHE:CD1   | 2.86                     | 0.49              |
| 3:B:18:ARG:NH1   | 3:B:54:ARG:O       | 2.46                     | 0.49              |
| 8:G:1378:C:H5''  | 14:M:6:ARG:HH12    | 1.77                     | 0.49              |
| 23:V:270(W):G:N7 | 23:V:270(X):G:N7   | 2.61                     | 0.49              |
| 23:V:1174:A:N3   | 23:V:1174:A:C2'    | 2.75                     | 0.49              |
| 23:V:2216:G:O5'  | 23:V:2216:G:H8     | 1.96                     | 0.49              |
| 23:V:2636:U:C1'  | 23:V:2783:G:N2     | 2.72                     | 0.49              |
| 25:Y:97:GLU:HA   | 25:Y:100:ILE:HD12  | 1.94                     | 0.49              |
| 30:d:11:VAL:HG12 | 30:d:48:GLY:O      | 2.13                     | 0.49              |
| 32:f:23:VAL:HG12 | 32:f:35:MET:CB     | 2.42                     | 0.49              |
| 45:s:70:LEU:CD2  | 45:s:91:LEU:HD21   | 2.41                     | 0.49              |
| 8:G:129(A):G:N3  | 8:G:191(A):G:C8    | 2.81                     | 0.48              |
| 8:G:266:G:O2'    | 8:G:268:C:OP2      | 2.26                     | 0.48              |
| 8:G:376:G:H5''   | 22:U:5:ARG:HD2     | 1.94                     | 0.48              |
| 9:H:77:ALA:O     | 9:H:79:ASP:N       | 2.45                     | 0.48              |
| 23:V:489:G:C4    | 23:V:1284:A:C6     | 3.01                     | 0.48              |
| 23:V:592:G:H21   | 53:AA:3:LYS:HZ1    | 1.60                     | 0.48              |
| 23:V:1169:G:C2   | 23:V:1170:G:C5     | 3.00                     | 0.48              |
| 23:V:1418:G:H8   | 23:V:1418:G:OP2    | 1.95                     | 0.48              |
| 23:V:1545:A:O3'  | 23:V:1545(A):A:H4' | 2.13                     | 0.48              |
| 23:V:1568:G:OP2  | 26:Z:63:ARG:NH2    | 2.38                     | 0.48              |
| 23:V:2126:A:N6   | 23:V:2164:C:P      | 2.86                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:2206:C:H3'    | 23:V:2206:C:H6    | 1.78                     | 0.48              |
| 29:c:47:LYS:CG     | 29:c:80:PHE:HD2   | 2.09                     | 0.48              |
| 8:G:920:U:O2'      | 8:G:1081:G:O2'    | 2.31                     | 0.48              |
| 8:G:1412:C:O5'     | 8:G:1412:C:H6     | 1.96                     | 0.48              |
| 17:P:82:VAL:HG11   | 17:P:98:LEU:HD11  | 1.95                     | 0.48              |
| 23:V:919:G:C6      | 23:V:2268:A:N7    | 2.81                     | 0.48              |
| 23:V:1169:G:N3     | 23:V:1170:G:C5    | 2.81                     | 0.48              |
| 23:V:1857:G:H21    | 23:V:1885:A:N6    | 2.11                     | 0.48              |
| 23:V:2881:C:H6     | 23:V:2881:C:O5'   | 1.97                     | 0.48              |
| 23:V:2883:A:H5'    | 23:V:2884:U:H5'   | 1.94                     | 0.48              |
| 25:Y:176:GLY:HA2   | 25:Y:180:PHE:CD2  | 2.47                     | 0.48              |
| 27:a:7:VAL:HA      | 27:a:25:VAL:HG12  | 1.94                     | 0.48              |
| 8:G:1242:C:H42     | 8:G:1295:G:H1     | 1.59                     | 0.48              |
| 18:Q:102:ARG:HD2   | 18:Q:107:ALA:HB1  | 1.95                     | 0.48              |
| 20:S:9:LYS:CE      | 20:S:21:TYR:CZ    | 2.96                     | 0.48              |
| 23:V:7:G:OP2       | 23:V:7:G:H4'      | 2.13                     | 0.48              |
| 23:V:271(A):G:H5'' | 23:V:271(B):U:H5' | 1.92                     | 0.48              |
| 23:V:370:G:N3      | 23:V:370:G:C2'    | 2.73                     | 0.48              |
| 23:V:602:G:H4'     | 23:V:603:A:H4'    | 1.95                     | 0.48              |
| 23:V:1452:A:H3'    | 23:V:1453:A:H4'   | 1.95                     | 0.48              |
| 25:Y:180:PHE:CG    | 25:Y:185:LEU:CD1  | 2.96                     | 0.48              |
| 29:c:39:ILE:HG23   | 29:c:92:VAL:HB    | 1.95                     | 0.48              |
| 8:G:403:C:O2'      | 11:J:122:ARG:NH1  | 2.42                     | 0.48              |
| 23:V:144:C:H2'     | 23:V:145:G:C8     | 2.49                     | 0.48              |
| 23:V:270:A:OP2     | 23:V:270(X):G:N2  | 2.37                     | 0.48              |
| 23:V:270(J):G:N1   | 23:V:270(K):C:C2  | 2.82                     | 0.48              |
| 23:V:1046:A:O2'    | 31:e:60:ARG:O     | 2.31                     | 0.48              |
| 23:V:1630:G:O5'    | 23:V:1630:G:H8    | 1.96                     | 0.48              |
| 23:V:2134:A:OP1    | 23:V:2159:G:N2    | 2.45                     | 0.48              |
| 23:V:2226:C:C2'    | 23:V:2227:A:C5'   | 2.92                     | 0.48              |
| 23:V:2343:C:O2'    | 23:V:2373:G:O2'   | 2.31                     | 0.48              |
| 23:V:2701:C:H5'    | 23:V:2702:U:H5''  | 1.95                     | 0.48              |
| 27:a:119:ARG:NH2   | 27:a:159:HIS:O    | 2.47                     | 0.48              |
| 36:j:12:GLN:HG3    | 36:j:13:GLN:HG2   | 1.96                     | 0.48              |
| 38:l:17:ARG:HH11   | 38:l:89:ARG:CB    | 2.27                     | 0.48              |
| 1:W:19:U:O2'       | 1:W:20:U:P        | 2.72                     | 0.48              |
| 8:G:92:G:OP1       | 8:G:92:G:H4'      | 2.14                     | 0.48              |
| 10:I:147:LYS:HB2   | 10:I:203:PHE:HD2  | 1.78                     | 0.48              |
| 23:V:1314:C:H42    | 23:V:1338:G:H1    | 1.61                     | 0.48              |
| 23:V:1458:C:O2'    | 23:V:1459:G:N2    | 2.46                     | 0.48              |
| 25:Y:127:LEU:HB3   | 25:Y:131:LEU:HD13 | 1.95                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:j:63:LYS:O      | 36:j:107:ALA:HB2  | 2.14                     | 0.48              |
| 51:y:24:GLU:OE1    | 51:y:37:ARG:NH1   | 2.46                     | 0.48              |
| 7:F:20:LYS:NZ      | 8:G:1267:C:O2     | 2.36                     | 0.48              |
| 21:T:4:THR:N       | 21:T:7:GLU:OE2    | 2.47                     | 0.48              |
| 23:V:255:A:O2'     | 23:V:384:U:OP1    | 2.32                     | 0.48              |
| 23:V:2056:G:N2     | 50:x:4:HIS:O      | 2.33                     | 0.48              |
| 23:V:2837:G:N2     | 23:V:2882:A:N3    | 2.61                     | 0.48              |
| 25:Y:66:HIS:ND1    | 25:Y:184:LYS:HG2  | 2.28                     | 0.48              |
| 32:f:23:VAL:CG1    | 32:f:35:MET:CB    | 2.92                     | 0.48              |
| 34:h:67:LYS:HZ3    | 34:h:77:ILE:HD13  | 1.78                     | 0.48              |
| 48:v:9:VAL:HG13    | 48:v:10:LYS:HD2   | 1.95                     | 0.48              |
| 5:D:1:MET:HE3      | 8:G:1311:G:OP1    | 2.14                     | 0.48              |
| 8:G:76:G:C2        | 8:G:95:G:C6       | 3.01                     | 0.48              |
| 8:G:503:C:OP2      | 18:Q:116:SER:OG   | 2.28                     | 0.48              |
| 23:V:140:A:N3      | 23:V:140:A:C2'    | 2.76                     | 0.48              |
| 23:V:270(P):C:O2'  | 23:V:270(Q):C:H5' | 2.12                     | 0.48              |
| 23:V:270(T):G:H2'  | 23:V:270(T):G:N3  | 2.29                     | 0.48              |
| 23:V:495:G:H21     | 42:p:61:ASN:HD21  | 1.62                     | 0.48              |
| 23:V:557:U:H2'     | 23:V:558:G:H8     | 1.79                     | 0.48              |
| 23:V:871:U:O2'     | 23:V:872:A:N7     | 2.40                     | 0.48              |
| 23:V:1173:G:N3     | 23:V:1173:G:C3'   | 2.77                     | 0.48              |
| 23:V:1530:G:H22    | 23:V:1542:G:H22   | 1.60                     | 0.48              |
| 23:V:2884:U:H5     | 50:x:43:HIS:HD2   | 1.60                     | 0.48              |
| 35:i:47:ASP:N      | 35:i:48:PRO:CD    | 2.74                     | 0.48              |
| 8:G:129(A):G:C2    | 8:G:191(A):G:C6   | 2.94                     | 0.48              |
| 23:V:43:G:N1       | 23:V:438:G:C6     | 2.82                     | 0.48              |
| 23:V:270(K):C:H5'' | 23:V:270(L):U:C5  | 2.49                     | 0.48              |
| 23:V:270(X):G:C4'  | 23:V:273:G:H5'    | 2.44                     | 0.48              |
| 23:V:1668:A:N3     | 23:V:1670:C:N4    | 2.62                     | 0.48              |
| 23:V:2124:G:H3'    | 25:Y:218:MET:C    | 2.39                     | 0.48              |
| 23:V:2791:C:H41    | 23:V:2892:A:H61   | 1.57                     | 0.48              |
| 8:G:776:G:N2       | 8:G:802:A:OP2     | 2.46                     | 0.48              |
| 8:G:1002:G:H2'     | 8:G:1003:G:C8     | 2.48                     | 0.48              |
| 8:G:1415:G:H2'     | 8:G:1416:G:H8     | 1.79                     | 0.48              |
| 8:G:1448:C:H2'     | 8:G:1449:C:O4'    | 2.14                     | 0.48              |
| 20:S:9:LYS:NZ      | 20:S:21:TYR:CG    | 2.77                     | 0.48              |
| 23:V:270(G):C:H2'  | 23:V:270(H):C:C5  | 2.48                     | 0.48              |
| 23:V:1138:G:O6     | 23:V:1139:G:O6    | 2.32                     | 0.48              |
| 23:V:1710:C:N4     | 23:V:1711:C:H42   | 2.10                     | 0.48              |
| 23:V:1823:G:OP1    | 26:Z:54:ARG:NH2   | 2.41                     | 0.48              |
| 23:V:2134:A:H2'    | 23:V:2136:C:H41   | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:b:157:VAL:HG23 | 28:b:194:MET:HA   | 1.94                     | 0.48              |
| 32:f:19:PRO:HB2   | 32:f:23:VAL:HG23  | 1.96                     | 0.48              |
| 34:h:87:ILE:HG12  | 34:h:91:LEU:HB3   | 1.95                     | 0.48              |
| 36:j:48:GLU:OE2   | 36:j:51:ARG:NH1   | 2.40                     | 0.48              |
| 39:m:32:TYR:HB2   | 39:m:48:ILE:HG23  | 1.96                     | 0.48              |
| 55:DD:37:U:C2'    | 55:DD:38:A:C5'    | 2.89                     | 0.48              |
| 55:DD:73:A:H2'    | 55:DD:74:A:H8     | 1.79                     | 0.48              |
| 23:V:276:A:H2'    | 23:V:276:A:N3     | 2.28                     | 0.48              |
| 23:V:852:G:C4     | 23:V:853:G:C8     | 3.02                     | 0.48              |
| 23:V:975:G:C2     | 23:V:990:A:N7     | 2.82                     | 0.48              |
| 23:V:1057:A:O2'   | 31:e:37:THR:N     | 2.34                     | 0.48              |
| 23:V:1964:G:O2'   | 23:V:1967:C:OP2   | 2.29                     | 0.48              |
| 23:V:2884:U:H5    | 50:x:43:HIS:CD2   | 2.32                     | 0.48              |
| 23:V:2898:U:O5'   | 23:V:2898:U:H6    | 1.96                     | 0.48              |
| 25:Y:127:LEU:O    | 25:Y:131:LEU:HB2  | 2.14                     | 0.48              |
| 26:Z:37:LEU:HD13  | 26:Z:64:ILE:HD11  | 1.95                     | 0.48              |
| 23:V:10:G:H2'     | 23:V:11:G:C2      | 2.49                     | 0.47              |
| 23:V:270(K):C:H3' | 23:V:270(L):U:C6  | 2.45                     | 0.47              |
| 23:V:527:C:H2'    | 23:V:2779:U:C6    | 2.49                     | 0.47              |
| 23:V:974:G:C6     | 23:V:1187:G:H1'   | 2.48                     | 0.47              |
| 23:V:1071:G:O6    | 23:V:1072:C:N4    | 2.47                     | 0.47              |
| 23:V:1084:A:N3    | 23:V:1106:G:O6    | 2.47                     | 0.47              |
| 23:V:1529:A:N7    | 23:V:1530:G:N1    | 2.62                     | 0.47              |
| 54:BB:17:ILE:HD12 | 54:BB:26:ILE:HD12 | 1.95                     | 0.47              |
| 23:V:644:A:H5''   | 23:V:2349:G:H21   | 1.79                     | 0.47              |
| 23:V:833:U:C4'    | 35:i:52:GLU:HB3   | 2.44                     | 0.47              |
| 40:n:28:ARG:HD3   | 40:n:38:THR:HG21  | 1.96                     | 0.47              |
| 43:q:52:VAL:HG12  | 43:q:53:LYS:HG3   | 1.97                     | 0.47              |
| 6:E:47:PHE:HE2    | 20:S:37:PHE:HZ    | 1.62                     | 0.47              |
| 8:G:738:C:OP2     | 13:L:92:LYS:NZ    | 2.46                     | 0.47              |
| 9:H:19:HIS:HB2    | 9:H:204:ASN:HD21  | 1.79                     | 0.47              |
| 23:V:270(L):U:O2' | 23:V:270(M):U:OP1 | 2.32                     | 0.47              |
| 23:V:270(N):G:C8  | 23:V:270(O):U:C6  | 3.02                     | 0.47              |
| 23:V:374:A:C2     | 23:V:401:A:C6     | 3.01                     | 0.47              |
| 23:V:1479:G:H4'   | 23:V:1559:G:N7    | 2.29                     | 0.47              |
| 23:V:1534:G:H1'   | 23:V:1537:C:H41   | 1.79                     | 0.47              |
| 23:V:1748:G:H8    | 23:V:1748:G:O5'   | 1.97                     | 0.47              |
| 23:V:1792:G:H5'   | 26:Z:205:VAL:HG13 | 1.96                     | 0.47              |
| 23:V:2124:G:P     | 25:Y:218:MET:HB2  | 2.47                     | 0.47              |
| 23:V:2485:G:OP1   | 36:j:46:GLN:NE2   | 2.46                     | 0.47              |
| 48:v:26:LEU:O     | 48:v:35:ARG:NH2   | 2.48                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:G:971:G:OP2    | 8:G:1231:G:N2     | 2.44                     | 0.47              |
| 8:G:1345:U:OP1   | 16:O:120:ARG:NH1  | 2.47                     | 0.47              |
| 13:L:15:ASP:OD1  | 13:L:15:ASP:N     | 2.47                     | 0.47              |
| 23:V:270(Z):U:O2 | 23:V:271(A):G:OP1 | 2.32                     | 0.47              |
| 23:V:557:U:H6    | 23:V:557:U:H3'    | 1.79                     | 0.47              |
| 30:d:102:ALA:CA  | 30:d:123:PHE:CE2  | 2.71                     | 0.47              |
| 41:o:85:LYS:HE2  | 41:o:85:LYS:HB3   | 1.75                     | 0.47              |
| 8:G:688:G:N2     | 8:G:699:C:O2      | 2.40                     | 0.47              |
| 8:G:1167:A:O2'   | 8:G:1169:A:H5'    | 2.14                     | 0.47              |
| 8:G:1360:A:P     | 8:G:1360:A:H8     | 2.37                     | 0.47              |
| 8:G:1442:G:N3    | 8:G:1442:G:C3'    | 2.73                     | 0.47              |
| 19:R:32:GLU:HA   | 19:R:35:GLU:HG3   | 1.96                     | 0.47              |
| 23:V:272:G:O6    | 23:V:364:C:N3     | 2.47                     | 0.47              |
| 23:V:852:G:N1    | 23:V:853:G:C6     | 2.82                     | 0.47              |
| 23:V:932:G:O2'   | 23:V:933:A:O4'    | 2.32                     | 0.47              |
| 30:d:27:LYS:HG2  | 30:d:32:GLU:CD    | 2.40                     | 0.47              |
| 45:s:70:LEU:CD1  | 45:s:98:MET:HE3   | 2.28                     | 0.47              |
| 45:s:119:GLU:HG2 | 45:s:173:ALA:H    | 1.79                     | 0.47              |
| 7:F:20:LYS:HG2   | 8:G:1327:C:H5''   | 1.97                     | 0.47              |
| 17:P:99:GLN:HE21 | 17:P:105:VAL:HG21 | 1.79                     | 0.47              |
| 23:V:2209:C:N4   | 23:V:2215:G:C6    | 2.69                     | 0.47              |
| 23:V:2312:U:O2'  | 29:c:89:GLY:CA    | 2.57                     | 0.47              |
| 8:G:440:A:N6     | 8:G:493:G:C2      | 2.35                     | 0.47              |
| 8:G:446:G:N2     | 8:G:489:C:O2      | 2.47                     | 0.47              |
| 8:G:842:C:H6     | 8:G:842:C:H3'     | 1.80                     | 0.47              |
| 8:G:1441:G:H4'   | 8:G:1442:G:C5     | 2.50                     | 0.47              |
| 9:H:78:GLN:O     | 9:H:94:ASN:ND2    | 2.47                     | 0.47              |
| 20:S:36:PHE:CD1  | 20:S:36:PHE:C     | 2.92                     | 0.47              |
| 23:V:234:C:H2'   | 23:V:235:U:H6     | 1.80                     | 0.47              |
| 23:V:270(W):G:C4 | 23:V:270(X):G:H8  | 2.32                     | 0.47              |
| 23:V:270(Z):U:H3 | 23:V:271(B):U:H1' | 1.73                     | 0.47              |
| 23:V:403:U:O2    | 23:V:403:U:O2'    | 2.22                     | 0.47              |
| 23:V:1048:A:N6   | 23:V:1111:A:O2'   | 2.29                     | 0.47              |
| 23:V:1441:G:O2'  | 23:V:1628:G:OP1   | 2.32                     | 0.47              |
| 23:V:1544:C:H4'  | 23:V:1544:C:OP1   | 2.15                     | 0.47              |
| 23:V:1712:C:O5'  | 23:V:1712:C:H6    | 1.97                     | 0.47              |
| 23:V:2206:C:C2'  | 23:V:2207:C:H5'   | 2.44                     | 0.47              |
| 25:Y:107:TRP:NE1 | 25:Y:109:ASP:OD2  | 2.43                     | 0.47              |
| 25:Y:167:LYS:HD3 | 25:Y:168:THR:HG23 | 1.97                     | 0.47              |
| 32:f:74:ALA:HB2  | 32:f:115:LEU:HD11 | 1.95                     | 0.47              |
| 32:f:86:LYS:CB   | 32:f:95:LYS:HB2   | 2.25                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:h:122:LEU:HD11  | 39:m:71:GLY:HA3   | 1.96                     | 0.47              |
| 41:o:7:THR:HB      | 41:o:37:VAL:HG13  | 1.97                     | 0.47              |
| 47:u:48:LEU:HG     | 47:u:51:GLN:HE21  | 1.79                     | 0.47              |
| 50:x:51:TYR:HB3    | 50:x:55:ARG:HA    | 1.96                     | 0.47              |
| 8:G:1020:U:H2'     | 8:G:1021:G:H8     | 1.78                     | 0.47              |
| 23:V:270(M):U:C3'  | 23:V:270(N):G:H4' | 2.44                     | 0.47              |
| 23:V:374:A:N6      | 23:V:401:A:C8     | 2.83                     | 0.47              |
| 23:V:1857:G:N2     | 23:V:1885:A:H62   | 2.13                     | 0.47              |
| 23:V:2714:G:H8     | 23:V:2714:G:O5'   | 1.98                     | 0.47              |
| 23:V:2813:A:H8     | 23:V:2813:A:O5'   | 1.98                     | 0.47              |
| 28:b:8:GLN:HG2     | 28:b:17:ARG:HG3   | 1.96                     | 0.47              |
| 32:f:115:LEU:HD23  | 32:f:116:ASN:H    | 1.80                     | 0.47              |
| 35:i:106:LEU:HG    | 35:i:109:GLY:HA2  | 1.96                     | 0.47              |
| 38:l:14:VAL:HG22   | 38:l:17:ARG:NH1   | 2.30                     | 0.47              |
| 53:AA:27:THR:O     | 53:AA:27:THR:OG1  | 2.31                     | 0.47              |
| 8:G:68:G:C2        | 8:G:102:G:N2      | 2.83                     | 0.47              |
| 8:G:474:G:H2'      | 8:G:475:G:C8      | 2.49                     | 0.47              |
| 8:G:1119:C:H2'     | 8:G:1120:G:H8     | 1.80                     | 0.47              |
| 23:V:371:A:N3      | 23:V:371:A:C2'    | 2.74                     | 0.47              |
| 23:V:840:C:H2'     | 23:V:841:A:C8     | 2.50                     | 0.47              |
| 23:V:1697:G:H5''   | 23:V:1698:A:H5''  | 1.97                     | 0.47              |
| 23:V:2807:G:N2     | 23:V:2892:A:N3    | 2.63                     | 0.47              |
| 25:Y:155:GLU:O     | 25:Y:158:ALA:N    | 2.43                     | 0.47              |
| 36:j:134:ARG:HH22  | 45:s:123:ASP:HB2  | 1.80                     | 0.47              |
| 41:o:36:PRO:HA     | 41:o:60:GLU:O     | 2.15                     | 0.47              |
| 45:s:145:GLU:HB3   | 45:s:148:ASP:HB2  | 1.96                     | 0.47              |
| 51:y:34:LEU:HD23   | 51:y:51:GLU:HG3   | 1.97                     | 0.47              |
| 2:A:9:VAL:HG12     | 2:A:56:VAL:HG22   | 1.97                     | 0.47              |
| 8:G:1023:G:H3'     | 8:G:1024:G:H8     | 1.80                     | 0.47              |
| 17:P:19:ALA:O      | 17:P:82:VAL:HA    | 2.15                     | 0.47              |
| 23:V:95:G:H2'      | 23:V:96:G:O2'     | 2.15                     | 0.47              |
| 23:V:270(P):C:O5'  | 23:V:270(P):C:H6  | 1.99                     | 0.47              |
| 23:V:270(R):G:C2   | 23:V:270(S):G:C4  | 3.03                     | 0.47              |
| 23:V:270(X):G:H5'' | 23:V:273:G:OP1    | 2.14                     | 0.47              |
| 23:V:882:G:H3'     | 23:V:883:G:H4'    | 1.97                     | 0.47              |
| 23:V:1528:A:H2'    | 23:V:1529:A:C4    | 2.50                     | 0.47              |
| 23:V:2521:C:O2'    | 23:V:2564:A:N3    | 2.41                     | 0.47              |
| 25:Y:176:GLY:HA2   | 25:Y:180:PHE:CD1  | 2.50                     | 0.47              |
| 8:G:31:G:N2        | 8:G:48:C:OP1      | 2.40                     | 0.46              |
| 8:G:1415:G:O6      | 8:G:1486:G:O6     | 2.33                     | 0.46              |
| 20:S:24:CYS:SG     | 20:S:25:VAL:N     | 2.88                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:V:486:C:O2'   | 42:p:60:ASN:ND2   | 2.39                     | 0.46              |
| 23:V:852:G:C6    | 23:V:926:A:C6     | 3.03                     | 0.46              |
| 23:V:1102:C:C2   | 23:V:1104:C:C4    | 3.03                     | 0.46              |
| 23:V:1935:G:O2'  | 23:V:1936:A:H5'   | 2.15                     | 0.46              |
| 25:Y:89:ALA:CB   | 25:Y:154:ARG:HG3  | 2.45                     | 0.46              |
| 55:DD:39:A:H8    | 55:DD:39:A:O5'    | 1.98                     | 0.46              |
| 8:G:1126:U:H2'   | 8:G:1127:G:C8     | 2.50                     | 0.46              |
| 12:K:8:GLU:HA    | 12:K:33:VAL:O     | 2.15                     | 0.46              |
| 23:V:270(K):C:N4 | 23:V:270(M):U:C6  | 2.83                     | 0.46              |
| 23:V:273(E):U:N3 | 23:V:273(F):C:H1' | 2.30                     | 0.46              |
| 23:V:931:G:H21   | 48:v:24:LYS:HG3   | 1.80                     | 0.46              |
| 23:V:974:G:C5    | 23:V:1187:G:C1'   | 2.88                     | 0.46              |
| 23:V:2216:G:H2'  | 23:V:2217:G:C8    | 2.50                     | 0.46              |
| 23:V:2807:G:OP1  | 23:V:2807:G:H4'   | 2.12                     | 0.46              |
| 24:X:40:U:O2'    | 24:X:45:A:N6      | 2.48                     | 0.46              |
| 32:f:52:ILE:HD11 | 32:f:76:TYR:CE1   | 2.50                     | 0.46              |
| 32:f:59:ILE:O    | 32:f:59:ILE:HG22  | 2.15                     | 0.46              |
| 37:k:13:HIS:HB3  | 37:k:16:HIS:HB3   | 1.98                     | 0.46              |
| 38:l:9:ARG:HA    | 38:l:12:PHE:CG    | 2.50                     | 0.46              |
| 8:G:129(A):G:N1  | 8:G:191(A):G:C4   | 2.81                     | 0.46              |
| 23:V:273:G:C5    | 23:V:273(A):G:N7  | 2.83                     | 0.46              |
| 23:V:280:C:C4    | 23:V:283:A:C5     | 3.03                     | 0.46              |
| 23:V:852:G:C6    | 23:V:853:G:C6     | 3.02                     | 0.46              |
| 23:V:910:A:N3    | 23:V:2264:C:O2'   | 2.47                     | 0.46              |
| 23:V:1084:A:C2'  | 23:V:1106:G:C5    | 2.96                     | 0.46              |
| 23:V:1102:C:N3   | 23:V:1104:C:C4    | 2.83                     | 0.46              |
| 23:V:1493:C:OP1  | 23:V:2210:G:C6    | 2.67                     | 0.46              |
| 23:V:2197:U:N3   | 23:V:2224:G:N1    | 2.62                     | 0.46              |
| 29:c:138:GLN:HB2 | 29:c:154:GLY:H    | 1.79                     | 0.46              |
| 55:DD:33:OMC:C3' | 55:DD:34:A:H5''   | 2.44                     | 0.46              |
| 3:B:50:ILE:N     | 8:G:719:C:O2      | 2.42                     | 0.46              |
| 8:G:167:G:H2'    | 8:G:168:G:C8      | 2.49                     | 0.46              |
| 8:G:375:U:H4'    | 22:U:6:LEU:HD11   | 1.97                     | 0.46              |
| 8:G:1125:U:OP2   | 8:G:1145:C:N4     | 2.48                     | 0.46              |
| 14:M:69:VAL:HG21 | 14:M:104:LEU:HD21 | 1.97                     | 0.46              |
| 23:V:375:C:H2'   | 23:V:376:C:C6     | 2.50                     | 0.46              |
| 23:V:376:C:O5'   | 23:V:376:C:H6     | 1.98                     | 0.46              |
| 23:V:873:G:H2'   | 23:V:874:G:C8     | 2.51                     | 0.46              |
| 23:V:2120:G:N1   | 23:V:2121:G:O6    | 2.48                     | 0.46              |
| 23:V:2124:G:H21  | 25:Y:221:SER:H    | 1.49                     | 0.46              |
| 23:V:2897:U:H2'  | 23:V:2898:U:C6    | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:l:60:GLY:HA3   | 38:l:62:LYS:HE3   | 1.97                     | 0.46              |
| 55:DD:7:G:H3'     | 55:DD:8:4SU:H5''  | 1.97                     | 0.46              |
| 8:G:210:U:H4'     | 8:G:216:G:C8      | 2.50                     | 0.46              |
| 8:G:1006:C:H42    | 8:G:1024:G:H1'    | 1.80                     | 0.46              |
| 8:G:1356:G:H2'    | 8:G:1357:A:C8     | 2.51                     | 0.46              |
| 16:O:55:ALA:O     | 16:O:58:HIS:ND1   | 2.33                     | 0.46              |
| 17:P:86:GLY:N     | 17:P:112:THR:OG1  | 2.49                     | 0.46              |
| 23:V:89:G:H3'     | 23:V:90:U:H5''    | 1.98                     | 0.46              |
| 23:V:273:G:C4     | 23:V:273(A):G:N7  | 2.83                     | 0.46              |
| 23:V:542:C:C2     | 23:V:552:G:N2     | 2.84                     | 0.46              |
| 23:V:1084:A:N6    | 31:e:30:GLN:O     | 2.49                     | 0.46              |
| 23:V:1138:G:C6    | 23:V:1139:G:O6    | 2.68                     | 0.46              |
| 23:V:1544:C:C4    | 23:V:1545:A:N7    | 2.84                     | 0.46              |
| 23:V:1627:G:C2'   | 23:V:1628:G:H5'   | 2.46                     | 0.46              |
| 27:a:111:ARG:HB2  | 27:a:160:TYR:HD2  | 1.80                     | 0.46              |
| 28:b:7:TYR:HD2    | 28:b:21:ALA:HB3   | 1.80                     | 0.46              |
| 29:c:80:PHE:O     | 29:c:82:LEU:HG    | 2.15                     | 0.46              |
| 35:i:15:ARG:NH1   | 35:i:16:ARG:HA    | 2.31                     | 0.46              |
| 36:j:29:PHE:HE1   | 36:j:137:TYR:H    | 1.63                     | 0.46              |
| 37:k:38:VAL:HG22  | 37:k:112:ALA:HB2  | 1.98                     | 0.46              |
| 8:G:979:C:H41     | 8:G:1360:A:H61    | 1.64                     | 0.46              |
| 17:P:85:ARG:NH1   | 17:P:111:ASP:OD2  | 2.48                     | 0.46              |
| 23:V:270:A:O2'    | 23:V:270(A):A:OP1 | 2.32                     | 0.46              |
| 23:V:489:G:C6     | 23:V:1284:A:C2    | 3.04                     | 0.46              |
| 23:V:1079:C:H41   | 23:V:1088:A:H5'   | 1.80                     | 0.46              |
| 23:V:1860:G:C6    | 23:V:1861:G:C6    | 3.03                     | 0.46              |
| 23:V:2863:C:H2'   | 23:V:2864:G:H8    | 1.79                     | 0.46              |
| 39:m:110:ILE:HG23 | 39:m:113:LYS:HB2  | 1.97                     | 0.46              |
| 45:s:6:LYS:HG2    | 45:s:35:ARG:HH22  | 1.80                     | 0.46              |
| 45:s:100:VAL:HG23 | 45:s:100:VAL:O    | 2.15                     | 0.46              |
| 5:D:20:LEU:HD12   | 5:D:21:GLU:HG2    | 1.97                     | 0.46              |
| 9:H:71:VAL:HA     | 9:H:93:VAL:HB     | 1.98                     | 0.46              |
| 10:I:95:THR:O     | 10:I:97:LYS:NZ    | 2.48                     | 0.46              |
| 14:M:50:ILE:HD11  | 14:M:58:PRO:HB3   | 1.98                     | 0.46              |
| 23:V:364:C:H2'    | 23:V:365:C:C5     | 2.50                     | 0.46              |
| 23:V:1005:C:C5    | 23:V:1143:A:C8    | 3.04                     | 0.46              |
| 27:a:10:GLY:HA2   | 27:a:23:VAL:HA    | 1.97                     | 0.46              |
| 30:d:27:LYS:CD    | 30:d:32:GLU:OE2   | 2.64                     | 0.46              |
| 34:h:102:VAL:O    | 39:m:74:ARG:NH1   | 2.41                     | 0.46              |
| 51:y:13:CYS:O     | 51:y:21:TYR:HA    | 2.15                     | 0.46              |
| 7:F:8:THR:HG23    | 8:G:1243:C:H5''   | 1.98                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:G:101:A:OP1    | 8:G:101:A:H4'     | 2.15                     | 0.46              |
| 8:G:1413:A:C2    | 8:G:1488:G:C2     | 3.03                     | 0.46              |
| 23:V:278:A:H2    | 23:V:362:U:H3     | 1.53                     | 0.46              |
| 23:V:923:C:C4    | 23:V:924:C:C4     | 2.94                     | 0.46              |
| 23:V:1546:C:OP1  | 23:V:1547:C:H5'   | 2.16                     | 0.46              |
| 23:V:2630:G:C5   | 23:V:2894:G:H8    | 2.34                     | 0.46              |
| 34:h:35:VAL:HG11 | 34:h:64:ARG:HH11  | 1.80                     | 0.46              |
| 35:i:121:LYS:HD2 | 35:i:122:PRO:HD2  | 1.96                     | 0.46              |
| 51:y:45:LYS:CD   | 51:y:47:THR:HG22  | 2.45                     | 0.46              |
| 53:AA:29:LYS:HE3 | 53:AA:36:LYS:HG3  | 1.97                     | 0.46              |
| 54:BB:18:ARG:HG2 | 54:BB:23:VAL:HG22 | 1.98                     | 0.46              |
| 55:DD:9:G:N1     | 55:DD:47:7MG:C6   | 2.84                     | 0.46              |
| 8:G:959:A:O2'    | 8:G:984:C:O2'     | 2.32                     | 0.46              |
| 23:V:96:G:C5'    | 47:u:43:HIS:CE1   | 2.93                     | 0.46              |
| 23:V:888:C:H4'   | 23:V:889:C:C5'    | 2.46                     | 0.46              |
| 23:V:1083:U:H1'  | 23:V:1085:A:C6    | 2.50                     | 0.46              |
| 23:V:1202:C:H42  | 23:V:1243:G:H1    | 1.64                     | 0.46              |
| 23:V:2096:U:C2   | 23:V:2194:G:N2    | 2.84                     | 0.46              |
| 23:V:2156:G:H3'  | 23:V:2157:G:H21   | 1.81                     | 0.46              |
| 23:V:2827:C:H2'  | 23:V:2828:C:C6    | 2.51                     | 0.46              |
| 25:Y:13:LYS:HE2  | 25:Y:28:LEU:HG    | 1.98                     | 0.46              |
| 29:c:47:LYS:C    | 29:c:86:MET:HE1   | 2.41                     | 0.46              |
| 50:x:20:ARG:HA   | 50:x:23:HIS:HD2   | 1.81                     | 0.46              |
| 8:G:1205:U:OP1   | 10:I:190:ARG:NH1  | 2.42                     | 0.46              |
| 8:G:1359:C:C2'   | 8:G:1360:A:O5'    | 2.64                     | 0.46              |
| 23:V:10:G:N2     | 23:V:2629:A:C8    | 2.83                     | 0.46              |
| 23:V:925:C:H6    | 23:V:925:C:O5'    | 1.98                     | 0.46              |
| 23:V:1312:U:H2'  | 23:V:1313:U:O4'   | 2.15                     | 0.46              |
| 23:V:1527:G:N2   | 23:V:1542:G:N7    | 2.64                     | 0.46              |
| 23:V:1939:U:H3'  | 23:V:1940:U:H5''  | 1.97                     | 0.46              |
| 23:V:2805:G:H22  | 23:V:2892:A:H62   | 1.56                     | 0.46              |
| 23:V:2836:U:H2'  | 23:V:2837:G:C8    | 2.51                     | 0.46              |
| 26:Z:85:ASP:HB2  | 26:Z:92:ILE:HG12  | 1.98                     | 0.46              |
| 27:a:32:PRO:HA   | 27:a:47:VAL:O     | 2.16                     | 0.46              |
| 32:f:48:MET:CB   | 32:f:69:THR:CG2   | 2.78                     | 0.46              |
| 32:f:78:ILE:HD11 | 32:f:122:ALA:HB1  | 1.97                     | 0.46              |
| 32:f:103:GLN:HA  | 32:f:106:GLU:HG3  | 1.98                     | 0.46              |
| 34:h:15:GLY:HA3  | 34:h:47:ILE:HA    | 1.98                     | 0.46              |
| 8:G:1118:C:OP1   | 16:O:9:ARG:NE     | 2.49                     | 0.45              |
| 20:S:39:LEU:HD12 | 20:S:44:LEU:HD12  | 1.98                     | 0.45              |
| 23:V:13:A:N6     | 23:V:525:U:C5     | 2.84                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:280:C:N1     | 23:V:283:A:C8     | 2.84                     | 0.45              |
| 23:V:280:C:O2     | 23:V:280:C:O2'    | 2.26                     | 0.45              |
| 23:V:1270:C:H5''  | 23:V:1271:G:H5'   | 1.98                     | 0.45              |
| 23:V:2357:U:OP1   | 46:t:20:ARG:NH2   | 2.40                     | 0.45              |
| 26:Z:147:LEU:HD21 | 26:Z:183:ARG:HH21 | 1.80                     | 0.45              |
| 32:f:40:ALA:O     | 32:f:67:PHE:CE1   | 2.69                     | 0.45              |
| 55:DD:29:C:C4     | 55:DD:30:G:O6     | 2.69                     | 0.45              |
| 7:F:7:ARG:NH2     | 8:G:1327:C:OP2    | 2.49                     | 0.45              |
| 8:G:392:G:H2'     | 8:G:393:A:H8      | 1.82                     | 0.45              |
| 8:G:500:G:N1      | 8:G:546:G:C2      | 2.84                     | 0.45              |
| 8:G:1060:C:OP1    | 20:S:45:ARG:NH2   | 2.47                     | 0.45              |
| 8:G:1472:U:O4     | 8:G:1473:A:N6     | 2.49                     | 0.45              |
| 23:V:43:G:N1      | 23:V:438:G:C4     | 2.84                     | 0.45              |
| 23:V:270(C):C:C2' | 23:V:270(D):C:H6  | 2.02                     | 0.45              |
| 23:V:1447:G:OP2   | 23:V:1447:G:H8    | 1.99                     | 0.45              |
| 23:V:1537:C:H3'   | 23:V:1538:G:C8    | 2.49                     | 0.45              |
| 23:V:2226:C:C6    | 23:V:2226:C:C3'   | 3.00                     | 0.45              |
| 23:V:2226:C:C5    | 23:V:2227:A:C5    | 3.03                     | 0.45              |
| 25:Y:67:GLY:HA2   | 25:Y:157:LYS:O    | 2.16                     | 0.45              |
| 26:Z:146:GLU:HG2  | 26:Z:153:ALA:HA   | 1.98                     | 0.45              |
| 30:d:103:LEU:HD22 | 30:d:123:PHE:CE1  | 2.48                     | 0.45              |
| 34:h:106:LEU:HD12 | 34:h:115:VAL:HG21 | 1.97                     | 0.45              |
| 23:V:143:C:H2'    | 23:V:144:C:C6     | 2.52                     | 0.45              |
| 23:V:270(H):C:C2  | 23:V:270(I):G:C8  | 3.03                     | 0.45              |
| 23:V:880:G:H2'    | 23:V:881:G:H4'    | 1.98                     | 0.45              |
| 23:V:932:G:OP2    | 48:v:29:ARG:NH1   | 2.49                     | 0.45              |
| 23:V:974:G:N1     | 23:V:1187:G:N3    | 2.62                     | 0.45              |
| 23:V:2035:G:H5'   | 23:V:2036:C:H5    | 1.82                     | 0.45              |
| 35:i:46:LYS:HB3   | 35:i:47:ASP:H     | 1.65                     | 0.45              |
| 45:s:90:VAL:O     | 45:s:91:LEU:HD23  | 2.16                     | 0.45              |
| 49:w:44:THR:OG1   | 49:w:56:VAL:O     | 2.26                     | 0.45              |
| 3:B:44:LEU:HD11   | 3:B:80:PRO:HD2    | 1.98                     | 0.45              |
| 23:V:85:G:H1      | 23:V:98:G:N2      | 2.11                     | 0.45              |
| 23:V:134:C:N3     | 23:V:135:G:C6     | 2.85                     | 0.45              |
| 23:V:270:A:C5     | 23:V:270(A):A:C8  | 3.05                     | 0.45              |
| 23:V:270(N):G:H3' | 23:V:270(O):U:C5  | 2.50                     | 0.45              |
| 23:V:536:A:C5     | 23:V:558:G:N1     | 2.78                     | 0.45              |
| 23:V:1316:U:O2    | 23:V:1337:G:N2    | 2.49                     | 0.45              |
| 23:V:1448:G:H2'   | 23:V:1449:A:H5'   | 1.98                     | 0.45              |
| 23:V:2309:A:OP1   | 23:V:2310:A:N6    | 2.49                     | 0.45              |
| 27:a:61:ARG:HG2   | 27:a:62:PRO:HD3   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:d:9:ILE:HD11   | 30:d:69:ARG:HG3    | 1.98                     | 0.45              |
| 8:G:167:G:H2'     | 8:G:168:G:H8       | 1.82                     | 0.45              |
| 8:G:1412:C:H2'    | 8:G:1413:A:C8      | 2.51                     | 0.45              |
| 12:K:144:THR:O    | 12:K:147:ASP:N     | 2.37                     | 0.45              |
| 23:V:271(A):G:C3' | 23:V:271(B):U:H5'  | 2.46                     | 0.45              |
| 23:V:827:U:O2'    | 23:V:2068:U:N3     | 2.49                     | 0.45              |
| 23:V:1196:C:H2'   | 23:V:1197:G:C8     | 2.52                     | 0.45              |
| 29:c:67:LYS:HA    | 29:c:92:VAL:HG22   | 1.99                     | 0.45              |
| 4:C:26:ASN:HB2    | 4:C:71:THR:HG23    | 1.98                     | 0.45              |
| 5:D:19:VAL:HA     | 5:D:22:LEU:HB2     | 1.98                     | 0.45              |
| 10:I:188:LEU:HD21 | 10:I:195:VAL:HG13  | 1.98                     | 0.45              |
| 17:P:19:ALA:HA    | 17:P:31:THR:O      | 2.17                     | 0.45              |
| 23:V:631:A:OP2    | 53:AA:46:ARG:NH2   | 2.50                     | 0.45              |
| 23:V:852:G:O6     | 23:V:926:A:N6      | 2.50                     | 0.45              |
| 23:V:1545:A:C3'   | 23:V:1545(A):A:H4' | 2.47                     | 0.45              |
| 24:X:85:G:C2'     | 24:X:86:G:H5'      | 2.46                     | 0.45              |
| 25:Y:131:LEU:HD23 | 25:Y:137:LEU:HA    | 1.98                     | 0.45              |
| 32:f:41:PHE:O     | 32:f:45:THR:OG1    | 2.29                     | 0.45              |
| 44:r:88:LYS:HB3   | 44:r:91:GLU:HG3    | 1.99                     | 0.45              |
| 8:G:768:A:N3      | 8:G:1512:U:O2'     | 2.49                     | 0.45              |
| 14:M:30:ILE:HG22  | 14:M:39:ALA:HB1    | 1.98                     | 0.45              |
| 23:V:6:A:C2'      | 23:V:6:A:N3        | 2.80                     | 0.45              |
| 23:V:531:C:H5'    | 23:V:532:A:C2      | 2.51                     | 0.45              |
| 23:V:2124:G:C1'   | 25:Y:216:THR:CB    | 2.95                     | 0.45              |
| 23:V:2450:A:H62   | 23:V:2501:C:N4     | 2.10                     | 0.45              |
| 28:b:40:GLN:HE22  | 28:b:182:ASN:HB2   | 1.81                     | 0.45              |
| 29:c:40:ASN:OD1   | 29:c:89:GLY:O      | 2.35                     | 0.45              |
| 35:i:45:LEU:HB3   | 35:i:46:LYS:H      | 1.65                     | 0.45              |
| 45:s:36:LYS:HE3   | 45:s:38:TYR:HE1    | 1.81                     | 0.45              |
| 47:u:4:GLN:NE2    | 47:u:51:GLN:OE1    | 2.38                     | 0.45              |
| 8:G:199:G:C2'     | 8:G:200:G:H5'      | 2.46                     | 0.45              |
| 8:G:708:C:H2'     | 8:G:709:G:C8       | 2.52                     | 0.45              |
| 8:G:1485:U:H6     | 8:G:1485:U:O5'     | 1.99                     | 0.45              |
| 23:V:276:A:O4'    | 23:V:276:A:OP2     | 2.35                     | 0.45              |
| 23:V:856:C:O5'    | 23:V:856:C:H6      | 2.00                     | 0.45              |
| 27:a:61:ARG:HH21  | 27:a:62:PRO:HD3    | 1.81                     | 0.45              |
| 28:b:68:LYS:HD3   | 28:b:68:LYS:HA     | 1.86                     | 0.45              |
| 30:d:24:VAL:HG22  | 30:d:25:LYS:N      | 2.31                     | 0.45              |
| 45:s:100:VAL:HG12 | 45:s:133:ILE:CG1   | 2.45                     | 0.45              |
| 55:DD:47:7MG:H81  | 55:DD:47:7MG:H2'   | 1.71                     | 0.45              |
| 8:G:465:A:C5      | 8:G:467:G:C2       | 3.05                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:S:36:PHE:HD1   | 20:S:36:PHE:C     | 2.25                     | 0.45              |
| 23:V:153:C:C4     | 23:V:154:G:C6     | 3.05                     | 0.45              |
| 23:V:270(M):U:O3' | 23:V:270(N):G:H4' | 2.16                     | 0.45              |
| 23:V:270(V):G:C4  | 23:V:270(W):G:N7  | 2.85                     | 0.45              |
| 23:V:620:G:OP2    | 23:V:620:G:N2     | 2.43                     | 0.45              |
| 23:V:852:G:N1     | 23:V:853:G:C5     | 2.85                     | 0.45              |
| 23:V:1482:U:H6    | 23:V:1482:U:H5'   | 1.81                     | 0.45              |
| 23:V:1546:C:H3'   | 23:V:1546:C:H6    | 1.80                     | 0.45              |
| 23:V:1862:G:C2    | 23:V:1863:G:C5    | 3.04                     | 0.45              |
| 23:V:2792:G:H8    | 23:V:2792:G:O5'   | 1.99                     | 0.45              |
| 25:Y:61:THR:HG22  | 25:Y:143:GLY:HA3  | 1.99                     | 0.45              |
| 25:Y:71:GLN:HG2   | 25:Y:174:PRO:HB3  | 1.99                     | 0.45              |
| 30:d:18:GLU:CB    | 30:d:24:VAL:HB    | 2.47                     | 0.45              |
| 8:G:103:C:O5'     | 8:G:103:C:C6      | 2.70                     | 0.45              |
| 8:G:1163:C:O5'    | 8:G:1163:C:C6     | 2.70                     | 0.45              |
| 8:G:1323:G:H4'    | 8:G:1362:C:C5     | 2.51                     | 0.45              |
| 8:G:1485:U:O5'    | 8:G:1485:U:C6     | 2.70                     | 0.45              |
| 9:H:153:ARG:HG3   | 9:H:154:LEU:HD12  | 1.99                     | 0.45              |
| 14:M:85:TYR:HD2   | 14:M:154:TYR:HE2  | 1.65                     | 0.45              |
| 19:R:52:GLU:HB2   | 19:R:55:ARG:HG2   | 1.98                     | 0.45              |
| 23:V:270(C):C:O2  | 23:V:273:G:O2'    | 2.33                     | 0.45              |
| 23:V:270(E):G:C2  | 23:V:270(V):G:N2  | 2.85                     | 0.45              |
| 23:V:279:C:O5'    | 23:V:279:C:C6     | 2.70                     | 0.45              |
| 23:V:363(F):G:OP1 | 23:V:363(F):G:C8  | 2.71                     | 0.45              |
| 23:V:364:C:H6     | 23:V:364:C:H5''   | 1.82                     | 0.45              |
| 23:V:1084:A:O2'   | 23:V:1106:G:OP1   | 2.34                     | 0.45              |
| 23:V:1116:C:H6    | 23:V:1116:C:H5''  | 1.82                     | 0.45              |
| 23:V:1543:A:C8    | 23:V:1544:C:O4'   | 2.70                     | 0.45              |
| 23:V:1879:C:O5'   | 23:V:1879:C:H6    | 1.99                     | 0.45              |
| 23:V:2124:G:N2    | 25:Y:221:SER:H    | 2.11                     | 0.45              |
| 23:V:2795:G:C8    | 23:V:2795:G:OP2   | 2.70                     | 0.45              |
| 23:V:2840:C:H2'   | 23:V:2841:C:C6    | 2.52                     | 0.45              |
| 28:b:65:TRP:HZ3   | 28:b:75:HIS:HD2   | 1.65                     | 0.45              |
| 35:i:41:ARG:NH1   | 35:i:45:LEU:HD22  | 2.32                     | 0.45              |
| 39:m:52:ILE:HA    | 39:m:66:VAL:HG13  | 1.99                     | 0.45              |
| 44:r:76:CYS:HB3   | 44:r:99:CYS:HB2   | 1.75                     | 0.45              |
| 51:y:12:GLU:O     | 51:y:52:VAL:O     | 2.34                     | 0.45              |
| 55:DD:37:U:H6     | 55:DD:37:U:H5''   | 1.82                     | 0.45              |
| 8:G:75:C:O5'      | 8:G:75:C:C6       | 2.70                     | 0.44              |
| 8:G:97:U:O5'      | 8:G:97:U:C6       | 2.70                     | 0.44              |
| 8:G:235:C:H2'     | 8:G:236:G:H8      | 1.81                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:G:848:C:OP2      | 8:G:848:C:C6      | 2.70                     | 0.44              |
| 8:G:1286:A:H2'     | 8:G:1287:A:H4'    | 1.99                     | 0.44              |
| 8:G:1360:A:O5'     | 8:G:1360:A:H8     | 1.99                     | 0.44              |
| 23:V:372:G:H22     | 49:w:63:TYR:HB3   | 1.82                     | 0.44              |
| 23:V:998:C:OP1     | 40:n:84:LYS:NZ    | 2.49                     | 0.44              |
| 23:V:1447:G:C8     | 23:V:1447:G:OP2   | 2.71                     | 0.44              |
| 23:V:1449(A):G:C2' | 23:V:1450:C:O5'   | 2.63                     | 0.44              |
| 23:V:2785:C:O5'    | 23:V:2785:C:C6    | 2.71                     | 0.44              |
| 24:X:29:A:OP2      | 38:l:31:SER:OG    | 2.31                     | 0.44              |
| 32:f:19:PRO:CA     | 32:f:22:PRO:CD    | 2.94                     | 0.44              |
| 37:k:4:LEU:HD12    | 37:k:4:LEU:HA     | 1.74                     | 0.44              |
| 38:l:9:ARG:HB3     | 38:l:12:PHE:CE1   | 2.52                     | 0.44              |
| 55:DD:35:C:O2      | 55:DD:36:A:C8     | 2.70                     | 0.44              |
| 5:D:39:THR:HA      | 5:D:70:LYS:HA     | 1.97                     | 0.44              |
| 8:G:1161:C:N3      | 8:G:1176:A:N1     | 2.65                     | 0.44              |
| 8:G:1386:G:H2'     | 8:G:1387:G:H8     | 1.81                     | 0.44              |
| 8:G:1448:C:O5'     | 8:G:1448:C:C6     | 2.70                     | 0.44              |
| 8:G:1484:C:C6      | 8:G:1484:C:O5'    | 2.71                     | 0.44              |
| 23:V:270(L):U:O2   | 23:V:270(L):U:C2' | 2.65                     | 0.44              |
| 23:V:270(S):G:C2   | 23:V:270(T):G:C8  | 3.04                     | 0.44              |
| 23:V:730:C:OP1     | 23:V:1775:U:O2'   | 2.35                     | 0.44              |
| 23:V:847:U:H5''    | 23:V:929:G:O6     | 2.16                     | 0.44              |
| 23:V:856:C:O5'     | 23:V:856:C:C6     | 2.70                     | 0.44              |
| 23:V:1084:A:O2'    | 23:V:1106:G:C5    | 2.47                     | 0.44              |
| 23:V:1712:C:O5'    | 23:V:1712:C:C6    | 2.71                     | 0.44              |
| 23:V:1734:C:OP2    | 23:V:1734:C:C6    | 2.70                     | 0.44              |
| 23:V:1735:C:OP1    | 23:V:1735:C:C6    | 2.70                     | 0.44              |
| 23:V:2712(A):A:OP1 | 23:V:2712(A):A:C8 | 2.70                     | 0.44              |
| 23:V:2889:C:C6     | 23:V:2889:C:O5'   | 2.71                     | 0.44              |
| 25:Y:207:THR:HG22  | 25:Y:210:ARG:HA   | 2.00                     | 0.44              |
| 27:a:181:LEU:HD21  | 39:m:6:LEU:HD13   | 1.99                     | 0.44              |
| 29:c:35:GLU:HB2    | 29:c:160:VAL:HG23 | 1.99                     | 0.44              |
| 32:f:52:ILE:HG12   | 32:f:76:TYR:CG    | 2.47                     | 0.44              |
| 33:g:14:VAL:HB     | 33:g:52:VAL:HG23  | 1.99                     | 0.44              |
| 38:l:94:TYR:HA     | 38:l:98:VAL:HG11  | 1.98                     | 0.44              |
| 41:o:21:ARG:HD3    | 41:o:21:ARG:HA    | 1.82                     | 0.44              |
| 51:y:34:LEU:HD23   | 51:y:51:GLU:CG    | 2.48                     | 0.44              |
| 8:G:76:G:C2        | 8:G:95:G:C5       | 3.06                     | 0.44              |
| 8:G:672:U:O5'      | 8:G:672:U:C6      | 2.70                     | 0.44              |
| 8:G:1309:G:N3      | 8:G:1328:C:N4     | 2.66                     | 0.44              |
| 8:G:1454:G:H2'     | 8:G:1455:G:H8     | 1.81                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:1459:C:O5'    | 8:G:1459:C:C6     | 2.70                     | 0.44              |
| 16:O:79:LEU:HD22  | 16:O:101:PHE:HA   | 1.98                     | 0.44              |
| 20:S:25:VAL:CG1   | 20:S:39:LEU:CD2   | 2.89                     | 0.44              |
| 21:T:36:ILE:HD11  | 21:T:59:MET:HG3   | 1.99                     | 0.44              |
| 23:V:134:C:C2'    | 23:V:135:G:C8     | 2.97                     | 0.44              |
| 23:V:271(C):G:H2' | 23:V:272:G:H8     | 1.83                     | 0.44              |
| 23:V:925:C:H2'    | 23:V:926:A:C8     | 2.52                     | 0.44              |
| 23:V:1479:G:O5'   | 23:V:1479:G:C8    | 2.70                     | 0.44              |
| 23:V:2209:C:C4    | 23:V:2215:G:O6    | 2.60                     | 0.44              |
| 23:V:2508:G:O2'   | 23:V:2554:U:O2'   | 2.34                     | 0.44              |
| 23:V:2813:A:O5'   | 23:V:2813:A:C8    | 2.71                     | 0.44              |
| 25:Y:29:VAL:HA    | 25:Y:32:LEU:HB3   | 1.99                     | 0.44              |
| 29:c:138:GLN:HA   | 29:c:155:MET:HE2  | 1.99                     | 0.44              |
| 29:c:142:PRO:HG2  | 29:c:144:ILE:HG13 | 2.00                     | 0.44              |
| 39:m:65:LYS:HG3   | 39:m:75:ILE:HD11  | 1.99                     | 0.44              |
| 48:v:7:LYS:O      | 48:v:54:VAL:HA    | 2.17                     | 0.44              |
| 3:B:77:GLY:HA3    | 13:L:48:LEU:HD22  | 2.00                     | 0.44              |
| 6:E:5:ARG:HD2     | 6:E:71:LEU:HD11   | 2.00                     | 0.44              |
| 8:G:1310:G:H21    | 8:G:1328:C:H5     | 1.66                     | 0.44              |
| 15:N:70:GLN:HE21  | 15:N:72:PRO:HG2   | 1.82                     | 0.44              |
| 23:V:1107:G:H4'   | 31:e:81:VAL:HA    | 1.99                     | 0.44              |
| 23:V:1418:G:C6    | 23:V:1577:C:C5    | 3.06                     | 0.44              |
| 23:V:1455:G:OP2   | 23:V:1456:G:OP2   | 2.35                     | 0.44              |
| 23:V:2633:G:O5'   | 23:V:2633:G:C8    | 2.71                     | 0.44              |
| 23:V:2848:G:N1    | 23:V:2867:G:N3    | 2.65                     | 0.44              |
| 23:V:2885:C:O5'   | 23:V:2885:C:C6    | 2.71                     | 0.44              |
| 23:V:2898:U:O5'   | 23:V:2898:U:C6    | 2.71                     | 0.44              |
| 26:Z:147:LEU:HD12 | 26:Z:155:LEU:HD11 | 2.00                     | 0.44              |
| 32:f:89:HIS:HB3   | 32:f:90:LYS:H     | 1.62                     | 0.44              |
| 45:s:63:ASP:OD1   | 45:s:63:ASP:N     | 2.51                     | 0.44              |
| 55:DD:36:A:H8     | 55:DD:36:A:O5'    | 1.99                     | 0.44              |
| 3:B:45:SER:HB3    | 3:B:51:LEU:HD21   | 2.00                     | 0.44              |
| 8:G:1342:C:H2'    | 8:G:1343:G:H8     | 1.83                     | 0.44              |
| 8:G:1483:A:H5''   | 8:G:1484:C:OP2    | 2.18                     | 0.44              |
| 20:S:36:PHE:O     | 20:S:36:PHE:CD1   | 2.71                     | 0.44              |
| 20:S:39:LEU:H     | 20:S:39:LEU:HG    | 1.61                     | 0.44              |
| 23:V:41:C:O5'     | 23:V:41:C:C6      | 2.70                     | 0.44              |
| 23:V:138:G:O6     | 43:q:41:ASN:CG    | 2.61                     | 0.44              |
| 23:V:270(A):A:N6  | 23:V:270(Z):U:O5' | 2.50                     | 0.44              |
| 23:V:287:C:N3     | 23:V:355:G:N2     | 2.66                     | 0.44              |
| 23:V:878:A:H2'    | 23:V:879:G:C8     | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:925:C:O5'    | 23:V:925:C:C6     | 2.71                     | 0.44              |
| 23:V:1423:G:H2'   | 23:V:1424:G:C8    | 2.52                     | 0.44              |
| 23:V:1538:G:H2'   | 23:V:1539:G:C8    | 2.52                     | 0.44              |
| 23:V:1727:U:H3'   | 23:V:1728:G:H5''  | 1.99                     | 0.44              |
| 23:V:2126:A:OP1   | 25:Y:37:PHE:CZ    | 2.70                     | 0.44              |
| 23:V:2895:U:O2    | 23:V:2895:U:H2'   | 2.17                     | 0.44              |
| 25:Y:177:LYS:N    | 25:Y:180:PHE:HD1  | 1.76                     | 0.44              |
| 25:Y:180:PHE:HB2  | 25:Y:185:LEU:HD12 | 2.00                     | 0.44              |
| 36:j:58:PHE:O     | 36:j:60:ARG:N     | 2.49                     | 0.44              |
| 8:G:452:A:H2'     | 8:G:453:A:C8      | 2.53                     | 0.44              |
| 8:G:1169:A:H2'    | 8:G:1170:A:C8     | 2.53                     | 0.44              |
| 8:G:1295:G:O3'    | 19:R:14:ARG:NH2   | 2.50                     | 0.44              |
| 8:G:1358:U:H3     | 8:G:1363:A:H61    | 1.66                     | 0.44              |
| 8:G:1493:A:H1'    | 8:G:1494:G:C8     | 2.53                     | 0.44              |
| 23:V:270(B):A:C1' | 23:V:270(C):C:C5  | 2.92                     | 0.44              |
| 23:V:2795:G:OP1   | 23:V:2795:G:C5    | 2.70                     | 0.44              |
| 23:V:2897:U:C6    | 23:V:2897:U:O5'   | 2.71                     | 0.44              |
| 27:a:7:VAL:HG13   | 27:a:192:ASN:HA   | 1.99                     | 0.44              |
| 32:f:99:ILE:HD11  | 32:f:134:MET:HE2  | 2.00                     | 0.44              |
| 45:s:140:ASP:HB2  | 45:s:156:LYS:HE2  | 1.98                     | 0.44              |
| 51:y:11:LEU:HD22  | 51:y:26:ASN:HB2   | 1.99                     | 0.44              |
| 8:G:67:C:H2'      | 8:G:68:G:O4'      | 2.17                     | 0.44              |
| 8:G:138:G:H1      | 8:G:225:C:H42     | 1.66                     | 0.44              |
| 8:G:439:A:C5      | 8:G:496:A:C4      | 3.06                     | 0.44              |
| 8:G:501:C:C6      | 8:G:501:C:O5'     | 2.71                     | 0.44              |
| 8:G:676:A:H5'     | 17:P:113:PRO:HG3  | 1.99                     | 0.44              |
| 8:G:1258:G:O2'    | 8:G:1259:C:O4'    | 2.35                     | 0.44              |
| 9:H:51:LEU:HD22   | 9:H:55:PHE:HE2    | 1.82                     | 0.44              |
| 10:I:8:ILE:O      | 10:I:12:LEU:HB2   | 2.17                     | 0.44              |
| 23:V:270(X):G:C2  | 23:V:270(Y):G:H4' | 2.53                     | 0.44              |
| 23:V:1417:C:O5'   | 23:V:1417:C:C6    | 2.70                     | 0.44              |
| 23:V:2502:G:H5''  | 23:V:2503:A:H5''  | 1.99                     | 0.44              |
| 23:V:2884:U:C5    | 50:x:43:HIS:HD2   | 2.35                     | 0.44              |
| 26:Z:39:LYS:HD2   | 26:Z:62:TYR:HB2   | 1.99                     | 0.44              |
| 30:d:101:ARG:HB3  | 30:d:121:ILE:HD11 | 2.00                     | 0.44              |
| 32:f:20:ALA:CB    | 32:f:21:PRO:CD    | 2.76                     | 0.44              |
| 32:f:100:THR:O    | 32:f:103:GLN:N    | 2.50                     | 0.44              |
| 34:h:3:GLN:HE21   | 34:h:33:ALA:HB3   | 1.82                     | 0.44              |
| 55:DD:10:G:H2'    | 55:DD:11:A:C8     | 2.52                     | 0.44              |
| 1:W:17:U:H2'      | 1:W:18:G:H5'      | 1.98                     | 0.44              |
| 5:D:63:THR:OG1    | 5:D:64:GLU:N      | 2.47                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:G:209:U:C6       | 8:G:209:U:O5'     | 2.71                     | 0.44              |
| 8:G:1307:U:O5'     | 8:G:1307:U:C6     | 2.71                     | 0.44              |
| 9:H:22:LYS:HA      | 9:H:40:HIS:HE1    | 1.82                     | 0.44              |
| 9:H:81:VAL:HB      | 9:H:94:ASN:HD21   | 1.81                     | 0.44              |
| 15:N:21:LYS:O      | 15:N:65:TYR:OH    | 2.33                     | 0.44              |
| 18:Q:60:LEU:O      | 18:Q:63:GLY:N     | 2.51                     | 0.44              |
| 23:V:84:A:H5''     | 44:r:8:LYS:HE3    | 2.00                     | 0.44              |
| 23:V:1077:A:N6     | 23:V:1088:A:O3'   | 2.51                     | 0.44              |
| 23:V:1544:C:HO2'   | 23:V:1545:A:P     | 2.38                     | 0.44              |
| 23:V:1756:G:H4'    | 23:V:1758:G:H1'   | 2.00                     | 0.44              |
| 23:V:2198:A:N3     | 23:V:2198:A:C5'   | 2.74                     | 0.44              |
| 23:V:2212:A:H4'    | 23:V:2212:A:OP1   | 2.18                     | 0.44              |
| 23:V:2712(A):A:OP1 | 23:V:2712(A):A:H8 | 2.00                     | 0.44              |
| 23:V:2811:G:H2'    | 23:V:2812:G:H5'   | 1.98                     | 0.44              |
