



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:45 PM UTC

PDB ID : 8RDW / pdb\_00008rdw  
EMDB ID : EMD-19077  
Title : Cryo-EM structure of P. urativorans 70S ribosome in complex with hibernation factor Balon and EF-Tu(GDP) (structure 3).  
Authors : Helena-Bueno, K.; Rybak, M.Y.; Gagnon, M.G.; Hill, C.H.; Melnikov, S.V.  
Deposited on : 2023-12-08  
Resolution : 2.74 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:

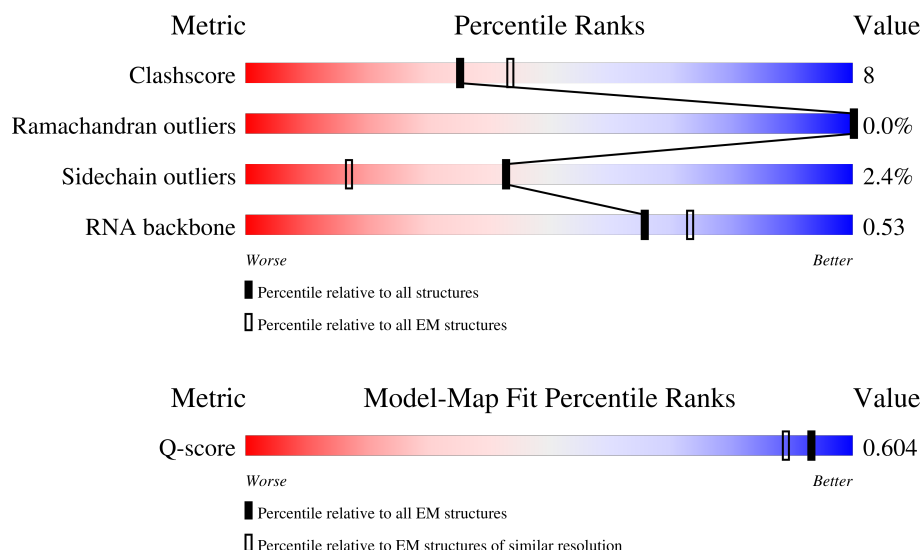
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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

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

The reported resolution of this entry is 2.74 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                       | 10492 ( 2.24 - 3.24 )                                    |

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   | B     | 369    |                  |
| 2   | D     | 123    |                  |
| 3   | F     | 128    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | H     