| 23:V:2885:C:O5'    | 23:V:2885:C:H6    | 2.01                     | 0.44              |
| 29:c:81:LYS:HB3    | 29:c:83:ARG:CZ    | 2.48                     | 0.44              |
| 44:r:13:VAL:HA     | 44:r:22:GLY:HA3   | 1.99                     | 0.44              |
| 2:A:10:VAL:HA      | 2:A:21:VAL:HG12   | 2.00                     | 0.44              |
| 8:G:101:A:H2       | 8:G:152:A:O2'     | 2.01                     | 0.44              |
| 11:J:25:ARG:HH12   | 11:J:30:LYS:HB2   | 1.83                     | 0.44              |
| 12:K:20:GLN:HG2    | 12:K:25:ARG:HH21  | 1.81                     | 0.44              |
| 23:V:99:U:C6       | 23:V:99:U:C3'     | 3.01                     | 0.44              |
| 23:V:1544:C:C2'    | 23:V:1545:A:C5'   | 2.86                     | 0.44              |
| 23:V:1728:G:OP1    | 23:V:1728:G:C8    | 2.71                     | 0.44              |
| 23:V:1879:C:O5'    | 23:V:1879:C:C6    | 2.71                     | 0.44              |
| 23:V:2275:C:O2'    | 36:j:84:GLY:O     | 2.29                     | 0.44              |
| 23:V:2794:C:C2     | 23:V:2799:A:C6    | 3.06                     | 0.44              |
| 25:Y:182:PRO:HD2   | 25:Y:183:GLU:OE1  | 2.17                     | 0.44              |
| 26:Z:43:ARG:HE     | 26:Z:44:ASN:ND2   | 2.15                     | 0.44              |
| 26:Z:143:HIS:ND1   | 26:Z:194:GLY:O    | 2.41                     | 0.44              |
| 30:d:105:LEU:HG    | 30:d:107:VAL:HG13 | 2.00                     | 0.44              |
| 31:e:25:PHE:HA     | 31:e:116:ILE:HA   | 2.00                     | 0.44              |
| 32:f:23:VAL:O      | 32:f:23:VAL:CG1   | 2.51                     | 0.44              |
| 35:i:101:VAL:HG13  | 35:i:106:LEU:HD23 | 2.00                     | 0.44              |
| 36:j:23:GLY:HA3    | 36:j:98:LYS:HB2   | 1.99                     | 0.44              |
| 44:r:34:LYS:HG2    | 44:r:63:LYS:HD3   | 2.00                     | 0.44              |
| 8:G:1159:U:O4'     | 8:G:1182:G:N2     | 2.51                     | 0.43              |
| 8:G:1309:G:C2      | 8:G:1328:C:N4     | 2.86                     | 0.43              |
| 14:M:48:LYS:HD2    | 14:M:48:LYS:HA    | 1.85                     | 0.43              |
| 23:V:43:G:C6       | 23:V:438:G:N2     | 2.84                     | 0.43              |
| 23:V:270(B):A:C1'  | 23:V:270(C):C:H5  | 2.30                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:1104:C:H6     | 23:V:1104:C:H5''  | 1.83                     | 0.43              |
| 23:V:2124:G:H1'    | 25:Y:216:THR:HB   | 1.99                     | 0.43              |
| 26:Z:254:THR:O     | 26:Z:254:THR:OG1  | 2.31                     | 0.43              |
| 54:BB:23:VAL:HB    | 54:BB:36:GLN:HG2  | 1.99                     | 0.43              |
| 8:G:452:A:H62      | 8:G:480:U:H3      | 1.65                     | 0.43              |
| 8:G:822:C:N4       | 8:G:823:G:O6      | 2.51                     | 0.43              |
| 18:Q:58:VAL:HG11   | 18:Q:85:ILE:HD11  | 2.00                     | 0.43              |
| 23:V:270(X):G:C2   | 23:V:270(Y):G:C1' | 3.02                     | 0.43              |
| 23:V:1533:C:H2'    | 23:V:1534:G:C8    | 2.54                     | 0.43              |
| 23:V:2166:G:H2'    | 23:V:2167:U:C2    | 2.53                     | 0.43              |
| 23:V:2208:U:H2'    | 23:V:2209:C:H5''  | 2.00                     | 0.43              |
| 23:V:2838:G:H2'    | 23:V:2839:G:C8    | 2.52                     | 0.43              |
| 24:X:89:G:C8       | 24:X:89:G:P       | 3.06                     | 0.43              |
| 25:Y:44:HIS:CE1    | 25:Y:172:HIS:HB3  | 2.53                     | 0.43              |
| 29:c:81:LYS:HB3    | 29:c:83:ARG:NH2   | 2.32                     | 0.43              |
| 32:f:19:PRO:HB2    | 32:f:23:VAL:HB    | 2.00                     | 0.43              |
| 32:f:131:ALA:HB1   | 32:f:136:VAL:HG13 | 2.00                     | 0.43              |
| 34:h:15:GLY:HA3    | 34:h:48:PRO:HD2   | 2.00                     | 0.43              |
| 35:i:61:ARG:H      | 35:i:61:ARG:HD2   | 1.83                     | 0.43              |
| 39:m:82:LEU:HG     | 39:m:84:GLN:H     | 1.82                     | 0.43              |
| 44:r:81:LYS:HZ1    | 44:r:94:LYS:HG2   | 1.83                     | 0.43              |
| 45:s:76:LEU:HD23   | 45:s:83:PRO:HB3   | 1.99                     | 0.43              |
| 8:G:45:U:H2'       | 8:G:46:G:H8       | 1.83                     | 0.43              |
| 8:G:138:G:C2       | 8:G:226:G:C2      | 3.06                     | 0.43              |
| 8:G:464:G:C6       | 8:G:466:C:H4'     | 2.53                     | 0.43              |
| 10:I:142:MET:HE1   | 10:I:170:GLN:HB2  | 1.99                     | 0.43              |
| 20:S:9:LYS:NZ      | 20:S:21:TYR:CD2   | 2.84                     | 0.43              |
| 23:V:37:C:H2'      | 23:V:38:A:C8      | 2.53                     | 0.43              |
| 23:V:155:C:O5'     | 23:V:155:C:C6     | 2.70                     | 0.43              |
| 23:V:172:C:C3'     | 23:V:172:C:C6     | 3.01                     | 0.43              |
| 23:V:249:C:O2      | 53:AA:11:LYS:NZ   | 2.49                     | 0.43              |
| 23:V:270(C):C:O2'  | 23:V:270(D):C:C5' | 2.62                     | 0.43              |
| 23:V:365:C:H3'     | 23:V:365:C:H6     | 1.83                     | 0.43              |
| 23:V:1066:U:H2'    | 32:f:13:PRO:HB3   | 2.00                     | 0.43              |
| 23:V:1197:G:O2'    | 23:V:1227:A:O2'   | 2.36                     | 0.43              |
| 23:V:1444(A):A:O5' | 23:V:1444(A):A:C8 | 2.70                     | 0.43              |
| 23:V:1589:C:C6     | 23:V:1589:C:O5'   | 2.71                     | 0.43              |
| 23:V:2789:C:C3'    | 23:V:2789:C:C6    | 3.01                     | 0.43              |
| 28:b:116:ASP:OD2   | 35:i:5:ASP:N      | 2.51                     | 0.43              |
| 30:d:167:GLU:HA    | 30:d:168:PRO:HD3  | 1.78                     | 0.43              |
| 39:m:50:ILE:HG12   | 39:m:66:VAL:HG12  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:DD:5:G:H2'     | 55:DD:6:G:C8      | 2.53                     | 0.43              |
| 2:A:63:ARG:NH1    | 8:G:190:G:O6      | 2.51                     | 0.43              |
| 8:G:110:C:H4'     | 22:U:25:ARG:HD3   | 2.01                     | 0.43              |
| 11:J:177:ASP:HB2  | 11:J:182:LYS:HB2  | 2.00                     | 0.43              |
| 23:V:137(A):G:OP2 | 23:V:137(A):G:C2  | 2.71                     | 0.43              |
| 23:V:373:U:O4     | 49:w:59:PHE:CD1   | 2.71                     | 0.43              |
| 23:V:852:G:C6     | 23:V:853:G:O6     | 2.71                     | 0.43              |
| 23:V:1544:C:N4    | 23:V:1545:A:N6    | 2.66                     | 0.43              |
| 23:V:1630:G:C4    | 23:V:1630(A):C:O2 | 2.71                     | 0.43              |
| 23:V:1750:G:H2'   | 23:V:1751:C:C6    | 2.53                     | 0.43              |
| 23:V:2312:U:H2'   | 29:c:40:ASN:HD21  | 1.83                     | 0.43              |
| 23:V:2782:G:N3    | 23:V:2782:G:C2'   | 2.79                     | 0.43              |
| 25:Y:38:ASP:HA    | 25:Y:178:ALA:HB2  | 2.00                     | 0.43              |
| 25:Y:39:GLU:HB3   | 25:Y:178:ALA:HA   | 2.01                     | 0.43              |
| 28:b:8:GLN:NE2    | 28:b:16:GLY:O     | 2.51                     | 0.43              |
| 28:b:158:THR:HG22 | 28:b:160:ASN:H    | 1.83                     | 0.43              |
| 30:d:46:GLU:HG3   | 30:d:47:GLU:H     | 1.82                     | 0.43              |
| 38:l:94:TYR:CD2   | 38:l:98:VAL:HG13  | 2.52                     | 0.43              |
| 8:G:740:U:OP1     | 21:T:38:ARG:NH1   | 2.51                     | 0.43              |
| 8:G:806:C:H2'     | 8:G:807:A:H8      | 1.83                     | 0.43              |
| 8:G:1161:C:H42    | 8:G:1176:A:N6     | 2.12                     | 0.43              |
| 17:P:57:THR:HG23  | 17:P:60:ALA:H     | 1.84                     | 0.43              |
| 23:V:265:A:H2     | 23:V:281:G:H5'    | 1.82                     | 0.43              |
| 23:V:974:G:N9     | 23:V:1187:G:O2'   | 2.41                     | 0.43              |
| 23:V:1106:G:C8    | 23:V:1106:G:O5'   | 2.70                     | 0.43              |
| 23:V:1363:C:H5'   | 23:V:1809:A:H62   | 1.83                     | 0.43              |
| 23:V:1435:G:N2    | 23:V:1477:A:O2'   | 2.45                     | 0.43              |
| 23:V:2226:C:H2'   | 23:V:2227:A:C4'   | 2.48                     | 0.43              |
| 23:V:2379:G:OP1   | 38:l:20:ARG:NH1   | 2.52                     | 0.43              |
| 23:V:2630:G:C8    | 23:V:2894:G:C8    | 3.06                     | 0.43              |
| 23:V:2814:C:H6    | 23:V:2814:C:O5'   | 2.01                     | 0.43              |
| 25:Y:150:GLY:O    | 25:Y:154:ARG:HB2  | 2.18                     | 0.43              |
| 29:c:71:THR:O     | 29:c:87:PRO:CA    | 2.65                     | 0.43              |
| 30:d:27:LYS:HB3   | 30:d:32:GLU:HA    | 1.99                     | 0.43              |
| 30:d:87:LEU:HD21  | 30:d:162:ILE:HD11 | 2.01                     | 0.43              |
| 8:G:344:A:H5''    | 8:G:345:C:H5      | 1.83                     | 0.43              |
| 10:I:6:HIS:CD2    | 10:I:8:ILE:HG12   | 2.54                     | 0.43              |
| 10:I:179:ARG:NE   | 10:I:206:GLU:OE2  | 2.49                     | 0.43              |
| 20:S:26:ARG:HD3   | 20:S:43:CYS:CB    | 2.40                     | 0.43              |
| 23:V:44:A:H2'     | 23:V:45:G:C8      | 2.53                     | 0.43              |
| 23:V:296:C:H2'    | 23:V:297:C:C6     | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:V:1450:C:H2'   | 23:V:1451:C:H4'   | 1.99                     | 0.43              |
| 23:V:2126:A:H62   | 23:V:2164:C:P     | 2.42                     | 0.43              |
| 23:V:2792:G:O5'   | 23:V:2792:G:C8    | 2.71                     | 0.43              |
| 25:Y:212:VAL:O    | 25:Y:223:ARG:NH2  | 2.49                     | 0.43              |
| 36:j:54:MET:HE2   | 36:j:118:LEU:HB3  | 2.01                     | 0.43              |
| 8:G:976:G:N3      | 8:G:1363:A:N6     | 2.66                     | 0.43              |
| 8:G:1007:C:N4     | 8:G:1023:G:O6     | 2.52                     | 0.43              |
| 8:G:1160:G:N2     | 8:G:1161:C:C2     | 2.87                     | 0.43              |
| 8:G:1256:A:H4'    | 8:G:1258:G:C8     | 2.53                     | 0.43              |
| 8:G:1309:G:N2     | 8:G:1328:C:N3     | 2.26                     | 0.43              |
| 8:G:1360:A:OP1    | 8:G:1360:A:C8     | 2.71                     | 0.43              |
| 9:H:54:THR:HG21   | 9:H:201:ILE:HD11  | 2.01                     | 0.43              |
| 10:I:70:VAL:HG12  | 10:I:72:LYS:H     | 1.84                     | 0.43              |
| 20:S:25:VAL:O     | 20:S:25:VAL:HG22  | 2.19                     | 0.43              |
| 23:V:270(M):U:O3' | 23:V:270(N):G:C4' | 2.66                     | 0.43              |
| 23:V:366:C:OP2    | 23:V:366:C:C6     | 2.71                     | 0.43              |
| 23:V:524:U:N3     | 23:V:525:U:O4     | 2.51                     | 0.43              |
| 23:V:542:C:O5'    | 23:V:542:C:H6     | 2.02                     | 0.43              |
| 23:V:1748:G:O5'   | 23:V:1748:G:C8    | 2.71                     | 0.43              |
| 25:Y:176:GLY:HA2  | 25:Y:180:PHE:CG   | 2.54                     | 0.43              |
| 25:Y:213:TYR:HA   | 25:Y:223:ARG:HB2  | 2.00                     | 0.43              |
| 29:c:71:THR:O     | 29:c:87:PRO:C     | 2.61                     | 0.43              |
| 32:f:72:PRO:HA    | 32:f:73:PRO:HD3   | 1.84                     | 0.43              |
| 38:l:62:LYS:HD2   | 38:l:65:VAL:HG13  | 2.01                     | 0.43              |
| 48:v:26:LEU:HD21  | 48:v:47:VAL:HG22  | 1.99                     | 0.43              |
| 8:G:718:G:H5''    | 8:G:720:C:H41     | 1.83                     | 0.43              |
| 8:G:971:G:H2'     | 8:G:1365:G:O2'    | 2.19                     | 0.43              |
| 8:G:1157:A:H61    | 8:G:1178:G:H1'    | 1.82                     | 0.43              |
| 8:G:1287:A:H2     | 8:G:1353:G:H1'    | 1.83                     | 0.43              |
| 8:G:1485:U:H2'    | 8:G:1486:G:H8     | 1.81                     | 0.43              |
| 9:H:181:PHE:HE1   | 15:N:72:PRO:HD3   | 1.82                     | 0.43              |
| 15:N:69:ARG:HG3   | 15:N:70:GLN:H     | 1.83                     | 0.43              |
| 23:V:106:C:O2     | 23:V:294:A:O2'    | 2.36                     | 0.43              |
| 23:V:1116:C:H2'   | 23:V:1117:G:C8    | 2.53                     | 0.43              |
| 23:V:1300:U:H6    | 23:V:1300:U:H2'   | 1.64                     | 0.43              |
| 23:V:1838:C:N4    | 23:V:1898:U:OP2   | 2.28                     | 0.43              |
| 23:V:2787:C:C3'   | 23:V:2787:C:C6    | 3.01                     | 0.43              |
| 35:i:51:PHE:CA    | 35:i:57:THR:HG23  | 2.48                     | 0.43              |
| 36:j:22:LYS:HB3   | 36:j:22:LYS:HE3   | 1.80                     | 0.43              |
| 38:l:15:ARG:CG    | 38:l:15:ARG:NH2   | 2.79                     | 0.43              |
| 8:G:75:C:O5'      | 8:G:75:C:H6       | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:1010:G:H2'    | 8:G:1011:G:C8     | 2.54                     | 0.43              |
| 8:G:1099:G:H5'    | 9:H:96:ARG:HH12   | 1.83                     | 0.43              |
| 9:H:70:PHE:HB3    | 9:H:163:PHE:HB3   | 2.01                     | 0.43              |
| 20:S:9:LYS:NZ     | 20:S:21:TYR:CE2   | 2.86                     | 0.43              |
| 23:V:2813:A:HO2'  | 23:V:2814:C:H5'   | 1.81                     | 0.43              |
| 23:V:2894:G:N3    | 23:V:2894:G:H2'   | 2.33                     | 0.43              |
| 34:h:62:VAL:HG12  | 34:h:63:VAL:HG13  | 2.01                     | 0.43              |
| 38:l:28:VAL:HA    | 38:l:36:TYR:O     | 2.19                     | 0.43              |
| 38:l:75:GLU:HA    | 38:l:78:LEU:HD23  | 2.00                     | 0.43              |
| 8:G:1118:C:C2     | 8:G:1179:A:C6     | 3.07                     | 0.43              |
| 12:K:145:LYS:HA   | 12:K:148:VAL:HG12 | 1.99                     | 0.43              |
| 23:V:28:A:N6      | 23:V:512:G:O2'    | 2.52                     | 0.43              |
| 23:V:268:C:C2     | 23:V:269:U:C5     | 3.06                     | 0.43              |
| 23:V:535:C:O5'    | 23:V:535:C:C6     | 2.70                     | 0.43              |
| 23:V:1169:G:C3'   | 23:V:1170:G:H8    | 2.32                     | 0.43              |
| 23:V:1711:C:C6    | 23:V:1711:C:C3'   | 3.01                     | 0.43              |
| 23:V:2209:C:C4    | 23:V:2216:G:C2    | 3.02                     | 0.43              |
| 30:d:95:ARG:HB2   | 30:d:129:THR:CB   | 2.44                     | 0.43              |
| 35:i:146:VAL:HG12 | 35:i:147:LEU:H    | 1.84                     | 0.43              |
| 38:l:9:ARG:CA     | 38:l:12:PHE:CD1   | 3.01                     | 0.43              |
| 8:G:91:C:C4       | 8:G:92:G:N7       | 2.86                     | 0.42              |
| 23:V:16:G:O2'     | 23:V:17:G:H5'     | 2.18                     | 0.42              |
| 23:V:283:A:H5'    | 23:V:284:U:H5     | 1.83                     | 0.42              |
| 23:V:1716:U:C3'   | 23:V:1716:U:C6    | 3.02                     | 0.42              |
| 45:s:116:VAL:HG12 | 45:s:174:VAL:HG11 | 2.00                     | 0.42              |
| 8:G:456:C:O2      | 8:G:477:G:C2      | 2.72                     | 0.42              |
| 8:G:1015:A:H2'    | 8:G:1016:A:H8     | 1.84                     | 0.42              |
| 8:G:1448:C:O2'    | 8:G:1449:C:OP1    | 2.35                     | 0.42              |
| 23:V:271(B):U:O2' | 23:V:271(C):G:H4' | 2.20                     | 0.42              |
| 23:V:438:G:O5'    | 23:V:438:G:H8     | 2.02                     | 0.42              |
| 23:V:1414:G:N2    | 23:V:1589:C:O2    | 2.52                     | 0.42              |
| 23:V:1468:C:N3    | 23:V:1525:G:N2    | 2.68                     | 0.42              |
| 23:V:2209:C:H2'   | 23:V:2210:G:OP1   | 2.18                     | 0.42              |
| 23:V:2305:A:N6    | 29:c:153:ARG:O    | 2.52                     | 0.42              |
| 23:V:2791:C:N4    | 23:V:2893:G:H21   | 2.12                     | 0.42              |
| 24:X:23:G:N3      | 24:X:61:G:N2      | 2.68                     | 0.42              |
| 25:Y:180:PHE:CE2  | 25:Y:185:LEU:HB2  | 2.53                     | 0.42              |
| 8:G:1360:A:O5'    | 8:G:1360:A:C8     | 2.71                     | 0.42              |
| 20:S:22:THR:HB    | 20:S:33:VAL:HG21  | 2.01                     | 0.42              |
| 21:T:24:SER:OG    | 21:T:25:THR:N     | 2.52                     | 0.42              |
| 23:V:270(Z):U:O2  | 23:V:270(Z):U:C2' | 2.56                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:V:281:G:C2    | 23:V:281:G:OP1    | 2.72                     | 0.42              |
| 23:V:374:A:N3    | 23:V:401:A:N1     | 2.67                     | 0.42              |
| 23:V:1441:G:N1   | 23:V:1442:G:C5    | 2.87                     | 0.42              |
| 23:V:2630:G:C2   | 23:V:2790:A:C2    | 3.02                     | 0.42              |
| 42:p:12:ILE:HG13 | 42:p:13:SER:H     | 1.84                     | 0.42              |
| 45:s:149:SER:O   | 45:s:151:HIS:ND1  | 2.43                     | 0.42              |
| 55:DD:48:U:C3'   | 55:DD:48:U:C6     | 3.02                     | 0.42              |
| 8:G:824:C:H2'    | 8:G:825:G:H8      | 1.85                     | 0.42              |
| 9:H:73:THR:HG23  | 9:H:96:ARG:HG2    | 2.02                     | 0.42              |
| 10:I:6:HIS:HA    | 10:I:7:PRO:HD3    | 1.90                     | 0.42              |
| 14:M:115:ARG:HB3 | 14:M:118:VAL:HG12 | 2.00                     | 0.42              |
| 22:U:39:TYR:HD1  | 22:U:49:LEU:HD13  | 1.84                     | 0.42              |
| 23:V:155:C:O5'   | 23:V:155:C:H6     | 2.02                     | 0.42              |
| 23:V:278:A:H2    | 23:V:362:U:O2     | 2.01                     | 0.42              |
| 23:V:630:G:N2    | 23:V:634:C:OP2    | 2.48                     | 0.42              |
| 23:V:926:A:O5'   | 23:V:926:A:C8     | 2.70                     | 0.42              |
| 23:V:973:A:O4'   | 23:V:1188:U:C2    | 2.72                     | 0.42              |
| 23:V:1106:G:C2   | 31:e:81:VAL:CB    | 3.02                     | 0.42              |
| 25:Y:49:ILE:HG13 | 25:Y:51:PRO:HD3   | 2.02                     | 0.42              |
| 28:b:122:LYS:HE2 | 28:b:122:LYS:HB3  | 1.89                     | 0.42              |
| 29:c:67:LYS:HZ1  | 29:c:90:LEU:HD12  | 1.78                     | 0.42              |
| 32:f:85:GLU:HB3  | 32:f:95:LYS:HG2   | 2.00                     | 0.42              |
| 37:k:73:VAL:HA   | 37:k:76:VAL:HG22  | 2.01                     | 0.42              |
| 43:q:12:VAL:HG12 | 43:q:29:TRP:NE1   | 2.34                     | 0.42              |
| 49:w:48:ARG:HB2  | 49:w:49:PHE:HD1   | 1.83                     | 0.42              |
| 8:G:103:C:O5'    | 8:G:103:C:H6      | 2.02                     | 0.42              |
| 8:G:191:G:H2'    | 8:G:192:U:C6      | 2.54                     | 0.42              |
| 8:G:1414:U:H2'   | 8:G:1415:G:C8     | 2.54                     | 0.42              |
| 9:H:187:LEU:HD22 | 9:H:205:ASP:HB3   | 2.01                     | 0.42              |
| 12:K:50:GLU:HB3  | 12:K:52:PRO:HD2   | 2.02                     | 0.42              |
| 13:L:45:LEU:HD21 | 13:L:57:GLN:HG3   | 2.02                     | 0.42              |
| 17:P:21:ILE:HG22 | 17:P:30:VAL:HG13  | 2.02                     | 0.42              |
| 23:V:270(J):G:C5 | 23:V:270(K):C:C4  | 3.06                     | 0.42              |
| 23:V:644:A:H8    | 23:V:2349:G:N3    | 2.18                     | 0.42              |
| 23:V:644:A:H4'   | 23:V:2350:C:C2    | 2.54                     | 0.42              |
| 23:V:923:C:C6    | 23:V:924:C:C5     | 3.06                     | 0.42              |
| 23:V:974:G:C6    | 23:V:1187:G:C4    | 2.98                     | 0.42              |
| 23:V:1173:G:C1'  | 23:V:1177:A:H61   | 2.19                     | 0.42              |
| 23:V:1547:C:O5'  | 23:V:1547:C:H6    | 2.03                     | 0.42              |
| 23:V:1585:C:H6   | 23:V:1585:C:H3'   | 1.85                     | 0.42              |
| 23:V:1586:A:O2'  | 23:V:1587:A:C8    | 2.73                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:V:2126:A:O3'   | 23:V:2127:G:C8     | 2.72                     | 0.42              |
| 32:f:35:MET:N     | 32:f:35:MET:SD     | 2.92                     | 0.42              |
| 40:n:21:ALA:HB2   | 40:n:39:LEU:HD12   | 2.02                     | 0.42              |
| 48:v:11:SER:O     | 48:v:11:SER:OG     | 2.29                     | 0.42              |
| 55:DD:30:G:H2'    | 55:DD:31:G:H8      | 1.81                     | 0.42              |
| 11:J:3:ARG:HH22   | 11:J:115:ARG:HE    | 1.68                     | 0.42              |
| 23:V:270(A):A:C2  | 23:V:270(X):G:N2   | 2.87                     | 0.42              |
| 23:V:537:C:O5'    | 23:V:537:C:C6      | 2.73                     | 0.42              |
| 23:V:552:G:C2'    | 23:V:553:U:C5'     | 2.97                     | 0.42              |
| 23:V:928:G:O5'    | 23:V:928:G:C8      | 2.70                     | 0.42              |
| 23:V:1169:G:N2    | 23:V:1180:C:O2     | 2.53                     | 0.42              |
| 23:V:1545:A:H2'   | 23:V:1545(A):A:O4' | 2.20                     | 0.42              |
| 23:V:1787:A:O5'   | 23:V:1787:A:C8     | 2.71                     | 0.42              |
| 23:V:1862:G:N2    | 23:V:1863:G:C6     | 2.88                     | 0.42              |
| 23:V:2181:G:H2'   | 23:V:2182:G:C2     | 2.55                     | 0.42              |
| 23:V:2209:C:C4    | 23:V:2212:A:C2     | 3.02                     | 0.42              |
| 23:V:2795:G:C8    | 23:V:2795:G:P      | 3.12                     | 0.42              |
| 25:Y:161:ILE:HG13 | 25:Y:162:GLU:N     | 2.35                     | 0.42              |
| 27:a:17:ASP:OD1   | 27:a:17:ASP:N      | 2.52                     | 0.42              |
| 29:c:76:SER:O     | 29:c:77:ILE:O      | 2.37                     | 0.42              |
| 30:d:23:ARG:HB3   | 30:d:36:PRO:CA     | 2.47                     | 0.42              |
| 34:h:10:VAL:HG12  | 34:h:17:ARG:HG3    | 2.01                     | 0.42              |
| 38:l:27:SER:O     | 38:l:37:ALA:HA     | 2.18                     | 0.42              |
| 38:l:57:LYS:HG2   | 38:l:59:LYS:HG3    | 2.01                     | 0.42              |
| 38:l:92:TYR:HB3   | 38:l:93:LYS:H      | 1.50                     | 0.42              |
| 45:s:158:PRO:O    | 45:s:160:GLY:N     | 2.52                     | 0.42              |
| 8:G:693:G:O2'     | 14:M:81:GLY:O      | 2.33                     | 0.42              |
| 8:G:1448:C:C5     | 8:G:1449:C:H5      | 2.37                     | 0.42              |
| 13:L:79:LEU:HB3   | 13:L:88:VAL:HG11   | 2.01                     | 0.42              |
| 18:Q:84:LEU:HD13  | 18:Q:104:VAL:HG11  | 2.01                     | 0.42              |
| 23:V:197:A:N6     | 23:V:2430:A:O2'    | 2.53                     | 0.42              |
| 23:V:276:A:N3     | 23:V:276:A:C2'     | 2.82                     | 0.42              |
| 23:V:290:G:H1     | 23:V:350:U:H3      | 1.67                     | 0.42              |
| 23:V:374:A:N3     | 23:V:401:A:C2      | 2.88                     | 0.42              |
| 23:V:506:G:HO2'   | 23:V:507:A:H8      | 1.65                     | 0.42              |
| 23:V:1541:U:O5'   | 23:V:1541:U:C6     | 2.70                     | 0.42              |
| 23:V:1735:C:H6    | 23:V:1735:C:H5''   | 1.85                     | 0.42              |
| 23:V:2295:C:H5    | 38:l:9:ARG:NH1     | 2.18                     | 0.42              |
| 23:V:2794:C:O2    | 23:V:2799:A:N1     | 2.52                     | 0.42              |
| 23:V:2802:G:O5'   | 23:V:2802:G:C8     | 2.70                     | 0.42              |
| 27:a:60:ASN:HA    | 27:a:63:LEU:HB2    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:c:22:ARG:HG3   | 29:c:23:PHE:CD2   | 2.53                     | 0.42              |
| 39:m:66:VAL:O     | 39:m:75:ILE:HA    | 2.19                     | 0.42              |
| 8:G:73:G:H2'      | 8:G:74:C:H5'      | 2.01                     | 0.42              |
| 8:G:85:U:O5'      | 8:G:85:U:C6       | 2.71                     | 0.42              |
| 8:G:1118:C:OP1    | 16:O:9:ARG:CZ     | 2.68                     | 0.42              |
| 8:G:1502:A:H2     | 8:G:1505:G:H22    | 1.66                     | 0.42              |
| 17:P:114:VAL:HG12 | 17:P:116:HIS:H    | 1.85                     | 0.42              |
| 23:V:1085:A:O2'   | 23:V:1086:A:OP2   | 2.35                     | 0.42              |
| 23:V:1418:G:N3    | 23:V:1581:G:N2    | 2.66                     | 0.42              |
| 23:V:1454:U:H3'   | 23:V:1454:U:O2    | 2.19                     | 0.42              |
| 23:V:2124:G:C5    | 25:Y:218:MET:HA   | 2.53                     | 0.42              |
| 23:V:2129:C:O5'   | 23:V:2129:C:C6    | 2.70                     | 0.42              |
| 23:V:2226:C:H2'   | 23:V:2227:A:O5'   | 2.20                     | 0.42              |
| 23:V:2313:C:O4'   | 29:c:40:ASN:ND2   | 2.53                     | 0.42              |
| 29:c:81:LYS:CG    | 29:c:83:ARG:HH22  | 2.32                     | 0.42              |
| 45:s:102:LEU:HD23 | 45:s:137:ILE:HD13 | 2.01                     | 0.42              |
| 8:G:375:U:H2'     | 8:G:376:G:H8      | 1.84                     | 0.42              |
| 8:G:877:C:H2'     | 8:G:878:G:H8      | 1.84                     | 0.42              |
| 8:G:1429:C:H2'    | 8:G:1430:C:H6     | 1.85                     | 0.42              |
| 17:P:121:PRO:HB2  | 17:P:125:PHE:HB2  | 2.00                     | 0.42              |
| 23:V:626:U:H5'    | 23:V:653:A:C6     | 2.55                     | 0.42              |
| 23:V:2046:G:H5''  | 50:x:19:ARG:HG2   | 2.00                     | 0.42              |
| 23:V:2206:C:C3'   | 23:V:2206:C:C6    | 3.03                     | 0.42              |
| 28:b:77:ASP:OD1   | 28:b:77:ASP:N     | 2.52                     | 0.42              |
| 8:G:1015:A:H2'    | 8:G:1016:A:C8     | 2.55                     | 0.42              |
| 23:V:13:A:C2      | 23:V:526:A:C5     | 3.08                     | 0.42              |
| 23:V:41:C:O5'     | 23:V:41:C:H6      | 2.03                     | 0.42              |
| 23:V:265:A:C4     | 23:V:281:G:N2     | 2.87                     | 0.42              |
| 23:V:270(W):G:C5  | 23:V:270(X):G:N7  | 2.88                     | 0.42              |
| 23:V:278:A:H2     | 23:V:362:U:C2     | 2.38                     | 0.42              |
| 23:V:614:U:N3     | 28:b:175:THR:O    | 2.49                     | 0.42              |
| 23:V:1058:G:C6    | 31:e:34:ALA:HB3   | 2.55                     | 0.42              |
| 23:V:1171:G:H3'   | 23:V:1173:G:H5''  | 2.01                     | 0.42              |
| 23:V:1417:C:O2    | 23:V:1582:C:O2'   | 2.23                     | 0.42              |
| 25:Y:180:PHE:CD2  | 25:Y:185:LEU:HB2  | 2.55                     | 0.42              |
| 39:m:31:SER:HA    | 39:m:48:ILE:O     | 2.20                     | 0.42              |
| 49:w:42:PHE:HD2   | 49:w:58:ARG:HB2   | 1.84                     | 0.42              |
| 51:y:14:THR:HG21  | 51:y:52:VAL:HG11  | 2.02                     | 0.42              |
| 54:BB:14:CYS:HA   | 54:BB:27:CYS:HA   | 2.02                     | 0.42              |
| 3:B:23:LYS:HE3    | 3:B:58:LEU:HD23   | 2.02                     | 0.41              |
| 8:G:458:C:O5'     | 8:G:458:C:H6      | 2.03                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:G:1312:G:N2    | 8:G:1313:U:H3     | 2.18                     | 0.41              |
| 11:J:145:GLU:HG2 | 11:J:184:LYS:HG2  | 2.02                     | 0.41              |
| 23:V:143:C:H3'   | 23:V:143:C:H6     | 1.85                     | 0.41              |
| 23:V:355:G:H2'   | 23:V:356:G:C4     | 2.55                     | 0.41              |
| 23:V:1113:U:H5'' | 23:V:1113:U:H6    | 1.85                     | 0.41              |
| 23:V:1782:C:C6   | 23:V:1782:C:H5'   | 2.54                     | 0.41              |
| 23:V:1854:A:H62  | 23:V:1888:G:H8    | 1.68                     | 0.41              |
| 25:Y:59:ARG:HD3  | 25:Y:139:ASN:HD22 | 1.85                     | 0.41              |
| 30:d:98:LEU:HD11 | 30:d:125:VAL:CG2  | 2.41                     | 0.41              |
| 54:BB:2:LYS:HG2  | 54:BB:35:ARG:HG3  | 2.02                     | 0.41              |
| 2:A:20:THR:HA    | 2:A:43:LEU:HA     | 2.02                     | 0.41              |
| 8:G:191(E):G:O5' | 8:G:191(E):G:C8   | 2.70                     | 0.41              |
| 8:G:817:C:H4'    | 8:G:818:G:H5'     | 2.02                     | 0.41              |
| 8:G:1356:G:H2'   | 8:G:1357:A:H8     | 1.84                     | 0.41              |
| 16:O:12:GLU:H    | 16:O:104:ARG:HH21 | 1.66                     | 0.41              |
| 23:V:13:A:C4     | 23:V:15:G:O6      | 2.73                     | 0.41              |
| 23:V:1539:G:O5'  | 23:V:1539:G:C8    | 2.71                     | 0.41              |
| 23:V:2713:A:O2'  | 23:V:2714:G:H5''  | 2.20                     | 0.41              |
| 23:V:2897:U:H3'  | 23:V:2897:U:H6    | 1.85                     | 0.41              |
| 24:X:2:C:H42     | 24:X:119:A:N6     | 2.18                     | 0.41              |
| 32:f:78:ILE:HG23 | 32:f:108:ALA:HB2  | 2.02                     | 0.41              |
| 43:q:5:TYR:CZ    | 47:u:21:ARG:HD2   | 2.55                     | 0.41              |
| 51:y:9:LEU:HD11  | 51:y:28:ARG:HG3   | 2.02                     | 0.41              |
| 8:G:842:C:C3'    | 8:G:842:C:C6      | 3.03                     | 0.41              |
| 8:G:932:C:H5'    | 14:M:4:ARG:HH11   | 1.84                     | 0.41              |
| 8:G:1049:U:C2    | 8:G:1201:A:H1'    | 2.56                     | 0.41              |
| 9:H:69:LEU:HB3   | 9:H:162:ILE:HG13  | 2.02                     | 0.41              |
| 9:H:214:ILE:H    | 9:H:214:ILE:HG13  | 1.71                     | 0.41              |
| 12:K:40:ARG:HG2  | 12:K:66:MET:HE3   | 2.02                     | 0.41              |
| 20:S:29:ARG:HB3  | 20:S:40:CYS:SG    | 2.60                     | 0.41              |
| 23:V:154:G:H8    | 23:V:154:G:P      | 2.43                     | 0.41              |
| 23:V:223:A:O2'   | 23:V:420:C:O2     | 2.30                     | 0.41              |
| 23:V:270(T):G:N1 | 23:V:270(U):C:C4  | 2.88                     | 0.41              |
| 23:V:630:G:OP1   | 53:AA:46:ARG:NH1  | 2.54                     | 0.41              |
| 23:V:1054:A:H2'  | 23:V:1055:G:C8    | 2.56                     | 0.41              |
| 23:V:1725:G:H2'  | 23:V:1726:G:H8    | 1.86                     | 0.41              |
| 23:V:2826:A:H2'  | 23:V:2827:C:C6    | 2.55                     | 0.41              |
| 29:c:81:LYS:HA   | 29:c:81:LYS:HD3   | 1.36                     | 0.41              |
| 32:f:66:THR:O    | 32:f:68:VAL:N     | 2.53                     | 0.41              |
| 38:l:33:LYS:HD2  | 38:l:33:LYS:HA    | 1.87                     | 0.41              |
| 45:s:95:PRO:HB3  | 45:s:98:MET:SD    | 2.60                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:68:LYS:NZ     | 8:G:196:A:OP1     | 2.39                     | 0.41              |
| 4:C:105:SER:HB3   | 8:G:191:G:H1'     | 2.03                     | 0.41              |
| 5:D:37:ARG:NH1    | 8:G:1318:A:O2'    | 2.53                     | 0.41              |
| 8:G:1355:G:H2'    | 8:G:1356:G:C8     | 2.55                     | 0.41              |
| 23:V:270(L):U:O2  | 23:V:270(M):U:C5  | 2.72                     | 0.41              |
| 23:V:270(M):U:O2  | 23:V:270(M):U:C2' | 2.68                     | 0.41              |
| 23:V:852:G:C5     | 23:V:853:G:N7     | 2.89                     | 0.41              |
| 23:V:1057:A:H5''  | 31:e:32:LEU:N     | 2.35                     | 0.41              |
| 23:V:1058:G:O4'   | 31:e:35:LYS:N     | 2.37                     | 0.41              |
| 23:V:1173:G:N3    | 23:V:1173:G:H5''  | 2.35                     | 0.41              |
| 23:V:1936:A:H2    | 23:V:1943:U:H3    | 1.68                     | 0.41              |
| 23:V:1938:A:N3    | 23:V:1938:A:C2'   | 2.82                     | 0.41              |
| 23:V:2140:C:H2'   | 23:V:2141:G:H8    | 1.85                     | 0.41              |
| 23:V:2414:G:H21   | 35:i:67:MET:HE1   | 1.85                     | 0.41              |
| 23:V:2839:G:O5'   | 23:V:2839:G:C8    | 2.70                     | 0.41              |
| 24:X:2:C:N3       | 24:X:119:A:N1     | 2.68                     | 0.41              |
| 26:Z:177:LEU:HA   | 26:Z:177:LEU:HD23 | 1.79                     | 0.41              |
| 27:a:13:ARG:HD3   | 27:a:13:ARG:HA    | 1.82                     | 0.41              |
| 28:b:78:ILE:HG23  | 28:b:83:PHE:HE1   | 1.86                     | 0.41              |
| 45:s:93:ASP:O     | 45:s:94:GLU:HG3   | 2.19                     | 0.41              |
| 17:P:21:ILE:HD11  | 17:P:84:VAL:HG12  | 2.03                     | 0.41              |
| 19:R:102:ARG:HH11 | 19:R:102:ARG:CG   | 2.26                     | 0.41              |
| 23:V:153:C:H3'    | 23:V:154:G:H8     | 1.62                     | 0.41              |
| 23:V:270(R):G:N2  | 23:V:270(S):G:C4  | 2.89                     | 0.41              |
| 23:V:293:U:H3     | 23:V:346:A:N6     | 2.16                     | 0.41              |
| 23:V:1071:G:N3    | 23:V:1089:G:H2'   | 2.36                     | 0.41              |
| 23:V:1191:G:H2'   | 23:V:1192:G:C8    | 2.56                     | 0.41              |
| 23:V:1446:C:H3'   | 23:V:1447:G:H8    | 1.84                     | 0.41              |
| 25:Y:165:ASN:HB2  | 25:Y:169:GLY:HA2  | 2.02                     | 0.41              |
| 32:f:54:PRO:CD    | 32:f:73:PRO:HD3   | 2.51                     | 0.41              |
| 37:k:2:ARG:HE     | 37:k:4:LEU:HD22   | 1.86                     | 0.41              |
| 38:l:9:ARG:HA     | 38:l:12:PHE:CZ    | 2.55                     | 0.41              |
| 2:A:11:VAL:HG22   | 2:A:22:LEU:HD22   | 2.02                     | 0.41              |
| 5:D:4:SER:OG      | 5:D:5:LEU:N       | 2.53                     | 0.41              |
| 8:G:82:U:C2       | 8:G:87:A:N1       | 2.88                     | 0.41              |
| 8:G:501:C:OP1     | 18:Q:117:ARG:NH2  | 2.54                     | 0.41              |
| 9:H:154:LEU:O     | 9:H:156:LYS:NZ    | 2.50                     | 0.41              |
| 10:I:91:LEU:HD23  | 10:I:91:LEU:HA    | 1.93                     | 0.41              |
| 23:V:270(B):A:C2' | 23:V:270(C):C:H6  | 2.34                     | 0.41              |
| 23:V:270(T):G:C6  | 23:V:270(U):C:C4  | 3.08                     | 0.41              |
| 23:V:1445:C:C5    | 23:V:1446:C:C4    | 3.05                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:V:1732:A:H2'    | 23:V:1733:G:OP1   | 2.21                     | 0.41              |
| 23:V:2786:U:O2     | 23:V:2786:U:H2'   | 2.20                     | 0.41              |
| 29:c:111:LEU:HD21  | 29:c:120:LEU:HG   | 2.02                     | 0.41              |
| 38:l:94:TYR:HH     | 38:l:99:LYS:HG3   | 1.83                     | 0.41              |
| 1:W:17:U:O5'       | 1:W:17:U:C6       | 2.70                     | 0.41              |
| 8:G:250:A:H2       | 8:G:274:A:N6      | 2.18                     | 0.41              |
| 8:G:490:G:H2'      | 8:G:491:G:H8      | 1.86                     | 0.41              |
| 23:V:852:G:N1      | 23:V:926:A:C6     | 2.89                     | 0.41              |
| 23:V:1546:C:C3'    | 23:V:1546:C:C6    | 3.03                     | 0.41              |
| 23:V:1583:A:H5''   | 23:V:1585:C:C5    | 2.56                     | 0.41              |
| 23:V:2108:C:O2'    | 23:V:2182:G:N2    | 2.54                     | 0.41              |
| 23:V:2572:A:H5'    | 23:V:2574:G:H4'   | 2.03                     | 0.41              |
| 25:Y:148:ASN:HB2   | 25:Y:151:GLU:HB2  | 2.02                     | 0.41              |
| 25:Y:160:ARG:O     | 25:Y:161:ILE:HG12 | 2.21                     | 0.41              |
| 34:h:10:VAL:HG12   | 34:h:17:ARG:HA    | 2.03                     | 0.41              |
| 38:l:17:ARG:NH1    | 38:l:89:ARG:CG    | 2.80                     | 0.41              |
| 3:B:23:LYS:NZ      | 3:B:57:GLY:O      | 2.46                     | 0.41              |
| 8:G:147:G:H2'      | 8:G:148:G:H8      | 1.85                     | 0.41              |
| 8:G:268:C:H2'      | 8:G:269:C:C6      | 2.56                     | 0.41              |
| 8:G:711:G:H2'      | 8:G:712:A:H8      | 1.85                     | 0.41              |
| 8:G:1429:C:H2'     | 8:G:1430:C:C6     | 2.55                     | 0.41              |
| 8:G:1455:G:C8      | 8:G:1455:G:O5'    | 2.71                     | 0.41              |
| 19:R:108:ARG:HD3   | 19:R:108:ARG:HA   | 1.84                     | 0.41              |
| 23:V:270(V):G:H2'  | 23:V:270(W):G:H8  | 1.85                     | 0.41              |
| 23:V:296:C:H2'     | 23:V:297:C:H6     | 1.86                     | 0.41              |
| 23:V:410:G:H1      | 23:V:417:C:H42    | 1.67                     | 0.41              |
| 23:V:487:C:H2'     | 23:V:488:G:H5'    | 2.03                     | 0.41              |
| 23:V:589:C:H2'     | 23:V:590:A:C8     | 2.55                     | 0.41              |
| 23:V:1444(A):A:H1' | 23:V:1732:A:N6    | 2.04                     | 0.41              |
| 23:V:1864:U:C6     | 23:V:1864:U:O5'   | 2.74                     | 0.41              |
| 23:V:2092:U:C5     | 23:V:2199:A:H2    | 2.39                     | 0.41              |
| 25:Y:64:LEU:O      | 25:Y:159:GLY:CA   | 2.63                     | 0.41              |
| 26:Z:39:LYS:NZ     | 26:Z:87:ASN:OD1   | 2.52                     | 0.41              |
| 26:Z:67:PHE:HB3    | 26:Z:153:ALA:HB3  | 2.03                     | 0.41              |
| 29:c:44:GLY:N      | 29:c:88:ILE:HD12  | 2.36                     | 0.41              |
| 29:c:47:LYS:CG     | 29:c:80:PHE:CE2   | 3.04                     | 0.41              |
| 29:c:103:LEU:HD11  | 29:c:178:PHE:HZ   | 1.85                     | 0.41              |
| 32:f:68:VAL:O      | 32:f:69:THR:OG1   | 2.36                     | 0.41              |
| 34:h:19:ILE:HG12   | 34:h:59:LYS:HE2   | 2.02                     | 0.41              |
| 38:l:35:ILE:CD1    | 38:l:97:ARG:HH12  | 2.18                     | 0.41              |
| 40:n:76:TYR:CZ     | 40:n:80:ILE:HD12  | 2.56                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:G:81:G:P         | 8:G:82:U:OP2      | 2.78                     | 0.41              |
| 8:G:222:U:H2'      | 8:G:223:U:H6      | 1.70                     | 0.41              |
| 8:G:475:G:O5'      | 8:G:475:G:C8      | 2.71                     | 0.41              |
| 8:G:546:G:OP1      | 11:J:71:SER:OG    | 2.39                     | 0.41              |
| 8:G:592:G:H2'      | 8:G:593:G:C8      | 2.56                     | 0.41              |
| 8:G:1099:G:OP2     | 9:H:148:TYR:OH    | 2.39                     | 0.41              |
| 8:G:1258:G:N2      | 8:G:1259:C:N3     | 2.68                     | 0.41              |
| 8:G:1322:C:H5'     | 19:R:100:GLY:HA3  | 2.02                     | 0.41              |
| 11:J:165:MET:HE3   | 11:J:168:ARG:HG3  | 2.02                     | 0.41              |
| 11:J:201:GLN:HA    | 11:J:204:ILE:HD13 | 2.02                     | 0.41              |
| 19:R:16:ASP:OD1    | 19:R:16:ASP:N     | 2.54                     | 0.41              |
| 19:R:23:TYR:CD1    | 19:R:67:GLU:HG2   | 2.56                     | 0.41              |
| 23:V:270(B):A:H4'  | 23:V:270(C):C:C6  | 2.55                     | 0.41              |
| 23:V:270(Z):U:HO2' | 23:V:271:C:P      | 2.40                     | 0.41              |
| 23:V:278:A:H2      | 23:V:362:U:N3     | 2.15                     | 0.41              |
| 23:V:363(F):G:H8   | 23:V:363(F):G:P   | 2.44                     | 0.41              |
| 23:V:553:U:C3'     | 23:V:553:U:C6     | 3.04                     | 0.41              |
| 23:V:972:G:C3'     | 23:V:973:A:C3'    | 2.96                     | 0.41              |
| 23:V:1589:C:O5'    | 23:V:1589:C:H6    | 2.04                     | 0.41              |
| 23:V:1631:A:H62    | 23:V:1683:C:H5'   | 1.86                     | 0.41              |
| 23:V:2127:G:C5     | 23:V:2128:C:N4    | 2.89                     | 0.41              |
| 23:V:2709:G:H2'    | 23:V:2710:C:H6    | 1.79                     | 0.41              |
| 23:V:2888:C:H3'    | 23:V:2888:C:H6    | 1.86                     | 0.41              |
| 27:a:8:LYS:HZ3     | 27:a:24:THR:HG22  | 1.86                     | 0.41              |
| 30:d:149:ARG:HG2   | 30:d:153:LYS:HG3  | 2.03                     | 0.41              |
| 32:f:114:ASP:OD1   | 32:f:114:ASP:N    | 2.54                     | 0.41              |
| 38:l:94:TYR:CD1    | 38:l:94:TYR:O     | 2.74                     | 0.41              |
| 44:r:86:ARG:O      | 44:r:88:LYS:N     | 2.54                     | 0.41              |
| 8:G:65:U:O2'       | 8:G:200:G:C5'     | 2.69                     | 0.41              |
| 8:G:197:A:N7       | 8:G:220:G:N2      | 2.63                     | 0.41              |
| 8:G:824:C:H2'      | 8:G:825:G:C8      | 2.56                     | 0.41              |
| 8:G:976:G:N2       | 8:G:1362(A):C:OP2 | 2.54                     | 0.41              |
| 23:V:270(D):C:O3'  | 23:V:270(E):G:O4' | 2.39                     | 0.41              |
| 23:V:270(V):G:H5'  | 23:V:270(W):G:OP2 | 2.21                     | 0.41              |
| 23:V:815:C:H5'     | 23:V:1224:G:H22   | 1.86                     | 0.41              |
| 23:V:852:G:N3      | 23:V:853:G:N7     | 2.69                     | 0.41              |
| 23:V:1860:G:C6     | 23:V:1861:G:C5    | 3.09                     | 0.41              |
| 23:V:1864:U:O5'    | 23:V:1864:U:H6    | 2.04                     | 0.41              |
| 23:V:2218:G:H2'    | 23:V:2219:G:H8    | 1.86                     | 0.41              |
| 23:V:2811:G:OP1    | 27:a:59:VAL:HB    | 2.21                     | 0.41              |
| 25:Y:175:VAL:O     | 25:Y:180:PHE:CZ   | 2.73                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:a:105:THR:HB   | 27:a:197:ILE:HG13 | 2.03                     | 0.41              |
| 29:c:80:PHE:HD1   | 29:c:80:PHE:HA    | 1.79                     | 0.41              |
| 43:q:87:GLN:HB3   | 43:q:88:LYS:H     | 1.44                     | 0.41              |
| 52:z:19:ARG:HA    | 52:z:19:ARG:HD3   | 1.78                     | 0.41              |
| 18:Q:86:ARG:HD3   | 18:Q:101:VAL:HG12 | 2.03                     | 0.40              |
| 23:V:270(B):A:O2' | 23:V:270(C):C:H3' | 2.21                     | 0.40              |
| 23:V:270(D):C:H2' | 23:V:270(E):G:C8  | 2.56                     | 0.40              |
| 23:V:537:C:H3'    | 23:V:537:C:H6     | 1.86                     | 0.40              |
| 23:V:840:C:H4'    | 23:V:1192:G:N3    | 2.36                     | 0.40              |
| 23:V:1171:G:H1    | 23:V:1178:C:N4    | 2.19                     | 0.40              |
| 23:V:1400:G:H2'   | 23:V:1401:G:H8    | 1.86                     | 0.40              |
| 23:V:1444:G:C6    | 23:V:1463:C:N4    | 2.86                     | 0.40              |
| 23:V:1548:C:O5'   | 23:V:1548:C:C6    | 2.70                     | 0.40              |
| 23:V:1592:C:H2'   | 23:V:1593:G:C8    | 2.56                     | 0.40              |
| 23:V:2630:G:C5    | 23:V:2894:G:C8    | 3.09                     | 0.40              |
| 23:V:2786:U:C6    | 23:V:2786:U:O5'   | 2.74                     | 0.40              |
| 23:V:2787:C:C5'   | 27:a:64:LYS:HE3   | 2.51                     | 0.40              |
| 23:V:2811:G:C2'   | 23:V:2812:G:H5'   | 2.51                     | 0.40              |
| 27:a:11:MET:HE1   | 27:a:13:ARG:HE    | 1.86                     | 0.40              |
| 28:b:205:ARG:O    | 28:b:209:GLU:HG2  | 2.21                     | 0.40              |
| 29:c:28:VAL:C     | 29:c:30:GLU:N     | 2.78                     | 0.40              |
| 38:l:94:TYR:CE1   | 38:l:99:LYS:HE2   | 2.56                     | 0.40              |
| 45:s:91:LEU:HD23  | 45:s:91:LEU:HA    | 1.86                     | 0.40              |
| 46:t:46:LYS:HB2   | 46:t:78:TYR:CD1   | 2.56                     | 0.40              |
| 14:M:74:GLU:O     | 14:M:88:PRO:HA    | 2.20                     | 0.40              |
| 18:Q:104:VAL:HG12 | 18:Q:105:TYR:H    | 1.87                     | 0.40              |
| 23:V:137(A):G:H2' | 23:V:138:G:H5'    | 2.02                     | 0.40              |
| 23:V:270(E):G:C6  | 23:V:270(F):U:C4  | 3.09                     | 0.40              |
| 23:V:377:C:H5''   | 23:V:377:C:H6     | 1.86                     | 0.40              |
| 23:V:380:U:H2'    | 23:V:381:G:H8     | 1.85                     | 0.40              |
| 23:V:1051:G:N3    | 23:V:2751:G:H5'   | 2.36                     | 0.40              |
| 23:V:1664:A:H2'   | 23:V:1665:A:C8    | 2.56                     | 0.40              |
| 23:V:2320:A:H62   | 38:l:3:ARG:HH12   | 1.68                     | 0.40              |
| 29:c:83:ARG:NH1   | 55:DD:58:A:OP2    | 2.47                     | 0.40              |
| 45:s:22:GLY:HA2   | 45:s:41:LEU:HD22  | 2.03                     | 0.40              |
| 7:F:4:GLY:H       | 8:G:1305:G:H5'    | 1.85                     | 0.40              |
| 8:G:728:A:H2'     | 8:G:729:A:H8      | 1.86                     | 0.40              |
| 8:G:1270:C:H2'    | 8:G:1271:G:C8     | 2.57                     | 0.40              |
| 9:H:93:VAL:HG11   | 9:H:97:TRP:HB2    | 2.03                     | 0.40              |
| 12:K:88:LYS:HD2   | 12:K:123:LEU:HB2  | 2.03                     | 0.40              |
| 17:P:34:ASP:HA    | 17:P:35:PRO:HD3   | 1.84                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 23:V:143:C:C3'    | 23:V:143:C:C6    | 3.05                     | 0.40              |
| 23:V:279:C:O5'    | 23:V:279:C:H6    | 2.05                     | 0.40              |
| 23:V:616:A:H3'    | 23:V:617:G:H21   | 1.87                     | 0.40              |
| 23:V:909:A:N6     | 23:V:912:C:O2    | 2.54                     | 0.40              |
| 23:V:1408:C:N3    | 23:V:1595:G:N2   | 2.69                     | 0.40              |
| 23:V:1480:G:H3'   | 23:V:1482:U:H5'' | 2.03                     | 0.40              |
| 23:V:2789:C:H3'   | 23:V:2789:C:C6   | 2.55                     | 0.40              |
| 24:X:89:G:C8      | 24:X:89:G:O5'    | 2.70                     | 0.40              |
| 29:c:81:LYS:HG3   | 29:c:83:ARG:NH1  | 2.31                     | 0.40              |
| 30:d:122:THR:O    | 30:d:122:THR:OG1 | 2.35                     | 0.40              |
| 36:j:73:PRO:HA    | 36:j:93:TYR:HB2  | 2.02                     | 0.40              |
| 37:k:5:LYS:HE3    | 37:k:5:LYS:HB3   | 1.91                     | 0.40              |
| 37:k:13:HIS:O     | 37:k:17:ARG:NE   | 2.49                     | 0.40              |
| 8:G:73:G:C6       | 8:G:99:C:O2      | 2.74                     | 0.40              |
| 8:G:718:G:C8      | 17:P:116:HIS:HD2 | 2.39                     | 0.40              |
| 22:U:60:LEU:HA    | 22:U:64:ALA:HB3  | 2.04                     | 0.40              |
| 23:V:270(S):G:H2' | 23:V:270(T):G:H8 | 1.86                     | 0.40              |
| 23:V:1005:C:N3    | 23:V:1006:C:N4   | 2.68                     | 0.40              |
| 23:V:1454:U:O2    | 23:V:1455:G:N7   | 2.54                     | 0.40              |
| 23:V:1727:U:O5'   | 23:V:1727:U:H6   | 2.04                     | 0.40              |
| 23:V:1778:U:C3'   | 23:V:1784:A:H61  | 2.33                     | 0.40              |
| 23:V:1860:G:H2'   | 23:V:1861:G:C8   | 2.57                     | 0.40              |
| 23:V:2209:C:N4    | 23:V:2216:G:N1   | 2.69                     | 0.40              |
| 23:V:2649:U:H2'   | 23:V:2650:U:C6   | 2.57                     | 0.40              |
| 23:V:2713:A:H3'   | 23:V:2714:G:C5'  | 2.52                     | 0.40              |
| 23:V:2720:U:C2'   | 23:V:2721:A:H8   | 2.22                     | 0.40              |
| 23:V:2807:G:N7    | 23:V:2891:G:C2   | 2.89                     | 0.40              |
| 24:X:28:C:H2'     | 24:X:29:A:C8     | 2.57                     | 0.40              |
| 45:s:145:GLU:HG2  | 45:s:146:ILE:H   | 1.86                     | 0.40              |
| 54:BB:28:GLU:H    | 54:BB:28:GLU:HG3 | 1.71                     | 0.40              |
| 55:DD:73:A:H2'    | 55:DD:74:A:C8    | 2.56                     | 0.40              |
| 8:G:501:C:O5'     | 8:G:501:C:H6     | 2.04                     | 0.40              |
| 9:H:60:ASP:HB2    | 9:H:64:ARG:HH12  | 1.86                     | 0.40              |
| 15:N:25:ASP:OD1   | 15:N:25:ASP:N    | 2.55                     | 0.40              |
| 19:R:25:ILE:HG13  | 19:R:29:ARG:HB3  | 2.04                     | 0.40              |
| 22:U:81:ARG:HG2   | 22:U:83:GLU:HG2  | 2.02                     | 0.40              |
| 23:V:252:G:OP2    | 35:i:50:ARG:NH2  | 2.55                     | 0.40              |
| 23:V:2897:U:O5'   | 23:V:2897:U:H6   | 2.04                     | 0.40              |
| 27:a:11:MET:HE1   | 27:a:13:ARG:NE   | 2.37                     | 0.40              |
| 27:a:41:LYS:HB2   | 27:a:41:LYS:HE2  | 1.85                     | 0.40              |
| 36:j:34:LEU:HD12  | 36:j:103:MET:HE2 | 2.03                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 38:l:83:LYS:HE2  | 38:l:83:LYS:HB2 | 1.94                     | 0.40              |
| 45:s:94:GLU:H    | 45:s:95:PRO:HD2 | 1.82                     | 0.40              |
| 45:s:152:ALA:HB2 | 45:s:171:ILE:HB | 2.02                     | 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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | A     | 95/104 (91%)  | 82 (86%)  | 12 (13%) | 1 (1%)   | 11          | 43  |
| 3   | B     | 71/73 (97%)   | 59 (83%)  | 12 (17%) | 0        | 100         | 100 |
| 4   | C     | 97/106 (92%)  | 85 (88%)  | 10 (10%) | 2 (2%)   | 5           | 31  |
| 5   | D     | 80/93 (86%)   | 64 (80%)  | 16 (20%) | 0        | 100         | 100 |
| 6   | E     | 96/105 (91%)  | 81 (84%)  | 14 (15%) | 1 (1%)   | 12          | 45  |
| 7   | F     | 22/27 (82%)   | 20 (91%)  | 2 (9%)   | 0        | 100         | 100 |
| 9   | H     | 220/256 (86%) | 195 (89%) | 23 (10%) | 2 (1%)   | 14          | 46  |
| 10  | I     | 204/239 (85%) | 174 (85%) | 30 (15%) | 0        | 100         | 100 |
| 11  | J     | 206/209 (99%) | 178 (86%) | 27 (13%) | 1 (0%)   | 24          | 57  |
| 12  | K     | 148/162 (91%) | 129 (87%) | 18 (12%) | 1 (1%)   | 18          | 51  |
| 13  | L     | 99/101 (98%)  | 84 (85%)  | 14 (14%) | 1 (1%)   | 12          | 45  |
| 14  | M     | 153/156 (98%) | 135 (88%) | 16 (10%) | 2 (1%)   | 9           | 39  |
| 15  | N     | 136/138 (99%) | 118 (87%) | 17 (12%) | 1 (1%)   | 18          | 51  |
| 16  | O     | 125/128 (98%) | 97 (78%)  | 28 (22%) | 0        | 100         | 100 |
| 17  | P     | 117/129 (91%) | 103 (88%) | 14 (12%) | 0        | 100         | 100 |
| 18  | Q     | 122/132 (92%) | 96 (79%)  | 25 (20%) | 1 (1%)   | 16          | 49  |
| 19  | R     | 112/126 (89%) | 86 (77%)  | 23 (20%) | 3 (3%)   | 4           | 27  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 20  | S     | 58/61 (95%)   | 39 (67%)  | 18 (31%) | 1 (2%)   | 7           | 35  |
| 21  | T     | 86/89 (97%)   | 83 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 22  | U     | 81/88 (92%)   | 70 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 25  | Y     | 226/229 (99%) | 179 (79%) | 39 (17%) | 8 (4%)   | 3           | 23  |
| 26  | Z     | 271/276 (98%) | 232 (86%) | 38 (14%) | 1 (0%)   | 30          | 61  |
| 27  | a     | 204/206 (99%) | 162 (79%) | 42 (21%) | 0        | 100         | 100 |
| 28  | b     | 206/210 (98%) | 156 (76%) | 48 (23%) | 2 (1%)   | 12          | 45  |
| 29  | c     | 177/182 (97%) | 121 (68%) | 45 (25%) | 11 (6%)  | 1           | 12  |
| 30  | d     | 174/180 (97%) | 135 (78%) | 27 (16%) | 12 (7%)  | 1           | 11  |
| 31  | e     | 124/173 (72%) | 79 (64%)  | 39 (32%) | 6 (5%)   | 2           | 16  |
| 32  | f     | 132/147 (90%) | 86 (65%)  | 34 (26%) | 12 (9%)  | 0           | 6   |
| 33  | g     | 115/140 (82%) | 92 (80%)  | 21 (18%) | 2 (2%)   | 7           | 35  |
| 34  | h     | 120/122 (98%) | 76 (63%)  | 39 (32%) | 5 (4%)   | 2           | 19  |
| 35  | i     | 143/150 (95%) | 95 (66%)  | 41 (29%) | 7 (5%)   | 1           | 16  |
| 36  | j     | 134/141 (95%) | 94 (70%)  | 37 (28%) | 3 (2%)   | 5           | 30  |
| 37  | k     | 115/118 (98%) | 97 (84%)  | 18 (16%) | 0        | 100         | 100 |
| 38  | l     | 108/112 (96%) | 82 (76%)  | 23 (21%) | 3 (3%)   | 4           | 26  |
| 39  | m     | 115/146 (79%) | 78 (68%)  | 34 (30%) | 3 (3%)   | 4           | 27  |
| 40  | n     | 115/118 (98%) | 103 (90%) | 12 (10%) | 0        | 100         | 100 |
| 41  | o     | 99/101 (98%)  | 79 (80%)  | 19 (19%) | 1 (1%)   | 12          | 45  |
| 42  | p     | 108/113 (96%) | 92 (85%)  | 15 (14%) | 1 (1%)   | 14          | 46  |
| 43  | q     | 92/96 (96%)   | 76 (83%)  | 14 (15%) | 2 (2%)   | 5           | 30  |
| 44  | r     | 108/110 (98%) | 66 (61%)  | 40 (37%) | 2 (2%)   | 6           | 33  |
| 45  | s     | 178/206 (86%) | 128 (72%) | 41 (23%) | 9 (5%)   | 1           | 15  |
| 46  | t     | 78/85 (92%)   | 64 (82%)  | 13 (17%) | 1 (1%)   | 9           | 39  |
| 47  | u     | 65/67 (97%)   | 55 (85%)  | 9 (14%)  | 1 (2%)   | 8           | 37  |
| 48  | v     | 57/60 (95%)   | 46 (81%)  | 10 (18%) | 1 (2%)   | 6           | 34  |
| 49  | CC    | 30/71 (42%)   | 18 (60%)  | 12 (40%) | 0        | 100         | 100 |
| 49  | w     | 69/71 (97%)   | 43 (62%)  | 23 (33%) | 3 (4%)   | 2           | 18  |
| 50  | x     | 55/60 (92%)   | 35 (64%)  | 18 (33%) | 2 (4%)   | 2           | 22  |
| 51  | y     | 47/54 (87%)   | 29 (62%)  | 17 (36%) | 1 (2%)   | 5           | 31  |

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| Mol | Chain | Analysed        | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|------------|----------|-------------|-----|
| 52  | z     | 47/49 (96%)     | 40 (85%)   | 7 (15%)    | 0        | 100         | 100 |
| 53  | AA    | 62/65 (95%)     | 50 (81%)   | 9 (14%)    | 3 (5%)   | 2           | 16  |
| 54  | BB    | 35/37 (95%)     | 32 (91%)   | 3 (9%)     | 0        | 100         | 100 |
| 56  | EE    | 488/497 (98%)   | 386 (79%)  | 98 (20%)   | 4 (1%)   | 16          | 49  |
| All | All   | 6425/6914 (93%) | 5084 (79%) | 1218 (19%) | 123 (2%) | 8           | 33  |

All (123) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 75  | ASN  |
| 9   | H     | 78  | GLN  |
| 25  | Y     | 161 | ILE  |
| 25  | Y     | 179 | SER  |
| 29  | c     | 31  | VAL  |
| 29  | c     | 32  | PRO  |
| 29  | c     | 77  | ILE  |
| 29  | c     | 81  | LYS  |
| 29  | c     | 86  | MET  |
| 29  | c     | 87  | PRO  |
| 30  | d     | 12  | PRO  |
| 30  | d     | 17  | VAL  |
| 30  | d     | 21  | PRO  |
| 30  | d     | 126 | PRO  |
| 30  | d     | 127 | GLU  |
| 30  | d     | 128 | PRO  |
| 31  | e     | 32  | LEU  |
| 32  | f     | 19  | PRO  |
| 32  | f     | 54  | PRO  |
| 32  | f     | 67  | PHE  |
| 32  | f     | 68  | VAL  |
| 32  | f     | 69  | THR  |
| 35  | i     | 48  | PRO  |
| 38  | l     | 100 | ALA  |
| 39  | m     | 59  | THR  |
| 43  | q     | 88  | LYS  |
| 43  | q     | 89  | ILE  |
| 45  | s     | 93  | ASP  |
| 45  | s     | 94  | GLU  |
| 45  | s     | 97  | GLU  |
| 49  | w     | 50  | VAL  |
| 53  | AA    | 12  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | AA    | 13  | ARG  |
| 56  | EE    | 150 | LEU  |
| 56  | EE    | 296 | PRO  |
| 4   | C     | 74  | LYS  |
| 6   | E     | 57  | LYS  |
| 9   | H     | 153 | ARG  |
| 25  | Y     | 37  | PHE  |
| 25  | Y     | 160 | ARG  |
| 25  | Y     | 184 | LYS  |
| 26  | Z     | 273 | ARG  |
| 29  | c     | 79  | ASN  |
| 29  | c     | 84  | LYS  |
| 30  | d     | 13  | LYS  |
| 30  | d     | 41  | MET  |
| 31  | e     | 7   | VAL  |
| 31  | e     | 12  | THR  |
| 32  | f     | 56  | GLU  |
| 34  | h     | 14  | THR  |
| 34  | h     | 103 | ALA  |
| 36  | j     | 99  | PRO  |
| 38  | l     | 91  | PRO  |
| 41  | o     | 46  | VAL  |
| 44  | r     | 87  | LYS  |
| 45  | s     | 90  | VAL  |
| 45  | s     | 92  | SER  |
| 45  | s     | 152 | ALA  |
| 49  | w     | 11  | PRO  |
| 56  | EE    | 100 | MET  |
| 56  | EE    | 347 | ASP  |
| 2   | A     | 67  | LYS  |
| 14  | M     | 113 | GLU  |
| 25  | Y     | 36  | LYS  |
| 25  | Y     | 182 | PRO  |
| 31  | e     | 10  | LEU  |
| 32  | f     | 61  | ALA  |
| 32  | f     | 101 | TRP  |
| 32  | f     | 110 | GLN  |
| 33  | g     | 66  | LYS  |
| 35  | i     | 33  | ARG  |
| 42  | p     | 90  | ARG  |
| 45  | s     | 42  | VAL  |
| 46  | t     | 8   | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | J     | 35  | ARG  |
| 12  | K     | 141 | GLN  |
| 25  | Y     | 162 | GLU  |
| 28  | b     | 62  | ARG  |
| 29  | c     | 29  | TRP  |
| 29  | c     | 78  | SER  |
| 29  | c     | 142 | PRO  |
| 30  | d     | 40  | GLU  |
| 30  | d     | 111 | HIS  |
| 32  | f     | 52  | ILE  |
| 35  | i     | 35  | HIS  |
| 36  | j     | 60  | ARG  |
| 39  | m     | 99  | LEU  |
| 45  | s     | 32  | HIS  |
| 47  | u     | 13  | PRO  |
| 19  | R     | 100 | GLY  |
| 19  | R     | 101 | GLN  |
| 19  | R     | 108 | ARG  |
| 30  | d     | 15  | VAL  |
| 31  | e     | 54  | ALA  |
| 32  | f     | 66  | THR  |
| 33  | g     | 45  | ASN  |
| 35  | i     | 46  | LYS  |
| 49  | w     | 58  | ARG  |
| 51  | y     | 19  | ARG  |
| 35  | i     | 47  | ASP  |
| 39  | m     | 97  | ALA  |
| 14  | M     | 112 | PRO  |
| 34  | h     | 119 | PRO  |
| 44  | r     | 38  | ILE  |
| 50  | x     | 40  | LYS  |
| 30  | d     | 39  | PRO  |
| 34  | h     | 15  | GLY  |
| 35  | i     | 34  | GLY  |
| 36  | j     | 78  | PRO  |
| 53  | AA    | 62  | LEU  |
| 13  | L     | 96  | PRO  |
| 31  | e     | 33  | PRO  |
| 45  | s     | 96  | VAL  |
| 48  | v     | 12  | PRO  |
| 18  | Q     | 7   | ILE  |
| 20  | S     | 14  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | b     | 178 | PRO  |
| 32  | f     | 21  | PRO  |
| 34  | h     | 4   | PRO  |
| 35  | i     | 71  | VAL  |
| 15  | N     | 74  | PRO  |
| 38  | l     | 96  | GLY  |
| 50  | x     | 5   | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | A     | 92/96 (96%)    | 90 (98%)   | 2 (2%)   | 45          | 65  |
| 3   | B     | 64/64 (100%)   | 64 (100%)  | 0        | 100         | 100 |
| 4   | C     | 76/82 (93%)    | 76 (100%)  | 0        | 100         | 100 |
| 5   | D     | 72/80 (90%)    | 72 (100%)  | 0        | 100         | 100 |
| 6   | E     | 88/92 (96%)    | 86 (98%)   | 2 (2%)   | 44          | 64  |
| 7   | F     | 19/22 (86%)    | 19 (100%)  | 0        | 100         | 100 |
| 9   | H     | 191/220 (87%)  | 190 (100%) | 1 (0%)   | 81          | 80  |
| 10  | I     | 160/188 (85%)  | 159 (99%)  | 1 (1%)   | 78          | 79  |
| 11  | J     | 180/181 (99%)  | 178 (99%)  | 2 (1%)   | 65          | 74  |
| 12  | K     | 115/123 (94%)  | 115 (100%) | 0        | 100         | 100 |
| 13  | L     | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 14  | M     | 126/127 (99%)  | 125 (99%)  | 1 (1%)   | 73          | 77  |
| 15  | N     | 119/119 (100%) | 118 (99%)  | 1 (1%)   | 73          | 77  |
| 16  | O     | 98/99 (99%)    | 98 (100%)  | 0        | 100         | 100 |
| 17  | P     | 90/99 (91%)    | 89 (99%)   | 1 (1%)   | 65          | 74  |
| 18  | Q     | 104/109 (95%)  | 104 (100%) | 0        | 100         | 100 |
| 19  | R     | 92/101 (91%)   | 90 (98%)   | 2 (2%)   | 45          | 65  |
| 20  | S     | 49/50 (98%)    | 42 (86%)   | 7 (14%)  | 3           | 19  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 21  | T     | 79/80 (99%)    | 78 (99%)   | 1 (1%)   | 61          | 72  |
| 22  | U     | 72/74 (97%)    | 72 (100%)  | 0        | 100         | 100 |
| 25  | Y     | 180/181 (99%)  | 176 (98%)  | 4 (2%)   | 45          | 65  |
| 26  | Z     | 215/218 (99%)  | 213 (99%)  | 2 (1%)   | 70          | 76  |
| 27  | a     | 166/166 (100%) | 164 (99%)  | 2 (1%)   | 63          | 73  |
| 28  | b     | 164/166 (99%)  | 161 (98%)  | 3 (2%)   | 51          | 68  |
| 29  | c     | 152/156 (97%)  | 140 (92%)  | 12 (8%)  | 11          | 37  |
| 30  | d     | 142/148 (96%)  | 132 (93%)  | 10 (7%)  | 14          | 41  |
| 32  | f     | 101/111 (91%)  | 90 (89%)   | 11 (11%) | 6           | 27  |
| 33  | g     | 99/119 (83%)   | 98 (99%)   | 1 (1%)   | 68          | 75  |
| 34  | h     | 100/100 (100%) | 99 (99%)   | 1 (1%)   | 68          | 75  |
| 35  | i     | 112/116 (97%)  | 107 (96%)  | 5 (4%)   | 24          | 51  |
| 36  | j     | 106/111 (96%)  | 106 (100%) | 0        | 100         | 100 |
| 37  | k     | 100/101 (99%)  | 100 (100%) | 0        | 100         | 100 |
| 38  | l     | 87/88 (99%)    | 76 (87%)   | 11 (13%) | 4           | 22  |
| 39  | m     | 105/127 (83%)  | 104 (99%)  | 1 (1%)   | 68          | 75  |
| 40  | n     | 93/94 (99%)    | 91 (98%)   | 2 (2%)   | 45          | 65  |
| 41  | o     | 82/82 (100%)   | 80 (98%)   | 2 (2%)   | 43          | 63  |
| 42  | p     | 90/92 (98%)    | 88 (98%)   | 2 (2%)   | 45          | 65  |
| 43  | q     | 76/78 (97%)    | 74 (97%)   | 2 (3%)   | 40          | 62  |
| 44  | r     | 91/91 (100%)   | 91 (100%)  | 0        | 100         | 100 |
| 45  | s     | 159/179 (89%)  | 155 (98%)  | 4 (2%)   | 42          | 63  |
| 46  | t     | 63/67 (94%)    | 61 (97%)   | 2 (3%)   | 34          | 58  |
| 47  | u     | 62/62 (100%)   | 62 (100%)  | 0        | 100         | 100 |
| 48  | v     | 51/52 (98%)    | 51 (100%)  | 0        | 100         | 100 |
| 49  | w     | 63/63 (100%)   | 62 (98%)   | 1 (2%)   | 55          | 69  |
| 50  | x     | 50/52 (96%)    | 47 (94%)   | 3 (6%)   | 17          | 45  |
| 51  | y     | 47/52 (90%)    | 43 (92%)   | 4 (8%)   | 10          | 35  |
| 52  | z     | 42/42 (100%)   | 42 (100%)  | 0        | 100         | 100 |
| 53  | AA    | 54/55 (98%)    | 53 (98%)   | 1 (2%)   | 50          | 67  |
| 54  | BB    | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 56  | EE    | 412/419 (98%)   | 386 (94%)  | 26 (6%)  | 16          | 44 |
| All | All   | 5274/5518 (96%) | 5141 (98%) | 133 (2%) | 42          | 63 |

All (133) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 84  | LEU  |
| 2   | A     | 90  | ILE  |
| 6   | E     | 16  | LEU  |
| 6   | E     | 49  | VAL  |
| 9   | H     | 162 | ILE  |
| 10  | I     | 10  | PHE  |
| 11  | J     | 21  | LEU  |
| 11  | J     | 204 | ILE  |
| 14  | M     | 30  | ILE  |
| 15  | N     | 97  | VAL  |
| 17  | P     | 82  | VAL  |
| 19  | R     | 96  | LEU  |
| 19  | R     | 102 | ARG  |
| 20  | S     | 21  | TYR  |
| 20  | S     | 26  | ARG  |
| 20  | S     | 29  | ARG  |
| 20  | S     | 31  | ARG  |
| 20  | S     | 35  | ARG  |
| 20  | S     | 39  | LEU  |
| 20  | S     | 42  | ILE  |
| 21  | T     | 87  | ILE  |
| 25  | Y     | 123 | VAL  |
| 25  | Y     | 155 | GLU  |
| 25  | Y     | 157 | LYS  |
| 25  | Y     | 216 | THR  |
| 26  | Z     | 65  | ILE  |
| 26  | Z     | 106 | ILE  |
| 27  | a     | 146 | THR  |
| 27  | a     | 170 | LEU  |
| 28  | b     | 11  | VAL  |
| 28  | b     | 64  | ILE  |
| 28  | b     | 106 | ARG  |
| 29  | c     | 28  | VAL  |
| 29  | c     | 31  | VAL  |
| 29  | c     | 77  | ILE  |
| 29  | c     | 79  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | c     | 80  | PHE  |
| 29  | c     | 81  | LYS  |
| 29  | c     | 82  | LEU  |
| 29  | c     | 86  | MET  |
| 29  | c     | 88  | ILE  |
| 29  | c     | 90  | LEU  |
| 29  | c     | 109 | VAL  |
| 29  | c     | 144 | ILE  |
| 30  | d     | 13  | LYS  |
| 30  | d     | 15  | VAL  |
| 30  | d     | 23  | ARG  |
| 30  | d     | 25  | LYS  |
| 30  | d     | 27  | LYS  |
| 30  | d     | 124 | GLU  |
| 30  | d     | 127 | GLU  |
| 30  | d     | 131 | VAL  |
| 30  | d     | 133 | VAL  |
| 30  | d     | 138 | LYS  |
| 32  | f     | 4   | VAL  |
| 32  | f     | 52  | ILE  |
| 32  | f     | 55  | VAL  |
| 32  | f     | 57  | ILE  |
| 32  | f     | 63  | ARG  |
| 32  | f     | 68  | VAL  |
| 32  | f     | 69  | THR  |
| 32  | f     | 77  | LEU  |
| 32  | f     | 89  | HIS  |
| 32  | f     | 95  | LYS  |
| 32  | f     | 115 | LEU  |
| 33  | g     | 25  | ARG  |
| 34  | h     | 19  | ILE  |
| 35  | i     | 15  | ARG  |
| 35  | i     | 46  | LYS  |
| 35  | i     | 51  | PHE  |
| 35  | i     | 52  | GLU  |
| 35  | i     | 146 | VAL  |
| 38  | l     | 9   | ARG  |
| 38  | l     | 10  | ARG  |
| 38  | l     | 12  | PHE  |
| 38  | l     | 14  | VAL  |
| 38  | l     | 15  | ARG  |
| 38  | l     | 17  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | l     | 78  | LEU  |
| 38  | l     | 88  | ASP  |
| 38  | l     | 92  | TYR  |
| 38  | l     | 97  | ARG  |
| 38  | l     | 98  | VAL  |
| 39  | m     | 66  | VAL  |
| 40  | n     | 27  | LEU  |
| 40  | n     | 80  | ILE  |
| 41  | o     | 38  | LEU  |
| 41  | o     | 66  | ARG  |
| 42  | p     | 10  | VAL  |
| 42  | p     | 71  | VAL  |
| 43  | q     | 9   | LEU  |
| 43  | q     | 12  | VAL  |
| 45  | s     | 31  | ARG  |
| 45  | s     | 90  | VAL  |
| 45  | s     | 93  | ASP  |
| 45  | s     | 94  | GLU  |
| 46  | t     | 9   | SER  |
| 46  | t     | 10  | THR  |
| 49  | w     | 10  | VAL  |
| 50  | x     | 33  | CYS  |
| 50  | x     | 37  | LYS  |
| 50  | x     | 39  | MET  |
| 51  | y     | 20  | ASN  |
| 51  | y     | 46  | HIS  |
| 51  | y     | 48  | VAL  |
| 51  | y     | 53  | LYS  |
| 53  | AA    | 59  | LYS  |
| 56  | EE    | 35  | LEU  |
| 56  | EE    | 43  | LYS  |
| 56  | EE    | 72  | GLN  |
| 56  | EE    | 92  | VAL  |
| 56  | EE    | 94  | ASN  |
| 56  | EE    | 95  | VAL  |
| 56  | EE    | 98  | ASP  |
| 56  | EE    | 100 | MET  |
| 56  | EE    | 101 | SER  |
| 56  | EE    | 104 | GLU  |
| 56  | EE    | 145 | PHE  |
| 56  | EE    | 291 | LEU  |
| 56  | EE    | 294 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | EE    | 331 | ASN  |
| 56  | EE    | 371 | LYS  |
| 56  | EE    | 373 | VAL  |
| 56  | EE    | 374 | LEU  |
| 56  | EE    | 376 | PHE  |
| 56  | EE    | 377 | MET  |
| 56  | EE    | 402 | ILE  |
| 56  | EE    | 403 | GLN  |
| 56  | EE    | 407 | SER  |
| 56  | EE    | 409 | LEU  |
| 56  | EE    | 410 | SER  |
| 56  | EE    | 413 | GLU  |
| 56  | EE    | 415 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | D     | 23  | ASN  |
| 9   | H     | 45  | GLN  |
| 9   | H     | 94  | ASN  |
| 9   | H     | 95  | GLN  |
| 9   | H     | 204 | ASN  |
| 10  | I     | 176 | HIS  |
| 11  | J     | 129 | ASN  |
| 12  | K     | 38  | GLN  |
| 13  | L     | 13  | ASN  |
| 14  | M     | 51  | GLN  |
| 14  | M     | 56  | GLN  |
| 14  | M     | 122 | HIS  |
| 15  | N     | 70  | GLN  |
| 16  | O     | 3   | GLN  |
| 16  | O     | 38  | GLN  |
| 16  | O     | 89  | ASN  |
| 17  | P     | 99  | GLN  |
| 17  | P     | 117 | ASN  |
| 18  | Q     | 99  | HIS  |
| 19  | R     | 62  | ASN  |
| 21  | T     | 37  | ASN  |
| 21  | T     | 46  | HIS  |
| 22  | U     | 76  | GLN  |
| 25  | Y     | 56  | GLN  |
| 25  | Y     | 57  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | Y     | 139 | ASN  |
| 25  | Y     | 188 | ASN  |
| 26  | Z     | 186 | HIS  |
| 27  | a     | 85  | ASN  |
| 28  | b     | 40  | GLN  |
| 28  | b     | 75  | HIS  |
| 29  | c     | 40  | ASN  |
| 29  | c     | 41  | GLN  |
| 29  | c     | 123 | ASN  |
| 32  | f     | 11  | GLN  |
| 32  | f     | 42  | ASN  |
| 32  | f     | 103 | GLN  |
| 32  | f     | 110 | GLN  |
| 34  | h     | 3   | GLN  |
| 34  | h     | 90  | GLN  |
| 35  | i     | 128 | HIS  |
| 37  | k     | 13  | HIS  |
| 40  | n     | 117 | GLN  |
| 41  | o     | 80  | GLN  |
| 42  | p     | 57  | ASN  |
| 42  | p     | 61  | ASN  |
| 43  | q     | 31  | HIS  |
| 43  | q     | 41  | ASN  |
| 44  | r     | 92  | ASN  |
| 45  | s     | 50  | GLN  |
| 46  | t     | 12  | ASN  |
| 46  | t     | 35  | ASN  |
| 47  | u     | 66  | ASN  |
| 49  | w     | 40  | HIS  |
| 49  | w     | 47  | GLN  |
| 50  | x     | 23  | HIS  |
| 50  | x     | 43  | HIS  |
| 51  | y     | 20  | ASN  |
| 51  | y     | 32  | ASN  |
| 51  | y     | 46  | HIS  |
| 53  | AA    | 35  | GLN  |
| 54  | BB    | 36  | GLN  |
| 56  | EE    | 194 | HIS  |
| 56  | EE    | 285 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | W     | 6/25 (24%)      | 6 (100%)          | 1 (16%)         |
| 23  | V     | 2874/2875 (99%) | 1143 (39%)        | 83 (2%)         |
| 24  | X     | 122/123 (99%)   | 41 (33%)          | 1 (0%)          |
| 55  | DD    | 76/77 (98%)     | 31 (40%)          | 4 (5%)          |
| 8   | G     | 1513/1514 (99%) | 480 (31%)         | 37 (2%)         |
| All | All   | 4591/4614 (99%) | 1701 (37%)        | 126 (2%)        |

All (1701) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 15  | A    |
| 1   | W     | 16  | A    |
| 1   | W     | 17  | U    |
| 1   | W     | 18  | G    |
| 1   | W     | 19  | U    |
| 1   | W     | 20  | U    |
| 8   | G     | 6   | G    |
| 8   | G     | 7   | G    |
| 8   | G     | 8   | A    |
| 8   | G     | 9   | G    |
| 8   | G     | 12  | U    |
| 8   | G     | 16  | A    |
| 8   | G     | 28  | G    |
| 8   | G     | 30  | U    |
| 8   | G     | 31  | G    |
| 8   | G     | 32  | A    |
| 8   | G     | 39  | G    |
| 8   | G     | 47  | C    |
| 8   | G     | 48  | C    |
| 8   | G     | 50  | A    |
| 8   | G     | 51  | A    |
| 8   | G     | 53  | A    |
| 8   | G     | 59  | A    |
| 8   | G     | 65  | U    |
| 8   | G     | 66  | G    |
| 8   | G     | 69  | G    |
| 8   | G     | 74  | C    |
| 8   | G     | 75  | C    |
| 8   | G     | 78  | G    |
| 8   | G     | 79  | G    |
| 8   | G     | 80  | G    |
| 8   | G     | 82  | U    |
| 8   | G     | 84  | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 8   | G     | 87     | A    |
| 8   | G     | 88     | C    |
| 8   | G     | 92     | G    |
| 8   | G     | 95     | G    |
| 8   | G     | 96     | G    |
| 8   | G     | 101    | A    |
| 8   | G     | 110    | C    |
| 8   | G     | 116    | A    |
| 8   | G     | 117    | G    |
| 8   | G     | 118    | U    |
| 8   | G     | 119    | A    |
| 8   | G     | 120    | A    |
| 8   | G     | 121    | C    |
| 8   | G     | 122    | G    |
| 8   | G     | 123    | C    |
| 8   | G     | 129(A) | G    |
| 8   | G     | 131    | C    |
| 8   | G     | 134    | A    |
| 8   | G     | 153    | C    |
| 8   | G     | 155    | C    |
| 8   | G     | 163    | C    |
| 8   | G     | 166    | G    |
| 8   | G     | 172    | A    |
| 8   | G     | 173    | U    |
| 8   | G     | 179    | A    |
| 8   | G     | 181    | G    |
| 8   | G     | 182    | U    |
| 8   | G     | 186(A) | C    |
| 8   | G     | 187    | C    |
| 8   | G     | 188    | U    |
| 8   | G     | 189    | U    |
| 8   | G     | 190    | G    |
| 8   | G     | 191(B) | G    |
| 8   | G     | 191(E) | G    |
| 8   | G     | 191    | G    |
| 8   | G     | 195    | A    |
| 8   | G     | 196    | A    |
| 8   | G     | 197    | A    |
| 8   | G     | 200    | G    |
| 8   | G     | 201    | C    |
| 8   | G     | 208    | U    |
| 8   | G     | 209    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | G     | 210 | U    |
| 8   | G     | 216 | G    |
| 8   | G     | 220 | G    |
| 8   | G     | 222 | U    |
| 8   | G     | 226 | G    |
| 8   | G     | 230 | G    |
| 8   | G     | 231 | G    |
| 8   | G     | 240 | C    |
| 8   | G     | 244 | U    |
| 8   | G     | 245 | C    |
| 8   | G     | 247 | G    |
| 8   | G     | 251 | G    |
| 8   | G     | 263 | A    |
| 8   | G     | 266 | G    |
| 8   | G     | 267 | C    |
| 8   | G     | 274 | A    |
| 8   | G     | 279 | A    |
| 8   | G     | 280 | C    |
| 8   | G     | 281 | G    |
| 8   | G     | 283 | C    |
| 8   | G     | 288 | A    |
| 8   | G     | 289 | G    |
| 8   | G     | 291 | C    |
| 8   | G     | 293 | G    |
| 8   | G     | 298 | A    |
| 8   | G     | 301 | G    |
| 8   | G     | 302 | G    |
| 8   | G     | 304 | U    |
| 8   | G     | 306 | G    |
| 8   | G     | 309 | G    |
| 8   | G     | 315 | A    |
| 8   | G     | 321 | A    |
| 8   | G     | 328 | C    |
| 8   | G     | 329 | A    |
| 8   | G     | 330 | C    |
| 8   | G     | 332 | G    |
| 8   | G     | 340 | U    |
| 8   | G     | 345 | C    |
| 8   | G     | 347 | G    |
| 8   | G     | 352 | C    |
| 8   | G     | 353 | A    |
| 8   | G     | 354 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | G     | 356 | A    |
| 8   | G     | 358 | U    |
| 8   | G     | 363 | A    |
| 8   | G     | 365 | U    |
| 8   | G     | 366 | C    |
| 8   | G     | 367 | U    |
| 8   | G     | 372 | C    |
| 8   | G     | 373 | A    |
| 8   | G     | 384 | G    |
| 8   | G     | 388 | G    |
| 8   | G     | 389 | A    |
| 8   | G     | 390 | C    |
| 8   | G     | 397 | A    |
| 8   | G     | 398 | C    |
| 8   | G     | 406 | G    |
| 8   | G     | 412 | A    |
| 8   | G     | 413 | G    |
| 8   | G     | 414 | A    |
| 8   | G     | 420 | U    |
| 8   | G     | 421 | U    |
| 8   | G     | 422 | C    |
| 8   | G     | 423 | G    |
| 8   | G     | 424 | G    |
| 8   | G     | 429 | U    |
| 8   | G     | 434 | U    |
| 8   | G     | 438 | G    |
| 8   | G     | 439 | A    |
| 8   | G     | 448 | A    |
| 8   | G     | 465 | A    |
| 8   | G     | 466 | C    |
| 8   | G     | 467 | G    |
| 8   | G     | 468 | A    |
| 8   | G     | 474 | G    |
| 8   | G     | 481 | G    |
| 8   | G     | 482 | A    |
| 8   | G     | 483 | C    |
| 8   | G     | 484 | G    |
| 8   | G     | 485 | G    |
| 8   | G     | 489 | C    |
| 8   | G     | 492 | G    |
| 8   | G     | 494 | U    |
| 8   | G     | 496 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | G     | 497 | U    |
| 8   | G     | 505 | G    |
| 8   | G     | 515 | G    |
| 8   | G     | 517 | G    |
| 8   | G     | 518 | C    |
| 8   | G     | 527 | G    |
| 8   | G     | 532 | A    |
| 8   | G     | 533 | A    |
| 8   | G     | 543 | C    |
| 8   | G     | 545 | C    |
| 8   | G     | 547 | A    |
| 8   | G     | 548 | G    |
| 8   | G     | 557 | G    |
| 8   | G     | 559 | A    |
| 8   | G     | 560 | U    |
| 8   | G     | 563 | A    |
| 8   | G     | 564 | C    |
| 8   | G     | 567 | G    |
| 8   | G     | 568 | G    |
| 8   | G     | 571 | U    |
| 8   | G     | 572 | A    |
| 8   | G     | 573 | A    |
| 8   | G     | 576 | G    |
| 8   | G     | 577 | G    |
| 8   | G     | 579 | G    |
| 8   | G     | 586 | C    |
| 8   | G     | 592 | G    |
| 8   | G     | 596 | C    |
| 8   | G     | 598 | U    |
| 8   | G     | 602 | A    |
| 8   | G     | 607 | A    |
| 8   | G     | 609 | A    |
| 8   | G     | 618 | C    |
| 8   | G     | 619 | U    |
| 8   | G     | 623 | C    |
| 8   | G     | 627 | G    |
| 8   | G     | 629 | G    |
| 8   | G     | 639 | G    |
| 8   | G     | 642 | A    |
| 8   | G     | 643 | C    |
| 8   | G     | 648 | A    |
| 8   | G     | 652 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | G     | 653 | A    |
| 8   | G     | 654 | G    |
| 8   | G     | 661 | G    |
| 8   | G     | 663 | A    |
| 8   | G     | 665 | A    |
| 8   | G     | 666 | G    |
| 8   | G     | 667 | G    |
| 8   | G     | 674 | G    |
| 8   | G     | 679 | C    |
| 8   | G     | 686 | U    |
| 8   | G     | 687 | A    |
| 8   | G     | 688 | G    |
| 8   | G     | 694 | A    |
| 8   | G     | 696 | A    |
| 8   | G     | 701 | C    |
| 8   | G     | 702 | A    |
| 8   | G     | 703 | G    |
| 8   | G     | 707 | C    |
| 8   | G     | 714 | G    |
| 8   | G     | 715 | A    |
| 8   | G     | 717 | C    |
| 8   | G     | 718 | G    |
| 8   | G     | 719 | C    |
| 8   | G     | 721 | G    |
| 8   | G     | 724 | G    |
| 8   | G     | 725 | G    |
| 8   | G     | 729 | A    |
| 8   | G     | 731 | G    |
| 8   | G     | 733 | A    |
| 8   | G     | 748 | C    |
| 8   | G     | 755 | G    |
| 8   | G     | 761 | G    |
| 8   | G     | 773 | G    |
| 8   | G     | 777 | A    |
| 8   | G     | 781 | A    |
| 8   | G     | 782 | A    |
| 8   | G     | 785 | G    |
| 8   | G     | 793 | U    |
| 8   | G     | 794 | A    |
| 8   | G     | 801 | U    |
| 8   | G     | 803 | G    |
| 8   | G     | 810 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | G     | 812 | C    |
| 8   | G     | 813 | U    |
| 8   | G     | 816 | A    |
| 8   | G     | 817 | C    |
| 8   | G     | 818 | G    |
| 8   | G     | 819 | A    |
| 8   | G     | 820 | U    |
| 8   | G     | 821 | G    |
| 8   | G     | 828 | A    |
| 8   | G     | 838 | G    |
| 8   | G     | 843 | U    |
| 8   | G     | 848 | C    |
| 8   | G     | 852 | G    |
| 8   | G     | 869 | G    |
| 8   | G     | 870 | U    |
| 8   | G     | 871 | U    |
| 8   | G     | 872 | A    |
| 8   | G     | 873 | A    |
| 8   | G     | 885 | G    |
| 8   | G     | 890 | G    |
| 8   | G     | 891 | U    |
| 8   | G     | 900 | A    |
| 8   | G     | 902 | G    |
| 8   | G     | 905 | U    |
| 8   | G     | 907 | A    |
| 8   | G     | 914 | A    |
| 8   | G     | 919 | A    |
| 8   | G     | 927 | G    |
| 8   | G     | 934 | C    |
| 8   | G     | 941 | G    |
| 8   | G     | 945 | G    |
| 8   | G     | 947 | G    |
| 8   | G     | 960 | U    |
| 8   | G     | 962 | C    |
| 8   | G     | 966 | G    |
| 8   | G     | 967 | C    |
| 8   | G     | 968 | A    |
| 8   | G     | 969 | A    |
| 8   | G     | 971 | G    |
| 8   | G     | 972 | C    |
| 8   | G     | 974 | A    |
| 8   | G     | 975 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 8   | G     | 976     | G    |
| 8   | G     | 982     | U    |
| 8   | G     | 984     | C    |
| 8   | G     | 992     | U    |
| 8   | G     | 993     | G    |
| 8   | G     | 994     | A    |
| 8   | G     | 998     | G    |
| 8   | G     | 998(A)  | C    |
| 8   | G     | 999     | U    |
| 8   | G     | 1000    | A    |
| 8   | G     | 1001    | G    |
| 8   | G     | 1002    | G    |
| 8   | G     | 1003    | G    |
| 8   | G     | 1004    | A    |
| 8   | G     | 1005    | A    |
| 8   | G     | 1006    | C    |
| 8   | G     | 1009    | G    |
| 8   | G     | 1015    | A    |
| 8   | G     | 1016    | A    |
| 8   | G     | 1022    | G    |
| 8   | G     | 1024    | G    |
| 8   | G     | 1025    | U    |
| 8   | G     | 1026    | G    |
| 8   | G     | 1027    | C    |
| 8   | G     | 1028    | C    |
| 8   | G     | 1029    | G    |
| 8   | G     | 1030    | C    |
| 8   | G     | 1031    | G    |
| 8   | G     | 1032    | A    |
| 8   | G     | 1032(A) | G    |
| 8   | G     | 1032(B) | G    |
| 8   | G     | 1033    | G    |
| 8   | G     | 1035    | A    |
| 8   | G     | 1036    | G    |
| 8   | G     | 1042    | G    |
| 8   | G     | 1045    | C    |
| 8   | G     | 1046    | A    |
| 8   | G     | 1053    | G    |
| 8   | G     | 1054    | C    |
| 8   | G     | 1060    | C    |
| 8   | G     | 1061    | G    |
| 8   | G     | 1064    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | G     | 1065 | U    |
| 8   | G     | 1066 | C    |
| 8   | G     | 1067 | A    |
| 8   | G     | 1073 | U    |
| 8   | G     | 1078 | U    |
| 8   | G     | 1079 | G    |
| 8   | G     | 1084 | G    |
| 8   | G     | 1085 | U    |
| 8   | G     | 1086 | U    |
| 8   | G     | 1089 | G    |
| 8   | G     | 1090 | U    |
| 8   | G     | 1094 | G    |
| 8   | G     | 1095 | U    |
| 8   | G     | 1099 | G    |
| 8   | G     | 1101 | A    |
| 8   | G     | 1103 | C    |
| 8   | G     | 1117 | G    |
| 8   | G     | 1123 | A    |
| 8   | G     | 1124 | G    |
| 8   | G     | 1125 | U    |
| 8   | G     | 1126 | U    |
| 8   | G     | 1129 | C    |
| 8   | G     | 1130 | A    |
| 8   | G     | 1131 | G    |
| 8   | G     | 1132 | C    |
| 8   | G     | 1136 | U    |
| 8   | G     | 1137 | C    |
| 8   | G     | 1138 | G    |
| 8   | G     | 1139 | G    |
| 8   | G     | 1140 | C    |
| 8   | G     | 1146 | A    |
| 8   | G     | 1154 | G    |
| 8   | G     | 1158 | C    |
| 8   | G     | 1159 | U    |
| 8   | G     | 1166 | G    |
| 8   | G     | 1175 | G    |
| 8   | G     | 1181 | G    |
| 8   | G     | 1182 | G    |
| 8   | G     | 1183 | A    |
| 8   | G     | 1184 | G    |
| 8   | G     | 1186 | G    |
| 8   | G     | 1187 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | G     | 1189 | C    |
| 8   | G     | 1190 | G    |
| 8   | G     | 1192 | C    |
| 8   | G     | 1196 | U    |
| 8   | G     | 1197 | G    |
| 8   | G     | 1201 | A    |
| 8   | G     | 1207 | G    |
| 8   | G     | 1209 | C    |
| 8   | G     | 1211 | U    |
| 8   | G     | 1212 | U    |
| 8   | G     | 1213 | A    |
| 8   | G     | 1218 | C    |
| 8   | G     | 1226 | C    |
| 8   | G     | 1227 | A    |
| 8   | G     | 1236 | A    |
| 8   | G     | 1239 | A    |
| 8   | G     | 1240 | U    |
| 8   | G     | 1241 | G    |
| 8   | G     | 1249 | C    |
| 8   | G     | 1250 | A    |
| 8   | G     | 1253 | G    |
| 8   | G     | 1257 | U    |
| 8   | G     | 1258 | G    |
| 8   | G     | 1260 | C    |
| 8   | G     | 1270 | C    |
| 8   | G     | 1273 | G    |
| 8   | G     | 1275 | A    |
| 8   | G     | 1278 | U    |
| 8   | G     | 1279 | A    |
| 8   | G     | 1280 | A    |
| 8   | G     | 1281 | U    |
| 8   | G     | 1285 | A    |
| 8   | G     | 1286 | A    |
| 8   | G     | 1287 | A    |
| 8   | G     | 1288 | A    |
| 8   | G     | 1296 | C    |
| 8   | G     | 1298 | C    |
| 8   | G     | 1299 | A    |
| 8   | G     | 1300 | G    |
| 8   | G     | 1302 | U    |
| 8   | G     | 1305 | G    |
| 8   | G     | 1308 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 8   | G     | 1309    | G    |
| 8   | G     | 1310    | G    |
| 8   | G     | 1311    | G    |
| 8   | G     | 1312    | G    |
| 8   | G     | 1314    | C    |
| 8   | G     | 1317    | C    |
| 8   | G     | 1320    | C    |
| 8   | G     | 1322    | C    |
| 8   | G     | 1323    | G    |
| 8   | G     | 1329    | A    |
| 8   | G     | 1330    | U    |
| 8   | G     | 1331    | G    |
| 8   | G     | 1332    | A    |
| 8   | G     | 1336    | C    |
| 8   | G     | 1339    | A    |
| 8   | G     | 1347    | G    |
| 8   | G     | 1351    | U    |
| 8   | G     | 1353    | G    |
| 8   | G     | 1359    | C    |
| 8   | G     | 1360    | A    |
| 8   | G     | 1361    | G    |
| 8   | G     | 1362    | C    |
| 8   | G     | 1362(A) | C    |
| 8   | G     | 1363    | A    |
| 8   | G     | 1364    | U    |
| 8   | G     | 1365    | G    |
| 8   | G     | 1367    | C    |
| 8   | G     | 1372    | U    |
| 8   | G     | 1378    | C    |
| 8   | G     | 1379    | G    |
| 8   | G     | 1381    | U    |
| 8   | G     | 1396    | A    |
| 8   | G     | 1397    | C    |
| 8   | G     | 1398    | A    |
| 8   | G     | 1400    | C    |
| 8   | G     | 1401    | G    |
| 8   | G     | 1409    | C    |
| 8   | G     | 1416    | G    |
| 8   | G     | 1438    | G    |
| 8   | G     | 1442    | G    |
| 8   | G     | 1443    | G    |
| 8   | G     | 1446    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | G     | 1447 | G    |
| 8   | G     | 1449 | C    |
| 8   | G     | 1451 | A    |
| 8   | G     | 1452 | C    |
| 8   | G     | 1460 | A    |
| 8   | G     | 1461 | G    |
| 8   | G     | 1469 | G    |
| 8   | G     | 1477 | C    |
| 8   | G     | 1481 | U    |
| 8   | G     | 1492 | A    |
| 8   | G     | 1493 | A    |
| 8   | G     | 1494 | G    |
| 8   | G     | 1497 | G    |
| 8   | G     | 1498 | U    |
| 8   | G     | 1502 | A    |
| 8   | G     | 1503 | A    |
| 8   | G     | 1504 | G    |
| 8   | G     | 1505 | G    |
| 8   | G     | 1506 | U    |
| 8   | G     | 1507 | A    |
| 8   | G     | 1508 | G    |
| 8   | G     | 1510 | U    |
| 8   | G     | 1517 | G    |
| 8   | G     | 1520 | G    |
| 8   | G     | 1525 | G    |
| 8   | G     | 1529 | G    |
| 8   | G     | 1530 | G    |
| 8   | G     | 1531 | A    |
| 8   | G     | 1533 | C    |
| 8   | G     | 1535 | C    |
| 8   | G     | 1536 | C    |
| 8   | G     | 1538 | C    |
| 8   | G     | 1539 | C    |
| 23  | V     | 6    | A    |
| 23  | V     | 7    | G    |
| 23  | V     | 8    | A    |
| 23  | V     | 9    | U    |
| 23  | V     | 10   | G    |
| 23  | V     | 11   | G    |
| 23  | V     | 12   | U    |
| 23  | V     | 13   | A    |
| 23  | V     | 14   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | V     | 21  | A    |
| 23  | V     | 26  | G    |
| 23  | V     | 28  | A    |
| 23  | V     | 29  | U    |
| 23  | V     | 32  | C    |
| 23  | V     | 34  | C    |
| 23  | V     | 35  | G    |
| 23  | V     | 43  | G    |
| 23  | V     | 46  | C    |
| 23  | V     | 47  | C    |
| 23  | V     | 49  | A    |
| 23  | V     | 50  | U    |
| 23  | V     | 51  | G    |
| 23  | V     | 52  | A    |
| 23  | V     | 63  | U    |
| 23  | V     | 71  | A    |
| 23  | V     | 72  | U    |
| 23  | V     | 74  | A    |
| 23  | V     | 75  | G    |
| 23  | V     | 83  | G    |
| 23  | V     | 84  | A    |
| 23  | V     | 85  | G    |
| 23  | V     | 88  | G    |
| 23  | V     | 90  | U    |
| 23  | V     | 91  | A    |
| 23  | V     | 93  | C    |
| 23  | V     | 94  | G    |
| 23  | V     | 96  | G    |
| 23  | V     | 97  | C    |
| 23  | V     | 98  | G    |
| 23  | V     | 99  | U    |
| 23  | V     | 101 | G    |
| 23  | V     | 102 | G    |
| 23  | V     | 118 | A    |
| 23  | V     | 120 | U    |
| 23  | V     | 121 | G    |
| 23  | V     | 125 | G    |
| 23  | V     | 126 | A    |
| 23  | V     | 131 | G    |
| 23  | V     | 134 | C    |
| 23  | V     | 136 | G    |
| 23  | V     | 137 | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 23  | V     | 137(A) | G    |
| 23  | V     | 138    | G    |
| 23  | V     | 139    | G    |
| 23  | V     | 140    | A    |
| 23  | V     | 141    | A    |
| 23  | V     | 142    | G    |
| 23  | V     | 143    | C    |
| 23  | V     | 145    | G    |
| 23  | V     | 146    | G    |
| 23  | V     | 149    | A    |
| 23  | V     | 161    | U    |
| 23  | V     | 164    | U    |
| 23  | V     | 171    | G    |
| 23  | V     | 177    | G    |
| 23  | V     | 178    | G    |
| 23  | V     | 181    | A    |
| 23  | V     | 182    | A    |
| 23  | V     | 190    | A    |
| 23  | V     | 196    | A    |
| 23  | V     | 198    | C    |
| 23  | V     | 199    | A    |
| 23  | V     | 204    | A    |
| 23  | V     | 205    | G    |
| 23  | V     | 207    | A    |
| 23  | V     | 216    | A    |
| 23  | V     | 217    | G    |
| 23  | V     | 221    | A    |
| 23  | V     | 222    | A    |
| 23  | V     | 223    | A    |
| 23  | V     | 224    | G    |
| 23  | V     | 226    | G    |
| 23  | V     | 228    | A    |
| 23  | V     | 229    | A    |
| 23  | V     | 230    | U    |
| 23  | V     | 233    | A    |
| 23  | V     | 245    | G    |
| 23  | V     | 248    | G    |
| 23  | V     | 249    | C    |
| 23  | V     | 251    | A    |
| 23  | V     | 252    | G    |
| 23  | V     | 263    | C    |
| 23  | V     | 264    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 23  | V     | 265    | A    |
| 23  | V     | 266    | G    |
| 23  | V     | 267    | C    |
| 23  | V     | 270    | A    |
| 23  | V     | 270(A) | A    |
| 23  | V     | 270(B) | A    |
| 23  | V     | 270(C) | C    |
| 23  | V     | 270(E) | G    |
| 23  | V     | 270(G) | C    |
| 23  | V     | 270(K) | C    |
| 23  | V     | 270(L) | U    |
| 23  | V     | 270(M) | U    |
| 23  | V     | 270(N) | G    |
| 23  | V     | 270(V) | G    |
| 23  | V     | 270(Z) | U    |
| 23  | V     | 271    | C    |
| 23  | V     | 271(A) | G    |
| 23  | V     | 271(B) | U    |
| 23  | V     | 271(C) | G    |
| 23  | V     | 272    | G    |
| 23  | V     | 273(F) | C    |
| 23  | V     | 275    | G    |
| 23  | V     | 276    | A    |
| 23  | V     | 277    | C    |
| 23  | V     | 280    | C    |
| 23  | V     | 283    | A    |
| 23  | V     | 284    | U    |
| 23  | V     | 285    | C    |
| 23  | V     | 286    | C    |
| 23  | V     | 287    | C    |
| 23  | V     | 288    | C    |
| 23  | V     | 289    | A    |
| 23  | V     | 290    | G    |
| 23  | V     | 293    | U    |
| 23  | V     | 296    | C    |
| 23  | V     | 299    | A    |
| 23  | V     | 300    | A    |
| 23  | V     | 304    | G    |
| 23  | V     | 305    | U    |
| 23  | V     | 306    | U    |
| 23  | V     | 307    | G    |
| 23  | V     | 308    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 23  | V     | 310    | A    |
| 23  | V     | 311    | A    |
| 23  | V     | 312    | G    |
| 23  | V     | 323    | G    |
| 23  | V     | 324    | A    |
| 23  | V     | 327    | G    |
| 23  | V     | 329    | G    |
| 23  | V     | 330    | A    |
| 23  | V     | 332    | A    |
| 23  | V     | 333    | G    |
| 23  | V     | 334    | C    |
| 23  | V     | 338    | G    |
| 23  | V     | 339    | U    |
| 23  | V     | 340    | A    |
| 23  | V     | 341    | G    |
| 23  | V     | 345    | A    |
| 23  | V     | 347    | A    |
| 23  | V     | 348    | G    |
| 23  | V     | 349    | G    |
| 23  | V     | 350    | U    |
| 23  | V     | 351    | G    |
| 23  | V     | 352    | G    |
| 23  | V     | 354    | G    |
| 23  | V     | 356    | G    |
| 23  | V     | 358    | U    |
| 23  | V     | 359    | A    |
| 23  | V     | 360    | G    |
| 23  | V     | 361    | G    |
| 23  | V     | 363(A) | A    |
| 23  | V     | 363(E) | U    |
| 23  | V     | 363(F) | G    |
| 23  | V     | 365    | C    |
| 23  | V     | 366    | C    |
| 23  | V     | 370    | G    |
| 23  | V     | 371    | A    |
| 23  | V     | 372    | G    |
| 23  | V     | 373    | U    |
| 23  | V     | 374    | A    |
| 23  | V     | 380    | U    |
| 23  | V     | 383    | U    |
| 23  | V     | 386    | G    |
| 23  | V     | 388    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | V     | 394 | A    |
| 23  | V     | 399 | G    |
| 23  | V     | 403 | U    |
| 23  | V     | 404 | C    |
| 23  | V     | 405 | U    |
| 23  | V     | 411 | G    |
| 23  | V     | 412 | A    |
| 23  | V     | 413 | C    |
| 23  | V     | 417 | C    |
| 23  | V     | 418 | G    |
| 23  | V     | 419 | C    |
| 23  | V     | 428 | A    |
| 23  | V     | 433 | C    |
| 23  | V     | 434 | U    |
| 23  | V     | 435 | C    |
| 23  | V     | 443 | A    |
| 23  | V     | 444 | C    |
| 23  | V     | 446 | G    |
| 23  | V     | 447 | A    |
| 23  | V     | 448 | U    |
| 23  | V     | 449 | A    |
| 23  | V     | 451 | C    |
| 23  | V     | 452 | G    |
| 23  | V     | 455 | C    |
| 23  | V     | 456 | C    |
| 23  | V     | 457 | A    |
| 23  | V     | 458 | G    |
| 23  | V     | 459 | U    |
| 23  | V     | 467 | G    |
| 23  | V     | 471 | A    |
| 23  | V     | 473 | G    |
| 23  | V     | 479 | A    |
| 23  | V     | 480 | A    |
| 23  | V     | 481 | G    |
| 23  | V     | 485 | C    |
| 23  | V     | 489 | G    |
| 23  | V     | 491 | G    |
| 23  | V     | 501 | A    |
| 23  | V     | 504 | U    |
| 23  | V     | 505 | A    |
| 23  | V     | 508 | G    |
| 23  | V     | 512 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 23  | V     | 526    | A    |
| 23  | V     | 527    | C    |
| 23  | V     | 528    | A    |
| 23  | V     | 529    | A    |
| 23  | V     | 530    | G    |
| 23  | V     | 531    | C    |
| 23  | V     | 532    | A    |
| 23  | V     | 533    | G    |
| 23  | V     | 536    | A    |
| 23  | V     | 537    | C    |
| 23  | V     | 540    | G    |
| 23  | V     | 545    | G    |
| 23  | V     | 551    | G    |
| 23  | V     | 556    | G    |
| 23  | V     | 560    | C    |
| 23  | V     | 563    | G    |
| 23  | V     | 568    | U    |
| 23  | V     | 570    | G    |
| 23  | V     | 573    | G    |
| 23  | V     | 574    | C    |
| 23  | V     | 575    | A    |
| 23  | V     | 586    | A    |
| 23  | V     | 588    | U    |
| 23  | V     | 598    | G    |
| 23  | V     | 599    | G    |
| 23  | V     | 603    | A    |
| 23  | V     | 607    | U    |
| 23  | V     | 608    | A    |
| 23  | V     | 613    | U    |
| 23  | V     | 615    | G    |
| 23  | V     | 616    | A    |
| 23  | V     | 617    | G    |
| 23  | V     | 618(A) | C    |
| 23  | V     | 619    | G    |
| 23  | V     | 621    | A    |
| 23  | V     | 622    | G    |
| 23  | V     | 624    | C    |
| 23  | V     | 626    | U    |
| 23  | V     | 627    | A    |
| 23  | V     | 628    | G    |
| 23  | V     | 631    | A    |
| 23  | V     | 632    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | V     | 637 | A    |
| 23  | V     | 638 | G    |
| 23  | V     | 639 | U    |
| 23  | V     | 642 | G    |
| 23  | V     | 643 | A    |
| 23  | V     | 644 | A    |
| 23  | V     | 645 | C    |
| 23  | V     | 646 | A    |
| 23  | V     | 648 | G    |
| 23  | V     | 649 | G    |
| 23  | V     | 652 | C    |
| 23  | V     | 653 | A    |
| 23  | V     | 654 | A    |
| 23  | V     | 655 | A    |
| 23  | V     | 656 | G    |
| 23  | V     | 669 | G    |
| 23  | V     | 671 | C    |
| 23  | V     | 677 | A    |
| 23  | V     | 682 | G    |
| 23  | V     | 684 | G    |
| 23  | V     | 686 | G    |
| 23  | V     | 688 | U    |
| 23  | V     | 693 | C    |
| 23  | V     | 699 | A    |
| 23  | V     | 715 | G    |
| 23  | V     | 717 | G    |
| 23  | V     | 719 | C    |
| 23  | V     | 725 | G    |
| 23  | V     | 726 | G    |
| 23  | V     | 727 | A    |
| 23  | V     | 728 | G    |
| 23  | V     | 729 | G    |
| 23  | V     | 730 | C    |
| 23  | V     | 731 | C    |
| 23  | V     | 739 | G    |
| 23  | V     | 740 | U    |
| 23  | V     | 743 | G    |
| 23  | V     | 744 | G    |
| 23  | V     | 747 | U    |
| 23  | V     | 748 | G    |
| 23  | V     | 750 | A    |
| 23  | V     | 755 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | V     | 756 | C    |
| 23  | V     | 758 | C    |
| 23  | V     | 762 | U    |
| 23  | V     | 764 | A    |
| 23  | V     | 775 | G    |
| 23  | V     | 777 | A    |
| 23  | V     | 779 | U    |
| 23  | V     | 782 | A    |
| 23  | V     | 783 | A    |
| 23  | V     | 784 | A    |
| 23  | V     | 785 | G    |
| 23  | V     | 789 | A    |
| 23  | V     | 790 | C    |
| 23  | V     | 791 | C    |
| 23  | V     | 792 | G    |
| 23  | V     | 793 | A    |
| 23  | V     | 794 | G    |
| 23  | V     | 795 | C    |
| 23  | V     | 800 | A    |
| 23  | V     | 801 | G    |
| 23  | V     | 802 | A    |
| 23  | V     | 805 | G    |
| 23  | V     | 811 | U    |
| 23  | V     | 812 | C    |
| 23  | V     | 817 | C    |
| 23  | V     | 823 | G    |
| 23  | V     | 825 | C    |
| 23  | V     | 827 | U    |
| 23  | V     | 828 | U    |
| 23  | V     | 830 | G    |
| 23  | V     | 832 | G    |
| 23  | V     | 837 | C    |
| 23  | V     | 843 | G    |
| 23  | V     | 847 | U    |
| 23  | V     | 850 | C    |
| 23  | V     | 853 | G    |
| 23  | V     | 855 | G    |
| 23  | V     | 859 | G    |
| 23  | V     | 860 | U    |
| 23  | V     | 865 | C    |
| 23  | V     | 866 | A    |
| 23  | V     | 870 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 23  | V     | 873    | G    |
| 23  | V     | 874    | G    |
| 23  | V     | 875    | G    |
| 23  | V     | 876    | C    |
| 23  | V     | 881    | G    |
| 23  | V     | 882    | G    |
| 23  | V     | 883    | G    |
| 23  | V     | 884    | C    |
| 23  | V     | 886    | C    |
| 23  | V     | 887    | A    |
| 23  | V     | 889    | C    |
| 23  | V     | 890    | A    |
| 23  | V     | 892    | G    |
| 23  | V     | 893    | C    |
| 23  | V     | 894    | C    |
| 23  | V     | 895    | U    |
| 23  | V     | 896    | A    |
| 23  | V     | 898    | C    |
| 23  | V     | 900    | A    |
| 23  | V     | 901    | A    |
| 23  | V     | 902    | C    |
| 23  | V     | 903    | C    |
| 23  | V     | 904    | C    |
| 23  | V     | 906    | G    |
| 23  | V     | 907    | U    |
| 23  | V     | 910    | A    |
| 23  | V     | 915    | C    |
| 23  | V     | 926    | A    |
| 23  | V     | 929    | G    |
| 23  | V     | 930    | U    |
| 23  | V     | 931    | G    |
| 23  | V     | 932    | G    |
| 23  | V     | 941    | A    |
| 23  | V     | 945    | A    |
| 23  | V     | 946    | G    |
| 23  | V     | 957    | A    |
| 23  | V     | 961    | C    |
| 23  | V     | 966    | G    |
| 23  | V     | 968    | G    |
| 23  | V     | 973    | A    |
| 23  | V     | 974    | G    |
| 23  | V     | 974(A) | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 980  | A    |
| 23  | V     | 981  | A    |
| 23  | V     | 982  | C    |
| 23  | V     | 983  | A    |
| 23  | V     | 987  | G    |
| 23  | V     | 988  | A    |
| 23  | V     | 989  | G    |
| 23  | V     | 995  | C    |
| 23  | V     | 996  | A    |
| 23  | V     | 999  | U    |
| 23  | V     | 1000 | A    |
| 23  | V     | 1004 | C    |
| 23  | V     | 1005 | C    |
| 23  | V     | 1006 | C    |
| 23  | V     | 1007 | C    |
| 23  | V     | 1008 | C    |
| 23  | V     | 1011 | G    |
| 23  | V     | 1013 | C    |
| 23  | V     | 1016 | G    |
| 23  | V     | 1021 | A    |
| 23  | V     | 1022 | G    |
| 23  | V     | 1023 | U    |
| 23  | V     | 1024 | G    |
| 23  | V     | 1025 | G    |
| 23  | V     | 1026 | U    |
| 23  | V     | 1027 | A    |
| 23  | V     | 1033 | U    |
| 23  | V     | 1034 | G    |
| 23  | V     | 1038 | C    |
| 23  | V     | 1041 | C    |
| 23  | V     | 1042 | G    |
| 23  | V     | 1044 | G    |
| 23  | V     | 1045 | A    |
| 23  | V     | 1046 | A    |
| 23  | V     | 1047 | G    |
| 23  | V     | 1050 | A    |
| 23  | V     | 1051 | G    |
| 23  | V     | 1052 | C    |
| 23  | V     | 1053 | C    |
| 23  | V     | 1054 | A    |
| 23  | V     | 1055 | G    |
| 23  | V     | 1056 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 1057 | A    |
| 23  | V     | 1058 | G    |
| 23  | V     | 1059 | G    |
| 23  | V     | 1060 | U    |
| 23  | V     | 1061 | U    |
| 23  | V     | 1062 | G    |
| 23  | V     | 1063 | G    |
| 23  | V     | 1064 | C    |
| 23  | V     | 1065 | U    |
| 23  | V     | 1066 | U    |
| 23  | V     | 1068 | G    |
| 23  | V     | 1069 | A    |
| 23  | V     | 1070 | A    |
| 23  | V     | 1071 | G    |
| 23  | V     | 1073 | A    |
| 23  | V     | 1075 | C    |
| 23  | V     | 1076 | C    |
| 23  | V     | 1077 | A    |
| 23  | V     | 1078 | U    |
| 23  | V     | 1079 | C    |
| 23  | V     | 1083 | U    |
| 23  | V     | 1085 | A    |
| 23  | V     | 1086 | A    |
| 23  | V     | 1087 | G    |
| 23  | V     | 1088 | A    |
| 23  | V     | 1089 | G    |
| 23  | V     | 1090 | U    |
| 23  | V     | 1093 | G    |
| 23  | V     | 1094 | U    |
| 23  | V     | 1096 | A    |
| 23  | V     | 1099 | G    |
| 23  | V     | 1101 | U    |
| 23  | V     | 1102 | C    |
| 23  | V     | 1104 | C    |
| 23  | V     | 1105 | U    |
| 23  | V     | 1106 | G    |
| 23  | V     | 1107 | G    |
| 23  | V     | 1110 | G    |
| 23  | V     | 1111 | A    |
| 23  | V     | 1112 | G    |
| 23  | V     | 1118 | C    |
| 23  | V     | 1124 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 23  | V     | 1126    | A    |
| 23  | V     | 1130    | U    |
| 23  | V     | 1131    | G    |
| 23  | V     | 1134    | G    |
| 23  | V     | 1135    | C    |
| 23  | V     | 1140    | C    |
| 23  | V     | 1141    | U    |
| 23  | V     | 1142    | U    |
| 23  | V     | 1142(A) | A    |
| 23  | V     | 1143    | A    |
| 23  | V     | 1144    | G    |
| 23  | V     | 1151    | G    |
| 23  | V     | 1155    | A    |
| 23  | V     | 1156    | A    |
| 23  | V     | 1158    | C    |
| 23  | V     | 1162    | G    |
| 23  | V     | 1170    | G    |
| 23  | V     | 1173    | G    |
| 23  | V     | 1174    | A    |
| 23  | V     | 1175    | U    |
| 23  | V     | 1176    | G    |
| 23  | V     | 1177    | A    |
| 23  | V     | 1178    | C    |
| 23  | V     | 1180    | C    |
| 23  | V     | 1183    | G    |
| 23  | V     | 1186    | G    |
| 23  | V     | 1190    | G    |
| 23  | V     | 1193    | G    |
| 23  | V     | 1195    | G    |
| 23  | V     | 1199    | U    |
| 23  | V     | 1200    | C    |
| 23  | V     | 1201    | C    |
| 23  | V     | 1203    | G    |
| 23  | V     | 1204    | A    |
| 23  | V     | 1205    | U    |
| 23  | V     | 1211    | U    |
| 23  | V     | 1215    | G    |
| 23  | V     | 1220    | A    |
| 23  | V     | 1221    | C    |
| 23  | V     | 1222    | C    |
| 23  | V     | 1229    | G    |
| 23  | V     | 1231    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 1233 | C    |
| 23  | V     | 1238 | G    |
| 23  | V     | 1240 | U    |
| 23  | V     | 1241 | A    |
| 23  | V     | 1242 | A    |
| 23  | V     | 1248 | G    |
| 23  | V     | 1250 | G    |
| 23  | V     | 1251 | C    |
| 23  | V     | 1252 | G    |
| 23  | V     | 1253 | A    |
| 23  | V     | 1255 | U    |
| 23  | V     | 1256 | G    |
| 23  | V     | 1258 | C    |
| 23  | V     | 1260 | G    |
| 23  | V     | 1262 | A    |
| 23  | V     | 1265 | A    |
| 23  | V     | 1266 | G    |
| 23  | V     | 1267 | U    |
| 23  | V     | 1268 | A    |
| 23  | V     | 1271 | G    |
| 23  | V     | 1272 | A    |
| 23  | V     | 1275 | A    |
| 23  | V     | 1284 | A    |
| 23  | V     | 1285 | G    |
| 23  | V     | 1286 | A    |
| 23  | V     | 1287 | A    |
| 23  | V     | 1289 | C    |
| 23  | V     | 1297 | C    |
| 23  | V     | 1300 | U    |
| 23  | V     | 1301 | A    |
| 23  | V     | 1302 | A    |
| 23  | V     | 1304 | C    |
| 23  | V     | 1308 | A    |
| 23  | V     | 1310 | G    |
| 23  | V     | 1313 | U    |
| 23  | V     | 1314 | C    |
| 23  | V     | 1321 | A    |
| 23  | V     | 1324 | G    |
| 23  | V     | 1325 | G    |
| 23  | V     | 1327 | C    |
| 23  | V     | 1329 | U    |
| 23  | V     | 1330 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 1332 | G    |
| 23  | V     | 1335 | U    |
| 23  | V     | 1338 | G    |
| 23  | V     | 1340 | U    |
| 23  | V     | 1341 | U    |
| 23  | V     | 1344 | G    |
| 23  | V     | 1351 | C    |
| 23  | V     | 1352 | U    |
| 23  | V     | 1354 | A    |
| 23  | V     | 1355 | G    |
| 23  | V     | 1359 | A    |
| 23  | V     | 1360 | A    |
| 23  | V     | 1362 | C    |
| 23  | V     | 1363 | C    |
| 23  | V     | 1364 | G    |
| 23  | V     | 1365 | A    |
| 23  | V     | 1366 | A    |
| 23  | V     | 1367 | A    |
| 23  | V     | 1368 | G    |
| 23  | V     | 1373 | A    |
| 23  | V     | 1376 | C    |
| 23  | V     | 1379 | A    |
| 23  | V     | 1384 | A    |
| 23  | V     | 1385 | G    |
| 23  | V     | 1390 | U    |
| 23  | V     | 1397 | U    |
| 23  | V     | 1398 | C    |
| 23  | V     | 1406 | U    |
| 23  | V     | 1411 | C    |
| 23  | V     | 1415 | U    |
| 23  | V     | 1416 | G    |
| 23  | V     | 1419 | A    |
| 23  | V     | 1420 | U    |
| 23  | V     | 1421 | G    |
| 23  | V     | 1428 | C    |
| 23  | V     | 1438 | U    |
| 23  | V     | 1443 | G    |
| 23  | V     | 1444 | G    |
| 23  | V     | 1445 | C    |
| 23  | V     | 1446 | C    |
| 23  | V     | 1447 | G    |
| 23  | V     | 1448 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 23  | V     | 1449    | A    |
| 23  | V     | 1449(A) | G    |
| 23  | V     | 1450    | C    |
| 23  | V     | 1451    | C    |
| 23  | V     | 1452    | A    |
| 23  | V     | 1453    | A    |
| 23  | V     | 1454    | U    |
| 23  | V     | 1455    | G    |
| 23  | V     | 1458    | C    |
| 23  | V     | 1460    | A    |
| 23  | V     | 1461    | G    |
| 23  | V     | 1462    | C    |
| 23  | V     | 1463    | C    |
| 23  | V     | 1467    | C    |
| 23  | V     | 1472    | A    |
| 23  | V     | 1474    | C    |
| 23  | V     | 1476    | C    |
| 23  | V     | 1477    | A    |
| 23  | V     | 1478    | G    |
| 23  | V     | 1479    | G    |
| 23  | V     | 1482    | U    |
| 23  | V     | 1483    | G    |
| 23  | V     | 1488    | G    |
| 23  | V     | 1490    | A    |
| 23  | V     | 1491    | G    |
| 23  | V     | 1492    | G    |
| 23  | V     | 1493    | C    |
| 23  | V     | 1494    | A    |
| 23  | V     | 1496    | A    |
| 23  | V     | 1497    | U    |
| 23  | V     | 1498    | C    |
| 23  | V     | 1503    | U    |
| 23  | V     | 1507    | A    |
| 23  | V     | 1508    | A    |
| 23  | V     | 1509    | C    |
| 23  | V     | 1513    | C    |
| 23  | V     | 1514    | U    |
| 23  | V     | 1515    | C    |
| 23  | V     | 1516    | U    |
| 23  | V     | 1519    | G    |
| 23  | V     | 1520    | U    |
| 23  | V     | 1522    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 23  | V     | 1523    | U    |
| 23  | V     | 1527    | G    |
| 23  | V     | 1528    | A    |
| 23  | V     | 1529    | A    |
| 23  | V     | 1530    | G    |
| 23  | V     | 1534    | G    |
| 23  | V     | 1537    | C    |
| 23  | V     | 1540    | G    |
| 23  | V     | 1542    | G    |
| 23  | V     | 1543    | A    |
| 23  | V     | 1544    | C    |
| 23  | V     | 1545    | A    |
| 23  | V     | 1545(A) | A    |
| 23  | V     | 1546    | C    |
| 23  | V     | 1548    | C    |
| 23  | V     | 1549    | C    |
| 23  | V     | 1554    | A    |
| 23  | V     | 1555    | G    |
| 23  | V     | 1558    | A    |
| 23  | V     | 1559    | G    |
| 23  | V     | 1560    | G    |
| 23  | V     | 1561    | G    |
| 23  | V     | 1562    | A    |
| 23  | V     | 1563    | G    |
| 23  | V     | 1565    | C    |
| 23  | V     | 1566    | A    |
| 23  | V     | 1567    | A    |
| 23  | V     | 1568    | G    |
| 23  | V     | 1569    | A    |
| 23  | V     | 1571    | A    |
| 23  | V     | 1572    | A    |
| 23  | V     | 1573    | G    |
| 23  | V     | 1574    | C    |
| 23  | V     | 1577    | C    |
| 23  | V     | 1578    | U    |
| 23  | V     | 1579    | A    |
| 23  | V     | 1580    | A    |
| 23  | V     | 1581    | G    |
| 23  | V     | 1582    | C    |
| 23  | V     | 1583    | A    |
| 23  | V     | 1585    | C    |
| 23  | V     | 1586    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 23  | V     | 1587    | A    |
| 23  | V     | 1588    | C    |
| 23  | V     | 1589    | C    |
| 23  | V     | 1591    | G    |
| 23  | V     | 1602    | U    |
| 23  | V     | 1603    | A    |
| 23  | V     | 1604    | C    |
| 23  | V     | 1607    | C    |
| 23  | V     | 1608    | A    |
| 23  | V     | 1609    | A    |
| 23  | V     | 1610    | A    |
| 23  | V     | 1612    | C    |
| 23  | V     | 1614    | A    |
| 23  | V     | 1617    | C    |
| 23  | V     | 1618    | A    |
| 23  | V     | 1619    | G    |
| 23  | V     | 1626    | G    |
| 23  | V     | 1627    | G    |
| 23  | V     | 1628    | G    |
| 23  | V     | 1630    | G    |
| 23  | V     | 1630(A) | C    |
| 23  | V     | 1632    | A    |
| 23  | V     | 1638    | C    |
| 23  | V     | 1640    | C    |
| 23  | V     | 1644    | C    |
| 23  | V     | 1646    | C    |
| 23  | V     | 1648    | C    |
| 23  | V     | 1653    | G    |
| 23  | V     | 1665    | A    |
| 23  | V     | 1672    | C    |
| 23  | V     | 1673    | U    |
| 23  | V     | 1674    | G    |
| 23  | V     | 1675    | C    |
| 23  | V     | 1680    | U    |
| 23  | V     | 1681    | G    |
| 23  | V     | 1694    | C    |
| 23  | V     | 1695    | G    |
| 23  | V     | 1696    | G    |
| 23  | V     | 1697    | G    |
| 23  | V     | 1698    | A    |
| 23  | V     | 1704    | G    |
| 23  | V     | 1710    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 1712 | C    |
| 23  | V     | 1716 | U    |
| 23  | V     | 1717 | G    |
| 23  | V     | 1718 | G    |
| 23  | V     | 1725 | G    |
| 23  | V     | 1726 | G    |
| 23  | V     | 1728 | G    |
| 23  | V     | 1729 | A    |
| 23  | V     | 1730 | U    |
| 23  | V     | 1731 | G    |
| 23  | V     | 1732 | A    |
| 23  | V     | 1733 | G    |
| 23  | V     | 1734 | C    |
| 23  | V     | 1735 | C    |
| 23  | V     | 1741 | C    |
| 23  | V     | 1743 | G    |
| 23  | V     | 1747 | G    |
| 23  | V     | 1753 | G    |
| 23  | V     | 1757 | U    |
| 23  | V     | 1758 | G    |
| 23  | V     | 1759 | A    |
| 23  | V     | 1762 | A    |
| 23  | V     | 1763 | G    |
| 23  | V     | 1764 | G    |
| 23  | V     | 1766 | U    |
| 23  | V     | 1773 | A    |
| 23  | V     | 1774 | C    |
| 23  | V     | 1776 | G    |
| 23  | V     | 1779 | U    |
| 23  | V     | 1780 | A    |
| 23  | V     | 1781 | C    |
| 23  | V     | 1782 | C    |
| 23  | V     | 1783 | A    |
| 23  | V     | 1784 | A    |
| 23  | V     | 1785 | A    |
| 23  | V     | 1786 | A    |
| 23  | V     | 1787 | A    |
| 23  | V     | 1788 | C    |
| 23  | V     | 1791 | A    |
| 23  | V     | 1799 | G    |
| 23  | V     | 1800 | C    |
| 23  | V     | 1801 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 1802 | A    |
| 23  | V     | 1809 | A    |
| 23  | V     | 1810 | A    |
| 23  | V     | 1811 | G    |
| 23  | V     | 1813 | G    |
| 23  | V     | 1814 | G    |
| 23  | V     | 1815 | A    |
| 23  | V     | 1816 | G    |
| 23  | V     | 1818 | U    |
| 23  | V     | 1819 | A    |
| 23  | V     | 1820 | U    |
| 23  | V     | 1821 | A    |
| 23  | V     | 1829 | A    |
| 23  | V     | 1834 | U    |
| 23  | V     | 1835 | G    |
| 23  | V     | 1838 | C    |
| 23  | V     | 1839 | G    |
| 23  | V     | 1846 | G    |
| 23  | V     | 1847 | A    |
| 23  | V     | 1848 | A    |
| 23  | V     | 1858 | G    |
| 23  | V     | 1860 | G    |
| 23  | V     | 1861 | G    |
| 23  | V     | 1864 | U    |
| 23  | V     | 1869 | G    |
| 23  | V     | 1870 | C    |
| 23  | V     | 1871 | A    |
| 23  | V     | 1872 | A    |
| 23  | V     | 1878 | G    |
| 23  | V     | 1880 | C    |
| 23  | V     | 1882 | C    |
| 23  | V     | 1884 | A    |
| 23  | V     | 1889 | A    |
| 23  | V     | 1898 | U    |
| 23  | V     | 1903 | G    |
| 23  | V     | 1905 | C    |
| 23  | V     | 1912 | A    |
| 23  | V     | 1913 | A    |
| 23  | V     | 1914 | C    |
| 23  | V     | 1916 | A    |
| 23  | V     | 1917 | U    |
| 23  | V     | 1919 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 1922 | G    |
| 23  | V     | 1929 | G    |
| 23  | V     | 1930 | G    |
| 23  | V     | 1934 | C    |
| 23  | V     | 1936 | A    |
| 23  | V     | 1937 | A    |
| 23  | V     | 1938 | A    |
| 23  | V     | 1939 | U    |
| 23  | V     | 1940 | U    |
| 23  | V     | 1943 | U    |
| 23  | V     | 1944 | U    |
| 23  | V     | 1945 | G    |
| 23  | V     | 1951 | U    |
| 23  | V     | 1955 | U    |
| 23  | V     | 1956 | U    |
| 23  | V     | 1963 | U    |
| 23  | V     | 1964 | G    |
| 23  | V     | 1965 | C    |
| 23  | V     | 1967 | C    |
| 23  | V     | 1970 | A    |
| 23  | V     | 1971 | A    |
| 23  | V     | 1972 | A    |
| 23  | V     | 1982 | C    |
| 23  | V     | 1987 | G    |
| 23  | V     | 1991 | U    |
| 23  | V     | 1993 | U    |
| 23  | V     | 1996 | C    |
| 23  | V     | 1997 | G    |
| 23  | V     | 2013 | A    |
| 23  | V     | 2018 | G    |
| 23  | V     | 2020 | A    |
| 23  | V     | 2021 | C    |
| 23  | V     | 2022 | U    |
| 23  | V     | 2023 | G    |
| 23  | V     | 2026 | C    |
| 23  | V     | 2028 | U    |
| 23  | V     | 2030 | A    |
| 23  | V     | 2031 | A    |
| 23  | V     | 2032 | G    |
| 23  | V     | 2033 | A    |
| 23  | V     | 2034 | U    |
| 23  | V     | 2036 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 2039 | C    |
| 23  | V     | 2040 | C    |
| 23  | V     | 2041 | U    |
| 23  | V     | 2049 | G    |
| 23  | V     | 2050 | C    |
| 23  | V     | 2055 | C    |
| 23  | V     | 2056 | G    |
| 23  | V     | 2060 | A    |
| 23  | V     | 2061 | G    |
| 23  | V     | 2062 | A    |
| 23  | V     | 2063 | C    |
| 23  | V     | 2064 | C    |
| 23  | V     | 2069 | G    |
| 23  | V     | 2070 | G    |
| 23  | V     | 2077 | A    |
| 23  | V     | 2087 | G    |
| 23  | V     | 2092 | U    |
| 23  | V     | 2093 | G    |
| 23  | V     | 2096 | U    |
| 23  | V     | 2097 | C    |
| 23  | V     | 2102 | U    |
| 23  | V     | 2105 | C    |
| 23  | V     | 2108 | C    |
| 23  | V     | 2109 | U    |
| 23  | V     | 2110 | G    |
| 23  | V     | 2111 | C    |
| 23  | V     | 2113 | U    |
| 23  | V     | 2114 | A    |
| 23  | V     | 2116 | G    |
| 23  | V     | 2117 | A    |
| 23  | V     | 2120 | G    |
| 23  | V     | 2122 | U    |
| 23  | V     | 2123 | G    |
| 23  | V     | 2125 | G    |
| 23  | V     | 2126 | A    |
| 23  | V     | 2128 | C    |
| 23  | V     | 2129 | C    |
| 23  | V     | 2131 | G    |
| 23  | V     | 2132 | U    |
| 23  | V     | 2133 | G    |
| 23  | V     | 2134 | A    |
| 23  | V     | 2135 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 2136 | C    |
| 23  | V     | 2138 | C    |
| 23  | V     | 2144 | U    |
| 23  | V     | 2147 | G    |
| 23  | V     | 2156 | G    |
| 23  | V     | 2158 | A    |
| 23  | V     | 2159 | G    |
| 23  | V     | 2167 | U    |
| 23  | V     | 2168 | G    |
| 23  | V     | 2171 | A    |
| 23  | V     | 2172 | U    |
| 23  | V     | 2173 | A    |
| 23  | V     | 2175 | C    |
| 23  | V     | 2177 | C    |
| 23  | V     | 2182 | G    |
| 23  | V     | 2183 | C    |
| 23  | V     | 2187 | G    |
| 23  | V     | 2189 | U    |
| 23  | V     | 2190 | G    |
| 23  | V     | 2194 | G    |
| 23  | V     | 2195 | C    |
| 23  | V     | 2199 | A    |
| 23  | V     | 2205 | C    |
| 23  | V     | 2206 | C    |
| 23  | V     | 2207 | C    |
| 23  | V     | 2208 | U    |
| 23  | V     | 2209 | C    |
| 23  | V     | 2210 | G    |
| 23  | V     | 2212 | A    |
| 23  | V     | 2213 | U    |
| 23  | V     | 2215 | G    |
| 23  | V     | 2218 | G    |
| 23  | V     | 2226 | C    |
| 23  | V     | 2238 | G    |
| 23  | V     | 2239 | G    |
| 23  | V     | 2243 | U    |
| 23  | V     | 2246 | G    |
| 23  | V     | 2247 | A    |
| 23  | V     | 2258 | C    |
| 23  | V     | 2259 | G    |
| 23  | V     | 2268 | A    |
| 23  | V     | 2270 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 2273 | A    |
| 23  | V     | 2283 | C    |
| 23  | V     | 2284 | C    |
| 23  | V     | 2286 | A    |
| 23  | V     | 2287 | A    |
| 23  | V     | 2288 | A    |
| 23  | V     | 2292 | C    |
| 23  | V     | 2294 | C    |
| 23  | V     | 2295 | C    |
| 23  | V     | 2296 | U    |
| 23  | V     | 2297 | C    |
| 23  | V     | 2304 | G    |
| 23  | V     | 2305 | A    |
| 23  | V     | 2308 | G    |
| 23  | V     | 2309 | A    |
| 23  | V     | 2310 | A    |
| 23  | V     | 2311 | A    |
| 23  | V     | 2312 | U    |
| 23  | V     | 2319 | G    |
| 23  | V     | 2320 | A    |
| 23  | V     | 2322 | A    |
| 23  | V     | 2325 | G    |
| 23  | V     | 2327 | A    |
| 23  | V     | 2333 | A    |
| 23  | V     | 2334 | G    |
| 23  | V     | 2335 | A    |
| 23  | V     | 2337 | G    |
| 23  | V     | 2338 | G    |
| 23  | V     | 2342 | C    |
| 23  | V     | 2343 | C    |
| 23  | V     | 2347 | C    |
| 23  | V     | 2348 | U    |
| 23  | V     | 2349 | G    |
| 23  | V     | 2350 | C    |
| 23  | V     | 2351 | G    |
| 23  | V     | 2356 | C    |
| 23  | V     | 2359 | C    |
| 23  | V     | 2361 | A    |
| 23  | V     | 2383 | G    |
| 23  | V     | 2385 | C    |
| 23  | V     | 2390 | U    |
| 23  | V     | 2403 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 2406 | U    |
| 23  | V     | 2407 | G    |
| 23  | V     | 2414 | G    |
| 23  | V     | 2417 | C    |
| 23  | V     | 2419 | U    |
| 23  | V     | 2423 | U    |
| 23  | V     | 2424 | C    |
| 23  | V     | 2425 | A    |
| 23  | V     | 2426 | A    |
| 23  | V     | 2429 | G    |
| 23  | V     | 2430 | A    |
| 23  | V     | 2437 | U    |
| 23  | V     | 2441 | C    |
| 23  | V     | 2443 | C    |
| 23  | V     | 2445 | G    |
| 23  | V     | 2448 | A    |
| 23  | V     | 2460 | U    |
| 23  | V     | 2462 | U    |
| 23  | V     | 2465 | C    |
| 23  | V     | 2467 | C    |
| 23  | V     | 2472 | G    |
| 23  | V     | 2475 | C    |
| 23  | V     | 2476 | A    |
| 23  | V     | 2482 | G    |
| 23  | V     | 2487 | G    |
| 23  | V     | 2493 | U    |
| 23  | V     | 2498 | C    |
| 23  | V     | 2502 | G    |
| 23  | V     | 2503 | A    |
| 23  | V     | 2504 | U    |
| 23  | V     | 2505 | G    |
| 23  | V     | 2510 | C    |
| 23  | V     | 2513 | G    |
| 23  | V     | 2514 | U    |
| 23  | V     | 2518 | A    |
| 23  | V     | 2519 | U    |
| 23  | V     | 2520 | C    |
| 23  | V     | 2530 | A    |
| 23  | V     | 2532 | G    |
| 23  | V     | 2534 | A    |
| 23  | V     | 2538 | C    |
| 23  | V     | 2553 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 2554 | U    |
| 23  | V     | 2556 | C    |
| 23  | V     | 2565 | A    |
| 23  | V     | 2566 | A    |
| 23  | V     | 2567 | G    |
| 23  | V     | 2570 | G    |
| 23  | V     | 2572 | A    |
| 23  | V     | 2573 | C    |
| 23  | V     | 2585 | U    |
| 23  | V     | 2599 | G    |
| 23  | V     | 2602 | A    |
| 23  | V     | 2603 | G    |
| 23  | V     | 2607 | G    |
| 23  | V     | 2608 | G    |
| 23  | V     | 2609 | U    |
| 23  | V     | 2611 | U    |
| 23  | V     | 2612 | C    |
| 23  | V     | 2613 | U    |
| 23  | V     | 2614 | A    |
| 23  | V     | 2615 | U    |
| 23  | V     | 2627 | G    |
| 23  | V     | 2628 | C    |
| 23  | V     | 2629 | A    |
| 23  | V     | 2630 | G    |
| 23  | V     | 2632 | A    |
| 23  | V     | 2638 | G    |
| 23  | V     | 2646 | C    |
| 23  | V     | 2652 | C    |
| 23  | V     | 2654 | A    |
| 23  | V     | 2655 | G    |
| 23  | V     | 2656 | U    |
| 23  | V     | 2659 | G    |
| 23  | V     | 2668 | G    |
| 23  | V     | 2670 | A    |
| 23  | V     | 2681 | C    |
| 23  | V     | 2682 | U    |
| 23  | V     | 2688 | U    |
| 23  | V     | 2689 | U    |
| 23  | V     | 2691 | C    |
| 23  | V     | 2693 | A    |
| 23  | V     | 2699 | C    |
| 23  | V     | 2701 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 23  | V     | 2702    | U    |
| 23  | V     | 2712    | U    |
| 23  | V     | 2712(A) | A    |
| 23  | V     | 2713    | A    |
| 23  | V     | 2714    | G    |
| 23  | V     | 2718    | G    |
| 23  | V     | 2721    | A    |
| 23  | V     | 2727    | G    |
| 23  | V     | 2728    | U    |
| 23  | V     | 2730    | C    |
| 23  | V     | 2732    | G    |
| 23  | V     | 2733    | A    |
| 23  | V     | 2741    | A    |
| 23  | V     | 2744    | G    |
| 23  | V     | 2746    | U    |
| 23  | V     | 2748    | A    |
| 23  | V     | 2750    | A    |
| 23  | V     | 2751    | G    |
| 23  | V     | 2752    | C    |
| 23  | V     | 2753    | A    |
| 23  | V     | 2756    | U    |
| 23  | V     | 2757    | A    |
| 23  | V     | 2758    | A    |
| 23  | V     | 2759    | G    |
| 23  | V     | 2764    | A    |
| 23  | V     | 2765    | A    |
| 23  | V     | 2766    | G    |
| 23  | V     | 2770    | G    |
| 23  | V     | 2772    | C    |
| 23  | V     | 2774    | C    |
| 23  | V     | 2776    | A    |
| 23  | V     | 2777    | G    |
| 23  | V     | 2778    | A    |
| 23  | V     | 2779    | U    |
| 23  | V     | 2780    | G    |
| 23  | V     | 2781    | A    |
| 23  | V     | 2782    | G    |
| 23  | V     | 2783    | G    |
| 23  | V     | 2786    | U    |
| 23  | V     | 2789    | C    |
| 23  | V     | 2790    | A    |
| 23  | V     | 2791    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 2793 | G    |
| 23  | V     | 2794 | C    |
| 23  | V     | 2795 | G    |
| 23  | V     | 2797 | U    |
| 23  | V     | 2799 | A    |
| 23  | V     | 2801 | A    |
| 23  | V     | 2804 | C    |
| 23  | V     | 2805 | G    |
| 23  | V     | 2807 | G    |
| 23  | V     | 2809 | A    |
| 23  | V     | 2810 | A    |
| 23  | V     | 2818 | G    |
| 23  | V     | 2820 | A    |
| 23  | V     | 2821 | A    |
| 23  | V     | 2832 | U    |
| 23  | V     | 2833 | G    |
| 23  | V     | 2834 | G    |
| 23  | V     | 2835 | A    |
| 23  | V     | 2837 | G    |
| 23  | V     | 2844 | G    |
| 23  | V     | 2847 | U    |
| 23  | V     | 2849 | U    |
| 23  | V     | 2850 | A    |
| 23  | V     | 2859 | G    |
| 23  | V     | 2861 | G    |
| 23  | V     | 2864 | G    |
| 23  | V     | 2865 | U    |
| 23  | V     | 2867 | G    |
| 23  | V     | 2868 | A    |
| 23  | V     | 2869 | G    |
| 23  | V     | 2872 | G    |
| 23  | V     | 2873 | A    |
| 23  | V     | 2874 | C    |
| 23  | V     | 2876 | G    |
| 23  | V     | 2877 | G    |
| 23  | V     | 2879 | C    |
| 23  | V     | 2883 | A    |
| 23  | V     | 2884 | U    |
| 23  | V     | 2893 | G    |
| 23  | V     | 2894 | G    |
| 23  | V     | 2895 | U    |
| 23  | V     | 2896 | C    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 24  | X     | 0     | A    |
| 24  | X     | 1     | U    |
| 24  | X     | 8     | U    |
| 24  | X     | 9     | G    |
| 24  | X     | 11    | C    |
| 24  | X     | 12    | C    |
| 24  | X     | 13    | A    |
| 24  | X     | 25    | A    |
| 24  | X     | 27    | C    |
| 24  | X     | 30    | C    |
| 24  | X     | 31    | C    |
| 24  | X     | 33    | G    |
| 24  | X     | 35    | U    |
| 24  | X     | 36    | C    |
| 24  | X     | 37    | C    |
| 24  | X     | 38    | C    |
| 24  | X     | 40    | U    |
| 24  | X     | 41    | U    |
| 24  | X     | 45    | A    |
| 24  | X     | 46    | A    |
| 24  | X     | 53    | A    |
| 24  | X     | 56    | G    |
| 24  | X     | 57    | A    |
| 24  | X     | 62    | C    |
| 24  | X     | 66    | A    |
| 24  | X     | 67    | G    |
| 24  | X     | 71    | C    |
| 24  | X     | 76    | G    |
| 24  | X     | 84    | C    |
| 24  | X     | 86    | G    |
| 24  | X     | 88    | C    |
| 24  | X     | 89    | G    |
| 24  | X     | 89(A) | A    |
| 24  | X     | 90    | C    |
| 24  | X     | 99    | A    |
| 24  | X     | 101   | A    |
| 24  | X     | 105   | G    |
| 24  | X     | 107   | U    |
| 24  | X     | 108   | C    |
| 24  | X     | 109   | G    |
| 24  | X     | 120   | U    |
| 55  | DD    | 3     | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | DD    | 4   | G    |
| 55  | DD    | 5   | G    |
| 55  | DD    | 6   | G    |
| 55  | DD    | 7   | G    |
| 55  | DD    | 8   | 4SU  |
| 55  | DD    | 9   | G    |
| 55  | DD    | 10  | G    |
| 55  | DD    | 11  | A    |
| 55  | DD    | 13  | C    |
| 55  | DD    | 16  | C    |
| 55  | DD    | 17  | C    |
| 55  | DD    | 18  | C    |
| 55  | DD    | 19  | G    |
| 55  | DD    | 20  | G    |
| 55  | DD    | 21  | U    |
| 55  | DD    | 22  | A    |
| 55  | DD    | 33  | OMC  |
| 55  | DD    | 34  | A    |
| 55  | DD    | 35  | C    |
| 55  | DD    | 36  | A    |
| 55  | DD    | 38  | A    |
| 55  | DD    | 47  | 7MG  |
| 55  | DD    | 48  | U    |
| 55  | DD    | 49  | C    |
| 55  | DD    | 50  | G    |
| 55  | DD    | 51  | U    |
| 55  | DD    | 56  | PSU  |
| 55  | DD    | 58  | A    |
| 55  | DD    | 65  | G    |
| 55  | DD    | 69  | C    |

All (126) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | W     | 19     | U    |
| 8   | G     | 115    | G    |
| 8   | G     | 119    | A    |
| 8   | G     | 129    | U    |
| 8   | G     | 129(A) | G    |
| 8   | G     | 196    | A    |
| 8   | G     | 208    | U    |
| 8   | G     | 243    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 8   | G     | 266     | G    |
| 8   | G     | 328     | C    |
| 8   | G     | 352     | C    |
| 8   | G     | 413     | G    |
| 8   | G     | 484     | G    |
| 8   | G     | 517     | G    |
| 8   | G     | 559     | A    |
| 8   | G     | 595     | G    |
| 8   | G     | 641     | U    |
| 8   | G     | 652     | U    |
| 8   | G     | 686     | U    |
| 8   | G     | 812     | C    |
| 8   | G     | 820     | U    |
| 8   | G     | 872     | A    |
| 8   | G     | 913     | A    |
| 8   | G     | 918     | A    |
| 8   | G     | 975     | A    |
| 8   | G     | 992     | U    |
| 8   | G     | 1065    | U    |
| 8   | G     | 1145    | C    |
| 8   | G     | 1182    | G    |
| 8   | G     | 1239    | A    |
| 8   | G     | 1257    | U    |
| 8   | G     | 1285    | A    |
| 8   | G     | 1331    | G    |
| 8   | G     | 1346    | A    |
| 8   | G     | 1359    | C    |
| 8   | G     | 1362(A) | C    |
| 8   | G     | 1399    | C    |
| 8   | G     | 1446    | A    |
| 23  | V     | 6       | A    |
| 23  | V     | 51      | G    |
| 23  | V     | 71      | A    |
| 23  | V     | 83      | G    |
| 23  | V     | 99      | U    |
| 23  | V     | 119     | A    |
| 23  | V     | 120     | U    |
| 23  | V     | 136     | G    |
| 23  | V     | 215     | G    |
| 23  | V     | 270(B)  | A    |
| 23  | V     | 270(L)  | U    |
| 23  | V     | 270(M)  | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 23  | V     | 270(Z)  | U    |
| 23  | V     | 271(A)  | G    |
| 23  | V     | 289     | A    |
| 23  | V     | 311     | A    |
| 23  | V     | 362     | U    |
| 23  | V     | 403     | U    |
| 23  | V     | 446     | G    |
| 23  | V     | 451     | C    |
| 23  | V     | 456     | C    |
| 23  | V     | 458     | G    |
| 23  | V     | 470     | A    |
| 23  | V     | 489     | G    |
| 23  | V     | 527     | C    |
| 23  | V     | 559     | G    |
| 23  | V     | 587     | C    |
| 23  | V     | 627     | A    |
| 23  | V     | 630     | G    |
| 23  | V     | 644     | A    |
| 23  | V     | 776     | G    |
| 23  | V     | 788     | A    |
| 23  | V     | 801     | G    |
| 23  | V     | 827     | U    |
| 23  | V     | 846     | C    |
| 23  | V     | 930     | U    |
| 23  | V     | 972     | G    |
| 23  | V     | 1051    | G    |
| 23  | V     | 1052    | C    |
| 23  | V     | 1057    | A    |
| 23  | V     | 1061    | U    |
| 23  | V     | 1062    | G    |
| 23  | V     | 1085    | A    |
| 23  | V     | 1106    | G    |
| 23  | V     | 1139    | G    |
| 23  | V     | 1143    | A    |
| 23  | V     | 1221    | C    |
| 23  | V     | 1247    | A    |
| 23  | V     | 1266    | G    |
| 23  | V     | 1267    | U    |
| 23  | V     | 1300    | U    |
| 23  | V     | 1312    | U    |
| 23  | V     | 1313    | U    |
| 23  | V     | 1449(A) | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 23  | V     | 1489 | U    |
| 23  | V     | 1544 | C    |
| 23  | V     | 1778 | U    |
| 23  | V     | 1782 | C    |
| 23  | V     | 1786 | A    |
| 23  | V     | 1799 | G    |
| 23  | V     | 1833 | U    |
| 23  | V     | 2017 | U    |
| 23  | V     | 2020 | A    |
| 23  | V     | 2049 | G    |
| 23  | V     | 2110 | G    |
| 23  | V     | 2157 | G    |
| 23  | V     | 2158 | A    |
| 23  | V     | 2171 | A    |
| 23  | V     | 2176 | A    |
| 23  | V     | 2181 | G    |
| 23  | V     | 2225 | A    |
| 23  | V     | 2238 | G    |
| 23  | V     | 2319 | G    |
| 23  | V     | 2349 | G    |
| 23  | V     | 2402 | C    |
| 23  | V     | 2436 | G    |
| 23  | V     | 2447 | G    |
| 23  | V     | 2481 | G    |
| 23  | V     | 2614 | A    |
| 23  | V     | 2637 | U    |
| 23  | V     | 2712 | U    |
| 23  | V     | 2750 | A    |
| 23  | V     | 2820 | A    |
| 24  | X     | 56   | G    |
| 55  | DD    | 8    | 4SU  |
| 55  | DD    | 18   | C    |
| 55  | DD    | 33   | OMC  |
| 55  | DD    | 47   | 7MG  |

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

5 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 |
| 55  | PSU  | DD    | 56  | 55   | 18,21,22     | 1.03 | 1 (5%)   | 21,30,33    | 1.80 | 5 (23%)  |
| 55  | OMC  | DD    | 33  | 55   | 19,22,23     | 0.81 | 0        | 25,31,34    | 1.08 | 1 (4%)   |
| 55  | 4SU  | DD    | 8   | 55   | 18,21,22     | 1.82 | 4 (22%)  | 25,30,33    | 2.39 | 6 (24%)  |
| 55  | 7MG  | DD    | 47  | 55   | 23,26,27     | 1.33 | 3 (13%)  | 27,39,42    | 2.78 | 8 (29%)  |
| 55  | 5MU  | DD    | 55  | 55   | 19,22,23     | 4.66 | 5 (26%)  | 27,32,35    | 3.69 | 10 (37%) |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 55  | PSU  | DD    | 56  | 55   | -       | 2/7/25/26 | 0/2/2/2 |
| 55  | OMC  | DD    | 33  | 55   | -       | 2/9/27/28 | 0/2/2/2 |
| 55  | 4SU  | DD    | 8   | 55   | -       | 1/7/25/26 | 0/2/2/2 |
| 55  | 7MG  | DD    | 47  | 55   | -       | 1/7/37/38 | 0/3/3/3 |
| 55  | 5MU  | DD    | 55  | 55   | -       | 1/7/25/26 | 0/2/2/2 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 55  | DD    | 55  | 5MU  | C2-N1 | 11.33 | 1.56        | 1.38     |
| 55  | DD    | 55  | 5MU  | C4-C5 | 10.04 | 1.61        | 1.44     |
| 55  | DD    | 55  | 5MU  | C4-N3 | -9.81 | 1.20        | 1.38     |
| 55  | DD    | 55  | 5MU  | C6-N1 | 8.01  | 1.51        | 1.38     |
| 55  | DD    | 8   | 4SU  | C4-S4 | -4.95 | 1.59        | 1.68     |
| 55  | DD    | 55  | 5MU  | C6-C5 | 4.43  | 1.41        | 1.34     |
| 55  | DD    | 47  | 7MG  | C5-C4 | 3.32  | 1.47        | 1.37     |
| 55  | DD    | 8   | 4SU  | C4-N3 | -3.25 | 1.34        | 1.37     |
| 55  | DD    | 56  | PSU  | C6-C5 | 3.12  | 1.38        | 1.35     |
| 55  | DD    | 47  | 7MG  | C4-N9 | -2.69 | 1.34        | 1.37     |
| 55  | DD    | 8   | 4SU  | C5-C4 | -2.59 | 1.39        | 1.42     |
| 55  | DD    | 47  | 7MG  | C6-N1 | -2.30 | 1.34        | 1.38     |
| 55  | DD    | 8   | 4SU  | C2-N3 | -2.12 | 1.34        | 1.38     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 55  | DD    | 55  | 5MU  | C5-C4-N3    | 12.03 | 125.78      | 115.32   |
| 55  | DD    | 47  | 7MG  | N9-C4-N3    | 9.35  | 139.16      | 125.46   |
| 55  | DD    | 55  | 5MU  | C5-C6-N1    | -9.30 | 113.21      | 123.31   |
| 55  | DD    | 8   | 4SU  | C4-N3-C2    | -6.94 | 120.66      | 127.31   |
| 55  | DD    | 8   | 4SU  | C5-C4-N3    | 5.85  | 120.20      | 114.75   |
| 55  | DD    | 47  | 7MG  | C5-C4-N3    | -5.58 | 117.66      | 128.13   |
| 55  | DD    | 55  | 5MU  | O4-C4-C5    | -5.51 | 118.62      | 124.92   |
| 55  | DD    | 47  | 7MG  | N9-C8-N7    | -5.33 | 95.82       | 103.37   |
| 55  | DD    | 55  | 5MU  | C4-N3-C2    | -4.74 | 121.12      | 127.34   |
| 55  | DD    | 55  | 5MU  | C5M-C5-C4   | 4.68  | 123.77      | 118.78   |
| 55  | DD    | 56  | PSU  | C4-N3-C2    | -4.65 | 119.97      | 126.37   |
| 55  | DD    | 47  | 7MG  | C2-N3-C4    | 4.46  | 119.98      | 112.30   |
| 55  | DD    | 56  | PSU  | N1-C2-N3    | 4.45  | 119.86      | 115.17   |
| 55  | DD    | 55  | 5MU  | C5M-C5-C6   | -4.40 | 116.90      | 122.85   |
| 55  | DD    | 55  | 5MU  | N3-C2-N1    | 4.27  | 120.45      | 114.89   |
| 55  | DD    | 8   | 4SU  | N3-C2-N1    | 4.13  | 120.27      | 114.89   |
| 55  | DD    | 8   | 4SU  | C5-C4-S4    | -3.86 | 119.90      | 124.31   |
| 55  | DD    | 47  | 7MG  | C5-C6-N1    | 2.71  | 115.72      | 110.94   |
| 55  | DD    | 47  | 7MG  | C3'-C2'-C1' | 2.56  | 106.30      | 101.46   |
| 55  | DD    | 8   | 4SU  | C3'-C2'-C1' | 2.53  | 106.26      | 101.46   |
| 55  | DD    | 56  | PSU  | O2-C2-N1    | -2.53 | 120.18      | 122.79   |
| 55  | DD    | 47  | 7MG  | C5-C4-N9    | -2.46 | 103.18      | 106.33   |
| 55  | DD    | 56  | PSU  | C6-N1-C2    | -2.44 | 120.43      | 122.69   |
| 55  | DD    | 55  | 5MU  | O4-C4-N3    | -2.40 | 115.60      | 120.11   |
| 55  | DD    | 33  | OMC  | C2'-C1'-N1  | -2.36 | 109.76      | 114.24   |
| 55  | DD    | 47  | 7MG  | O6-C6-C5    | -2.24 | 122.12      | 127.62   |
| 55  | DD    | 8   | 4SU  | O2-C2-N1    | -2.23 | 119.89      | 122.80   |
| 55  | DD    | 55  | 5MU  | C1'-N1-C2   | 2.21  | 121.56      | 117.59   |
| 55  | DD    | 55  | 5MU  | O2-C2-N1    | -2.10 | 120.06      | 122.80   |
| 55  | DD    | 56  | PSU  | O4'-C1'-C2' | 2.05  | 107.99      | 105.15   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | DD    | 33  | OMC  | O4'-C4'-C5'-O5' |
| 55  | DD    | 56  | PSU  | O4'-C4'-C5'-O5' |
| 55  | DD    | 56  | PSU  | C3'-C4'-C5'-O5' |
| 55  | DD    | 33  | OMC  | C3'-C4'-C5'-O5' |
| 55  | DD    | 8   | 4SU  | O4'-C4'-C5'-O5' |
| 55  | DD    | 47  | 7MG  | C3'-C4'-C5'-O5' |
| 55  | DD    | 55  | 5MU  | O4'-C4'-C5'-O5' |

There are no ring outliers.

3 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 55  | DD    | 33  | OMC  | 5       | 0            |
| 55  | DD    | 8   | 4SU  | 3       | 0            |
| 55  | DD    | 47  | 7MG  | 5       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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 | $\# Z  > 2$ |
| 58  | ANP  | EE    | 501 | -    | 33,33,33     | 2.04 | 10 (30%)    | 45,52,52    | 2.07 | 13 (28%)    |
| 58  | ANP  | EE    | 502 | -    | 33,33,33     | 2.04 | 9 (27%)     | 45,52,52    | 2.07 | 13 (28%)    |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 58  | ANP  | EE    | 501 | -    | -       | 6/18/38/38 | 0/3/3/3 |
| 58  | ANP  | EE    | 502 | -    | -       | 6/18/38/38 | 0/3/3/3 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 58  | EE    | 501 | ANP  | C5-C4 | 4.79 | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 58  | EE    | 502 | ANP  | C5-C4  | 4.72  | 1.47        | 1.39     |
| 58  | EE    | 501 | ANP  | PB-N3B | 4.63  | 1.75        | 1.63     |
| 58  | EE    | 502 | ANP  | PB-N3B | 4.62  | 1.75        | 1.63     |
| 58  | EE    | 502 | ANP  | PG-N3B | 4.62  | 1.75        | 1.63     |
| 58  | EE    | 501 | ANP  | PG-N3B | 4.60  | 1.75        | 1.63     |
| 58  | EE    | 502 | ANP  | PG-O1G | 3.51  | 1.51        | 1.46     |
| 58  | EE    | 501 | ANP  | PG-O1G | 3.51  | 1.51        | 1.46     |
| 58  | EE    | 502 | ANP  | PB-O1B | 3.48  | 1.51        | 1.46     |
| 58  | EE    | 501 | ANP  | PB-O1B | 3.45  | 1.51        | 1.46     |
| 58  | EE    | 501 | ANP  | C5-C6  | 2.76  | 1.48        | 1.41     |
| 58  | EE    | 502 | ANP  | C5-C6  | 2.76  | 1.48        | 1.41     |
| 58  | EE    | 502 | ANP  | C8-N7  | 2.35  | 1.36        | 1.31     |
| 58  | EE    | 501 | ANP  | C8-N7  | 2.32  | 1.36        | 1.31     |
| 58  | EE    | 501 | ANP  | C5-N7  | -2.22 | 1.35        | 1.39     |
| 58  | EE    | 502 | ANP  | C5-N7  | -2.20 | 1.35        | 1.39     |
| 58  | EE    | 502 | ANP  | PG-O2G | -2.01 | 1.51        | 1.56     |
| 58  | EE    | 501 | ANP  | PG-O3G | -2.01 | 1.51        | 1.56     |
| 58  | EE    | 501 | ANP  | PG-O2G | -2.01 | 1.51        | 1.56     |

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 58  | EE    | 501 | ANP  | C5-C4-N3    | -5.84 | 118.67      | 126.72   |
| 58  | EE    | 502 | ANP  | C5-C4-N3    | -5.83 | 118.69      | 126.72   |
| 58  | EE    | 502 | ANP  | O1G-PG-N3B  | -4.85 | 104.63      | 111.77   |
| 58  | EE    | 501 | ANP  | O1G-PG-N3B  | -4.84 | 104.64      | 111.77   |
| 58  | EE    | 501 | ANP  | N3-C4-N9    | 4.62  | 135.03      | 127.17   |
| 58  | EE    | 502 | ANP  | N3-C4-N9    | 4.59  | 134.97      | 127.17   |
| 58  | EE    | 501 | ANP  | O2B-PB-O1B  | 3.98  | 118.40      | 109.87   |
| 58  | EE    | 502 | ANP  | O2B-PB-O1B  | 3.98  | 118.40      | 109.87   |
| 58  | EE    | 502 | ANP  | C2-N3-C4    | 3.70  | 120.86      | 111.83   |
| 58  | EE    | 501 | ANP  | C2-N3-C4    | 3.70  | 120.86      | 111.83   |
| 58  | EE    | 501 | ANP  | C4-C5-N7    | -3.49 | 106.59      | 110.58   |
| 58  | EE    | 502 | ANP  | C4-C5-N7    | -3.49 | 106.59      | 110.58   |
| 58  | EE    | 502 | ANP  | N3-C2-N1    | -3.25 | 123.66      | 128.58   |
| 58  | EE    | 501 | ANP  | N3-C2-N1    | -3.21 | 123.73      | 128.58   |
| 58  | EE    | 501 | ANP  | C4-N9-C8    | 2.58  | 108.45      | 105.74   |
| 58  | EE    | 501 | ANP  | C5-N7-C8    | 2.54  | 107.45      | 103.45   |
| 58  | EE    | 502 | ANP  | C4-N9-C8    | 2.54  | 108.40      | 105.74   |
| 58  | EE    | 502 | ANP  | C5-N7-C8    | 2.52  | 107.40      | 103.45   |
| 58  | EE    | 501 | ANP  | O1B-PB-N3B  | -2.51 | 108.08      | 111.77   |
| 58  | EE    | 502 | ANP  | C3'-C2'-C1' | 2.48  | 106.15      | 101.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 58  | EE    | 502 | ANP  | O1B-PB-N3B  | -2.48 | 108.12      | 111.77   |
| 58  | EE    | 501 | ANP  | C3'-C2'-C1' | 2.43  | 106.05      | 101.46   |
| 58  | EE    | 502 | ANP  | O2G-PG-O3G  | 2.34  | 113.88      | 107.59   |
| 58  | EE    | 501 | ANP  | O2G-PG-O3G  | 2.31  | 113.81      | 107.59   |
| 58  | EE    | 501 | ANP  | C6-C5-N7    | 2.09  | 136.12      | 132.09   |
| 58  | EE    | 502 | ANP  | C6-C5-N7    | 2.09  | 136.11      | 132.09   |

There are no chirality outliers.

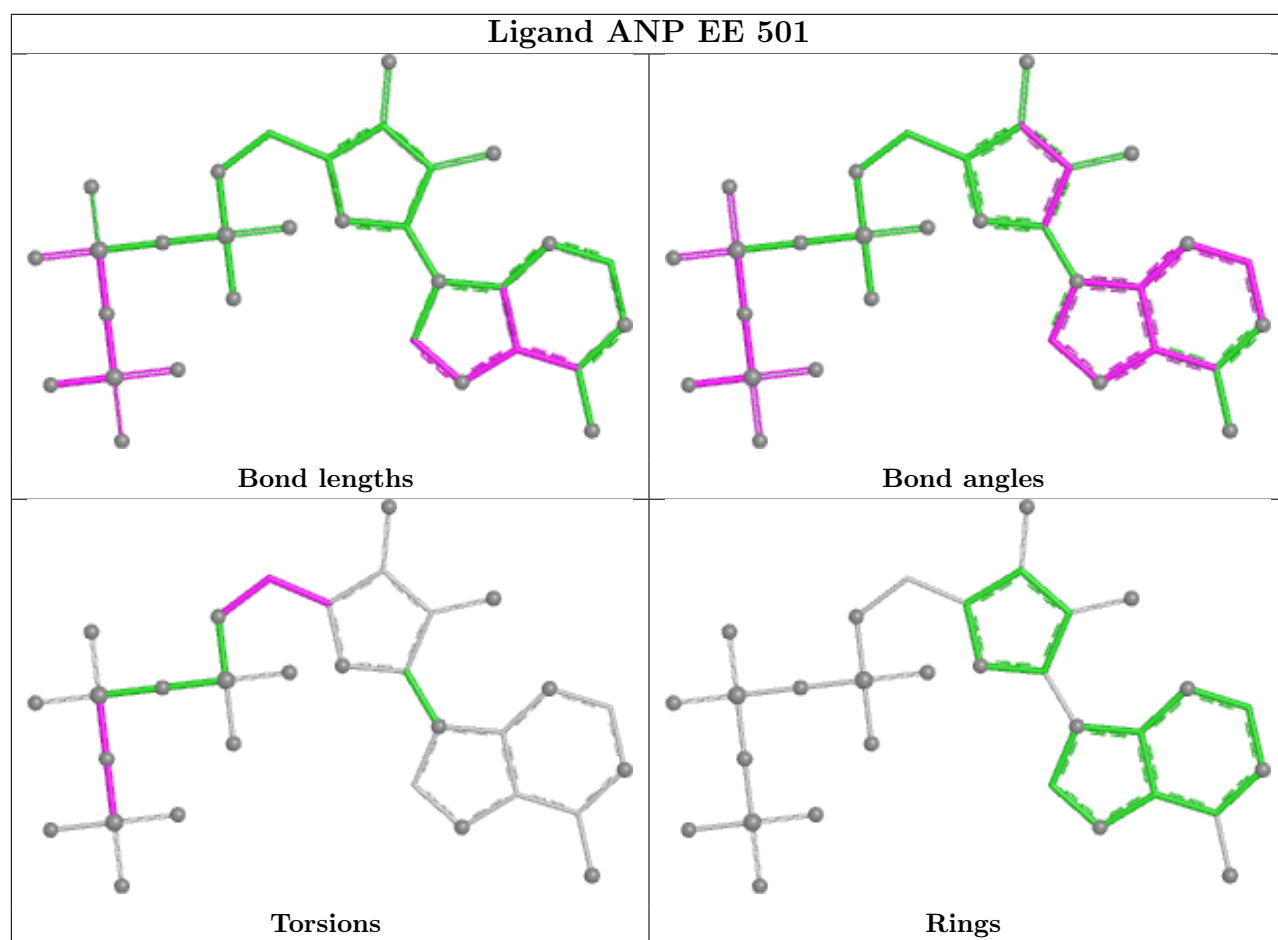
All (12) torsion outliers are listed below:

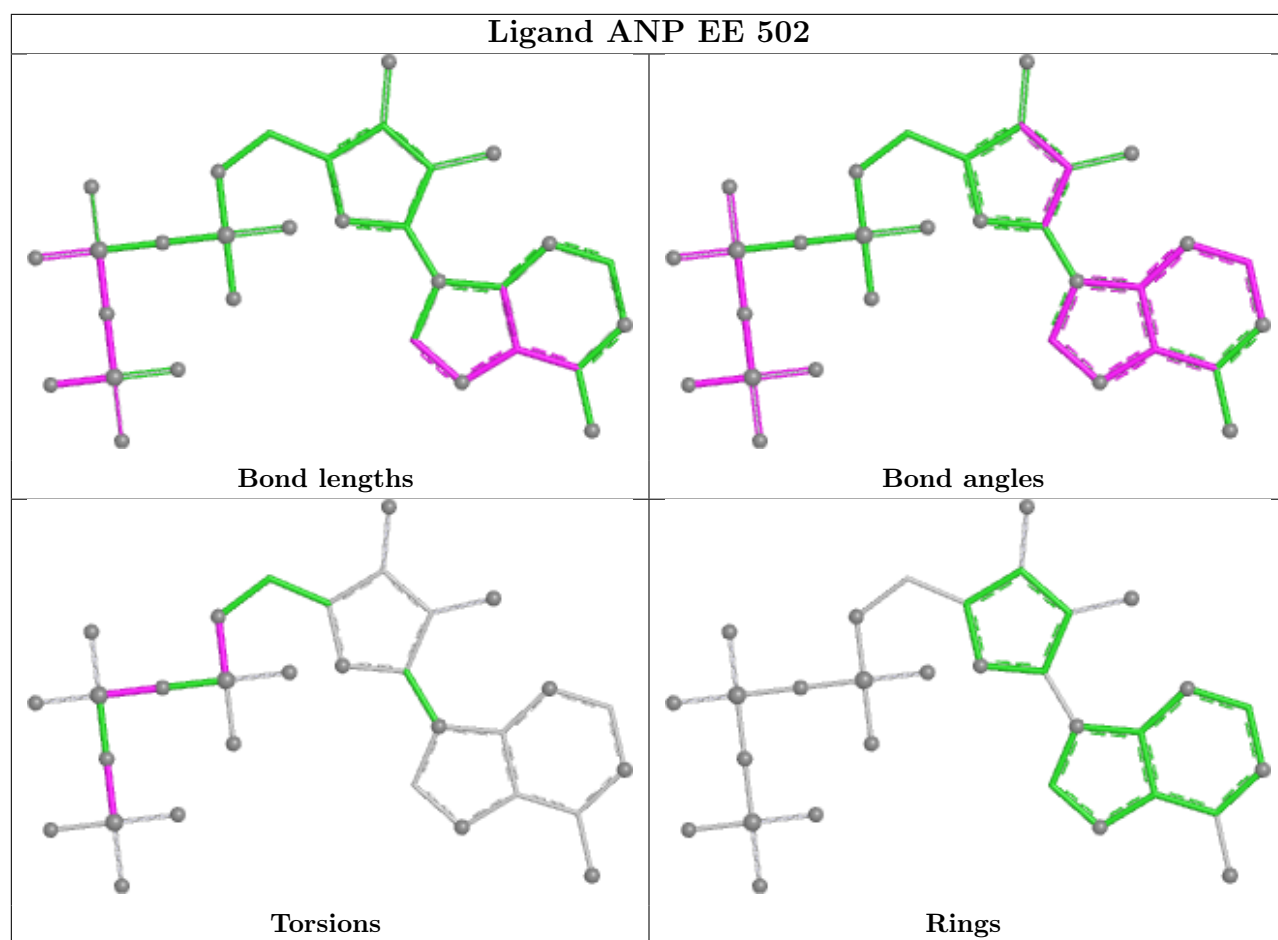
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 58  | EE    | 501 | ANP  | PB-N3B-PG-O1G   |
| 58  | EE    | 501 | ANP  | PG-N3B-PB-O1B   |
| 58  | EE    | 502 | ANP  | PB-N3B-PG-O1G   |
| 58  | EE    | 502 | ANP  | PA-O3A-PB-O2B   |
| 58  | EE    | 502 | ANP  | C5'-O5'-PA-O1A  |
| 58  | EE    | 502 | ANP  | C5'-O5'-PA-O2A  |
| 58  | EE    | 502 | ANP  | C5'-O5'-PA-O3A  |
| 58  | EE    | 501 | ANP  | C3'-C4'-C5'-O5' |
| 58  | EE    | 501 | ANP  | C4'-C5'-O5'-PA  |
| 58  | EE    | 501 | ANP  | O4'-C4'-C5'-O5' |
| 58  | EE    | 501 | ANP  | PG-N3B-PB-O3A   |
| 58  | EE    | 502 | ANP  | PA-O3A-PB-O1B   |

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

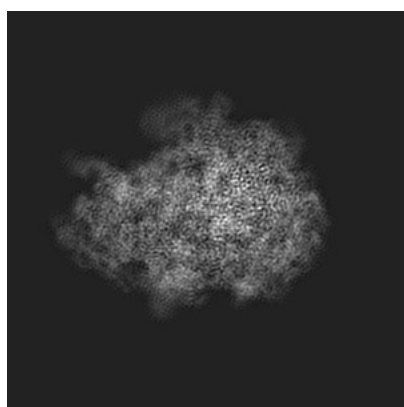
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6934. These allow visual inspection of the internal detail of the map and identification of artifacts.

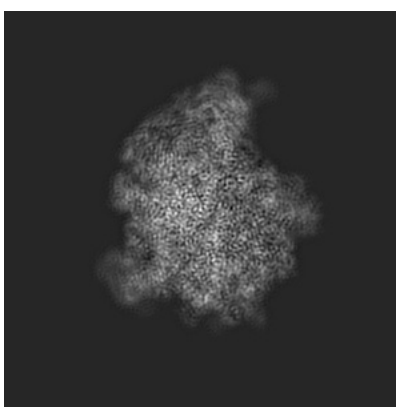
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

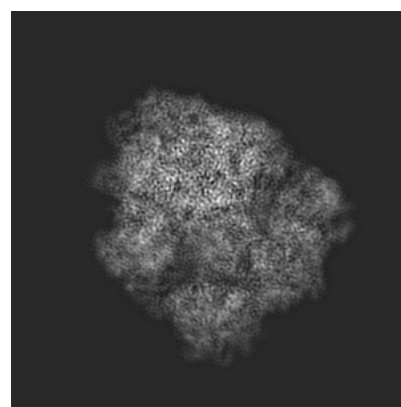
#### 6.1.1 Primary map



X



Y

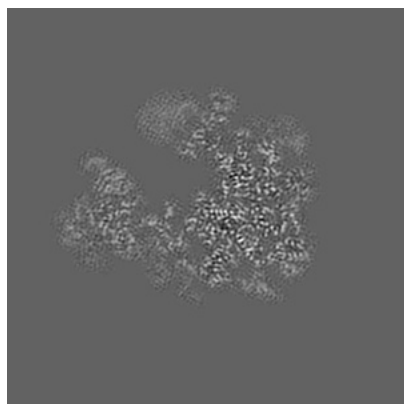


Z

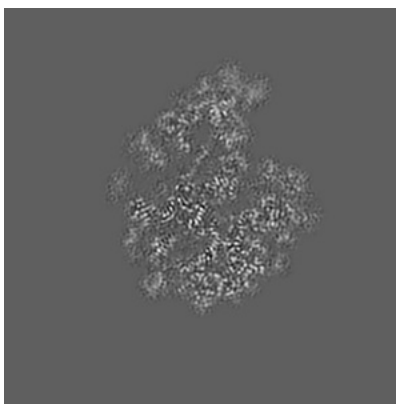
The images above show the map projected in three orthogonal directions.

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

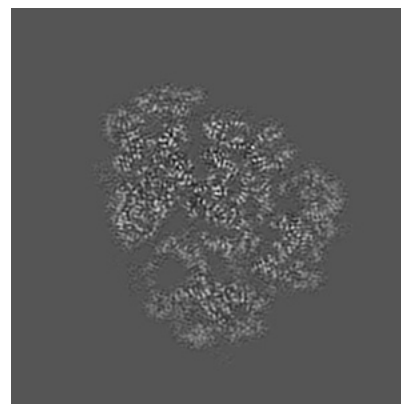
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

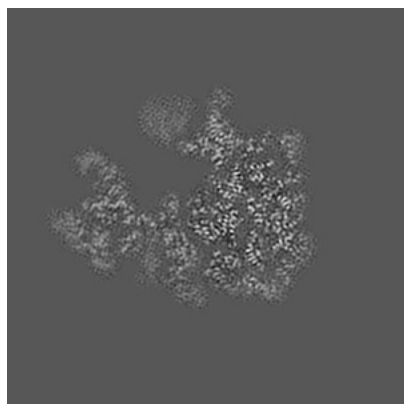


Z Index: 180

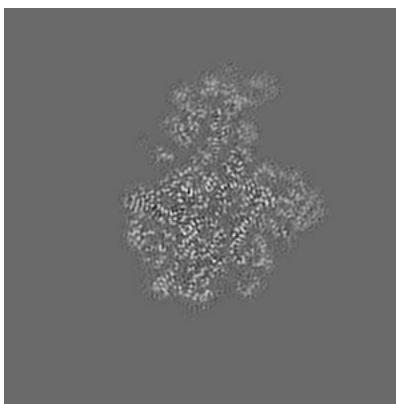
The images above show central slices of the map in three orthogonal directions.

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

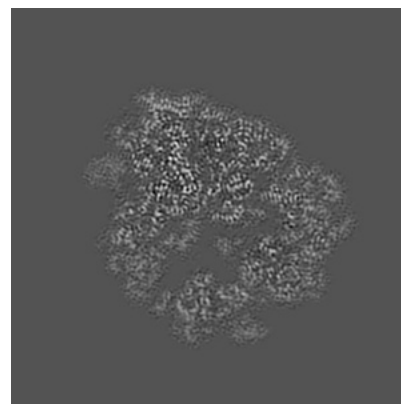
### 6.3.1 Primary map



X Index: 187



Y Index: 189

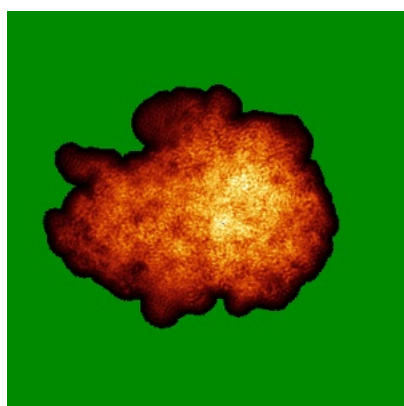


Z Index: 190

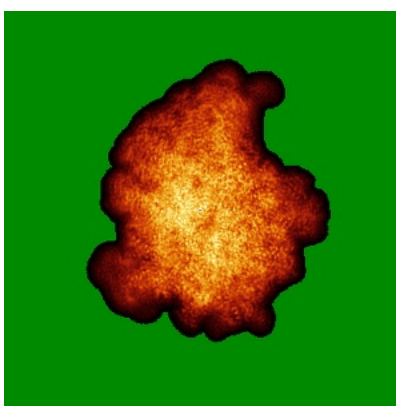
The images above show the largest variance slices of the map in three orthogonal directions.

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

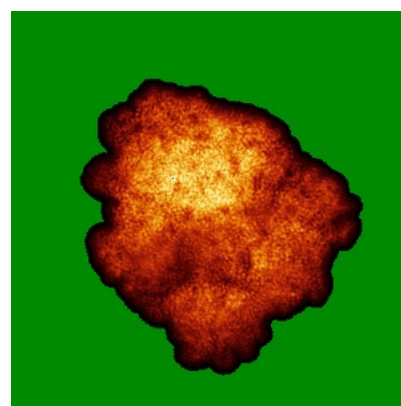
### 6.4.1 Primary map



X



Y

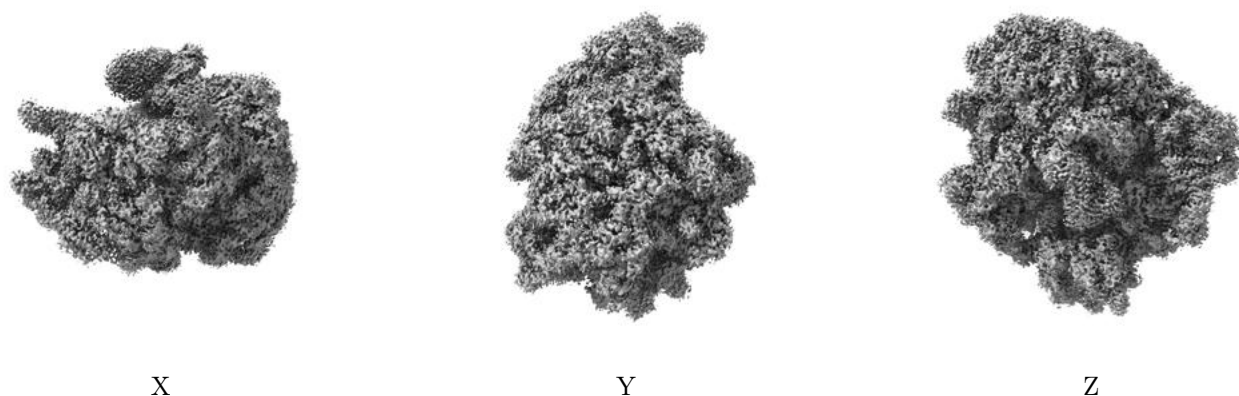


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.052. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

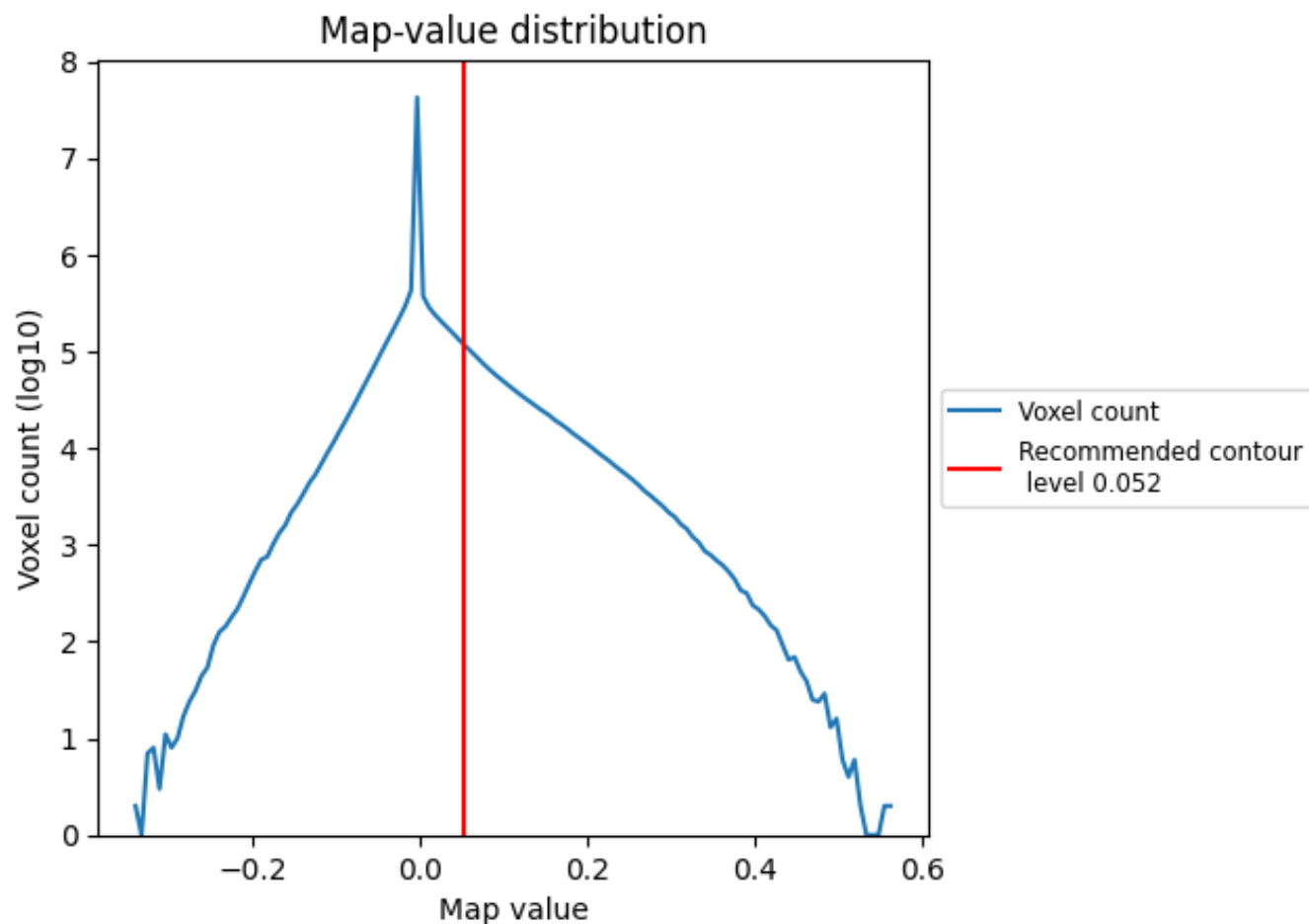
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

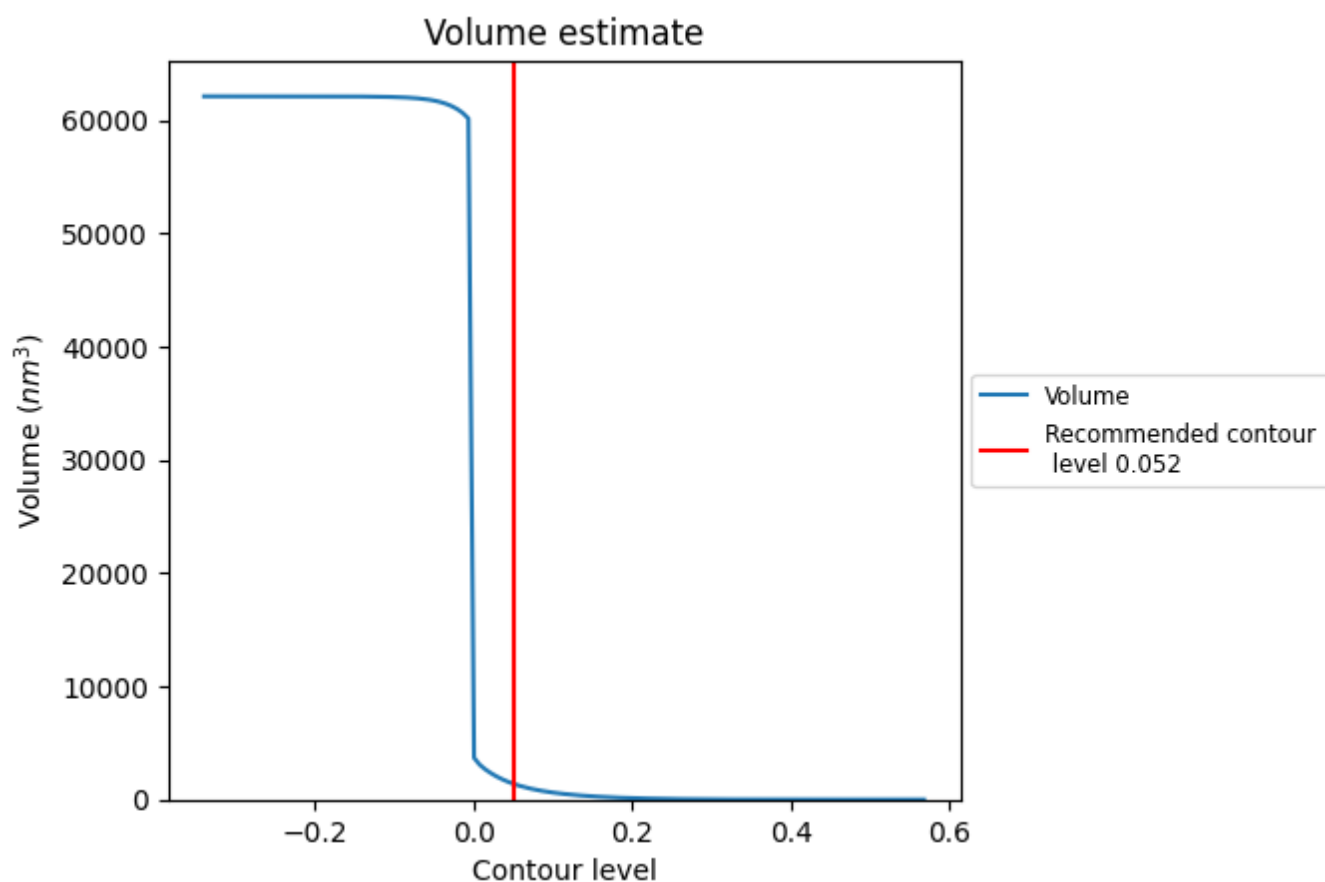
This section contains the results of statistical analysis of the map.

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



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

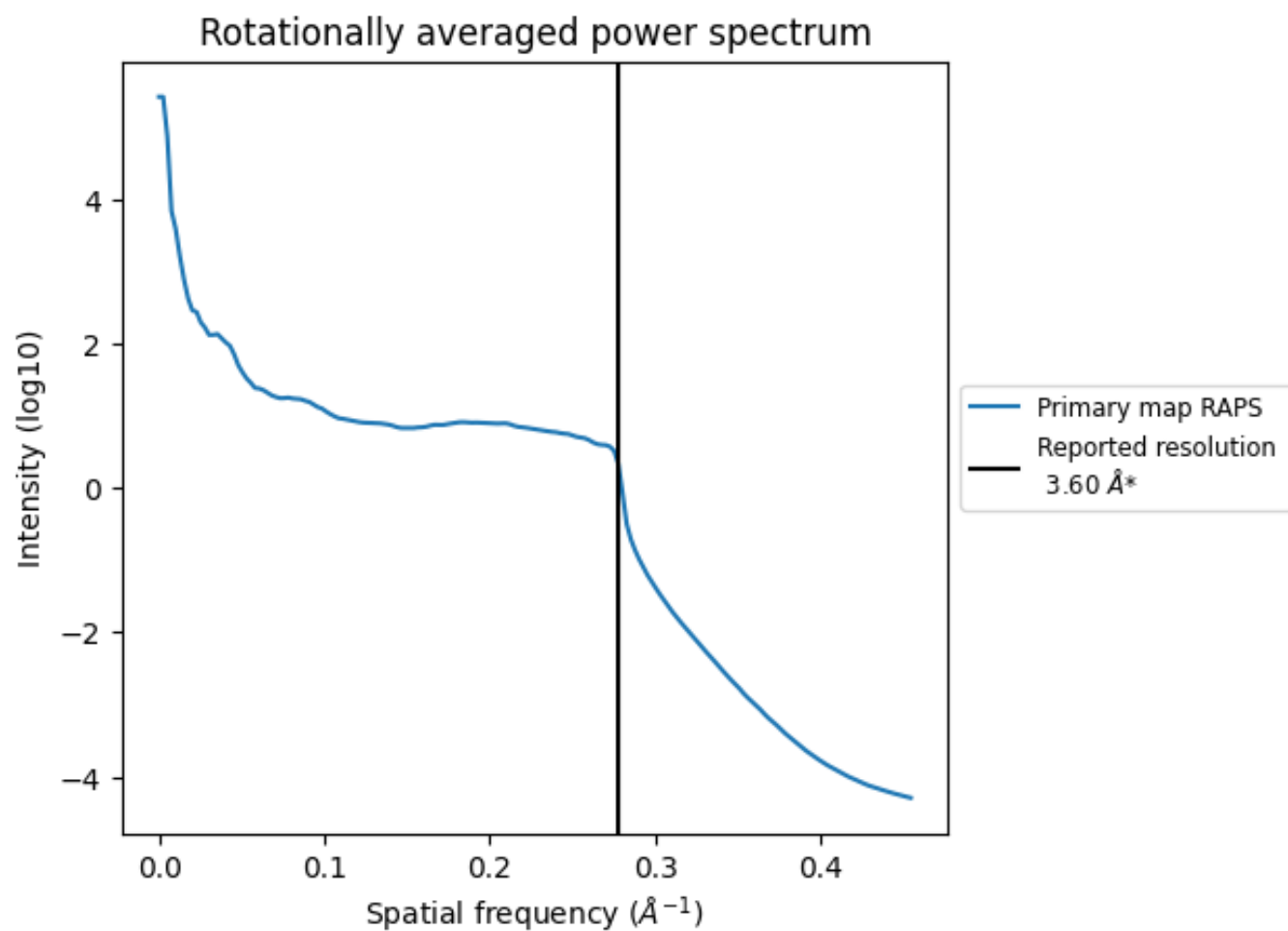
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1361 nm<sup>3</sup>; this corresponds to an approximate mass of 1230 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 ⓘ

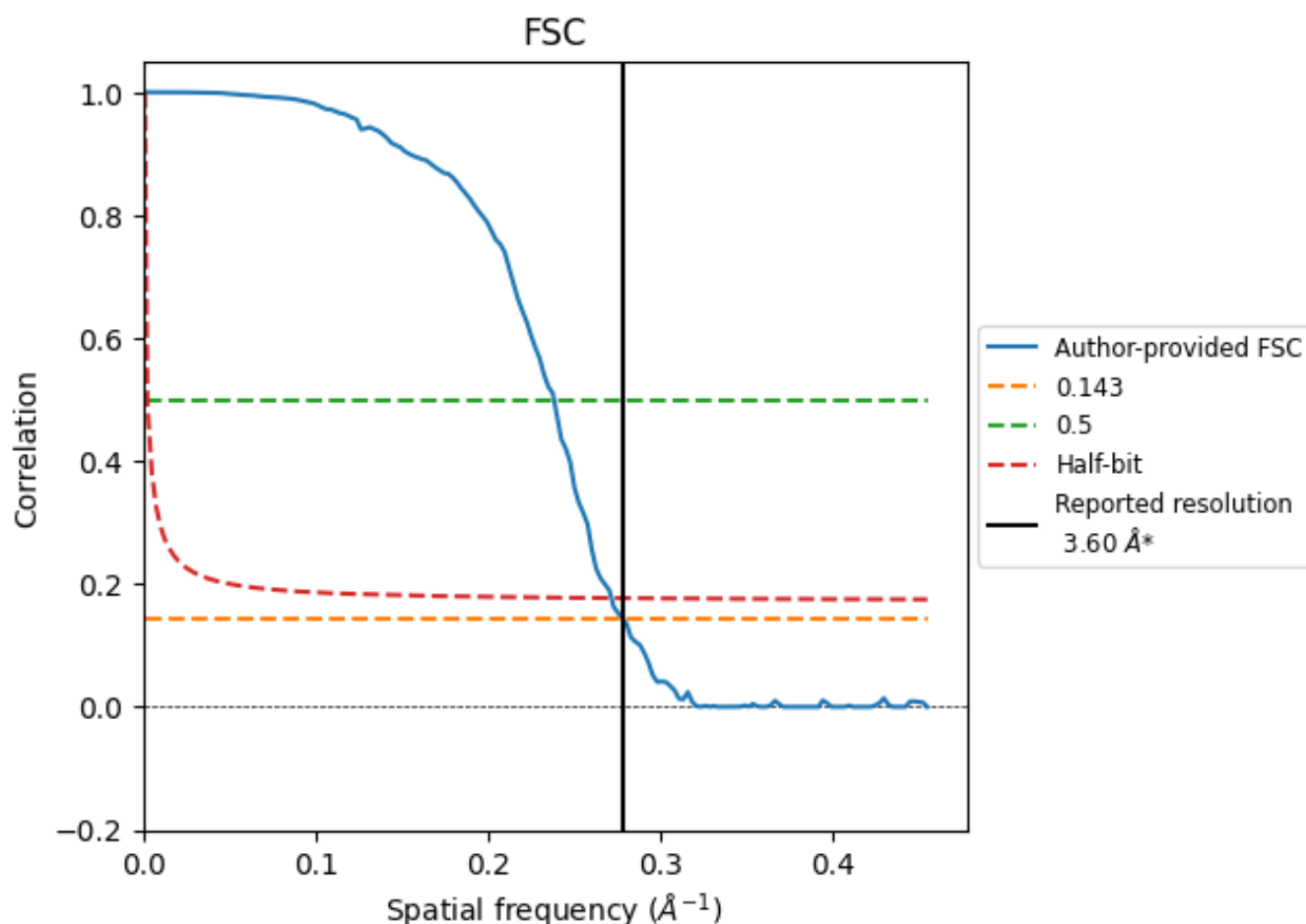


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

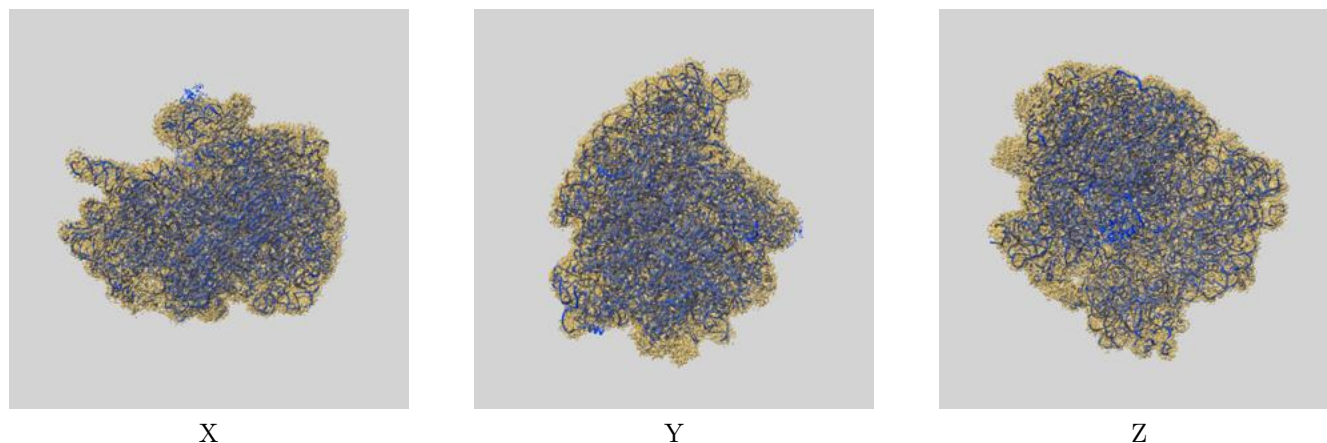
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.60                               | -    | -        |
| Author-provided FSC curve | 3.60                               | 4.20 | 3.68     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

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

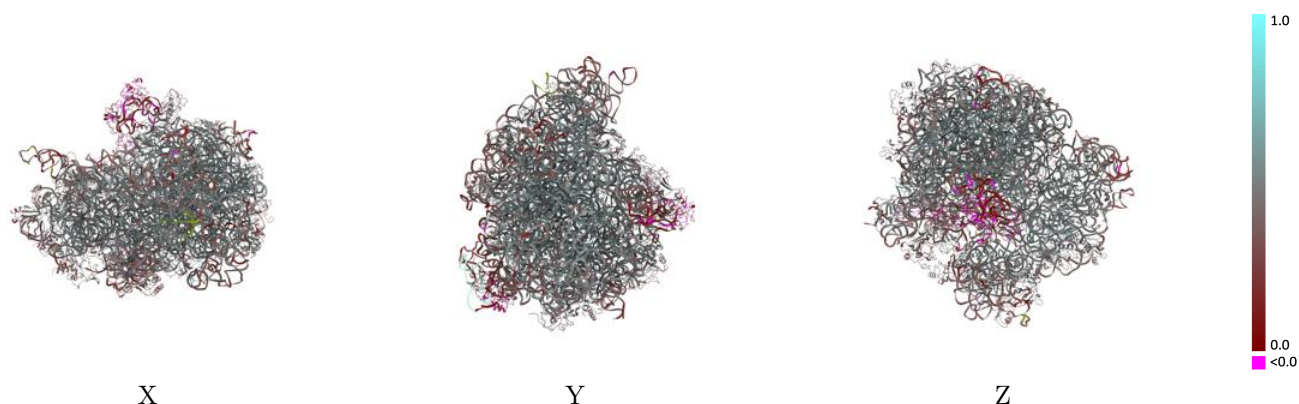
This section contains information regarding the fit between EMDB map EMD-6934 and PDB model 5ZLU. Per-residue inclusion information can be found in section 3 on page 16.

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



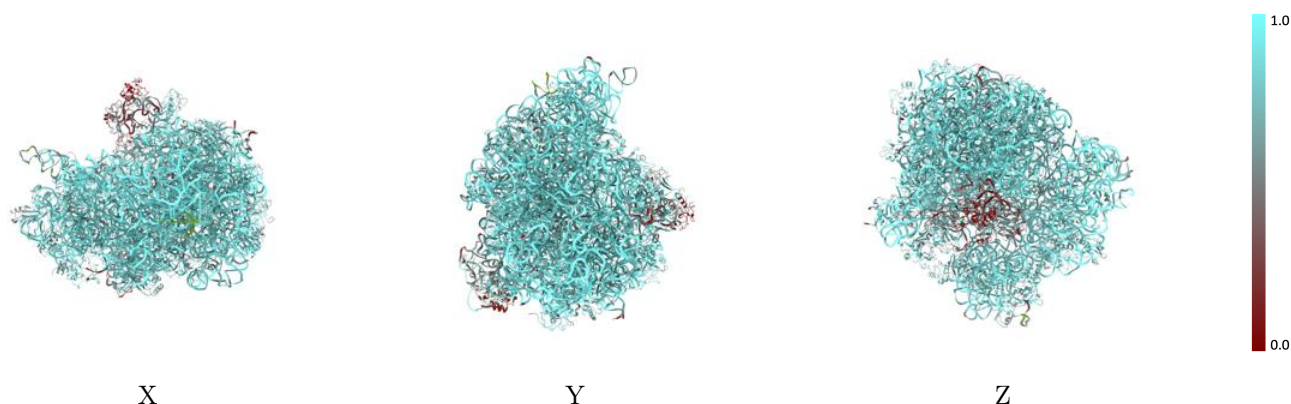
The images above show the 3D surface view of the map at the recommended contour level 0.052 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



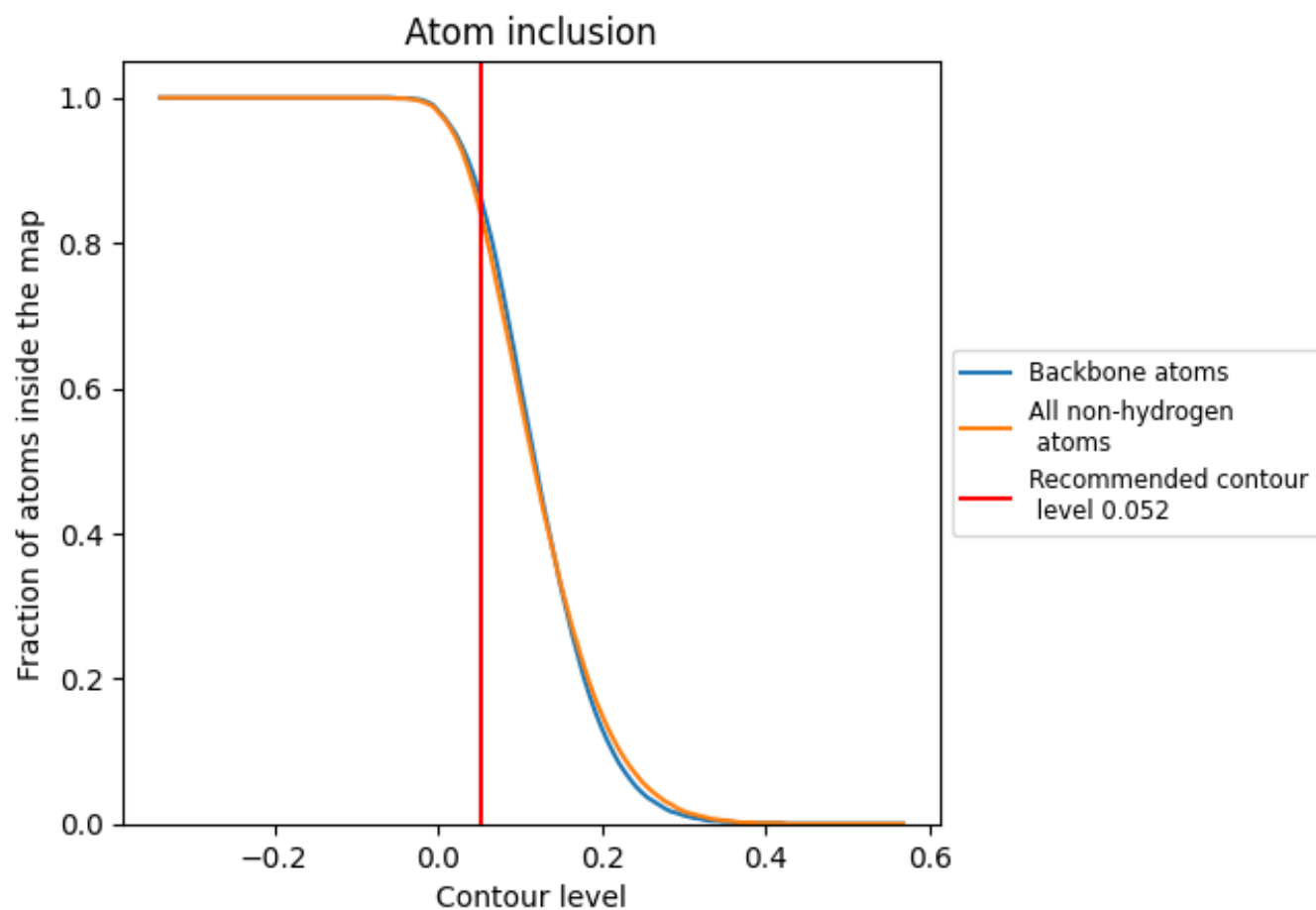
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.052).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.052) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8410   |  0.4410   |
| A     |  0.8120   |  0.4810   |
| AA    |  0.8010   |  0.4720   |
| B     |  0.7000   |  0.3950   |
| BB    |  0.8570   |  0.4720   |
| C     |  0.8420   |  0.4670   |
| CC    |  0.8280   |  0.3980   |
| D     |  0.7640   |  0.3880   |
| DD    |  0.7600   |  0.3870   |
| E     |  0.7220   |  0.4220   |
| EE    |  0.6980   |  0.4220   |
| F     |  0.8380   |  0.4520   |
| G     |  0.9120   |  0.4540   |
| H     |  0.7460   |  0.4140   |
| I     |  0.8110  |  0.4550  |
| J     |  0.8130 |  0.4490 |
| K     |  0.8210 |  0.4780 |
| L     |  0.6810 |  0.3630 |
| M     |  0.7670 |  0.4510 |
| N     |  0.8140 |  0.4580 |
| O     |  0.7820 |  0.4280 |
| P     |  0.7670 |  0.4050 |
| Q     |  0.7890 |  0.4870 |
| R     |  0.7650 |  0.4160 |
| S     |  0.8270 |  0.4560 |
| T     |  0.8360 |  0.4370 |
| U     |  0.8610 |  0.4590 |
| V     |  0.8800 |  0.4530 |
| W     |  0.7780 |  0.3830 |
| X     |  0.9080 |  0.4350 |
| Y     |  0.2400 |  0.1340 |
| Z     |  0.8710 |  0.5170 |
| a     |  0.8230 |  0.4760 |
| b     |  0.8270 |  0.4600 |
| c     |  0.7120 |  0.3730 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| d     |  0.7700   |  0.4070   |
| e     |  0.1420   |  0.0750   |
| f     |  0.2850   |  0.1400   |
| g     |  0.8150   |  0.4530   |
| h     |  0.7670   |  0.4310   |
| i     |  0.8180   |  0.4410   |
| j     |  0.7840   |  0.4440   |
| k     |  0.8840   |  0.5150   |
| l     |  0.7950   |  0.4110   |
| m     |  0.7420   |  0.4260   |
| n     |  0.8770   |  0.5010   |
| o     |  0.7760   |  0.4210   |
| p     |  0.8910   |  0.5200   |
| q     |  0.8490   |  0.4810   |
| r     |  0.6750   |  0.3630   |
| s     |  0.4750   |  0.2800   |
| t     |  0.8670   |  0.5210   |
| u     |  0.8260  |  0.4510  |
| v     |  0.8400 |  0.4780 |
| w     |  0.7270 |  0.3990 |
| x     |  0.8480 |  0.4760 |
| y     |  0.8070 |  0.4540 |
| z     |  0.8570 |  0.5170 |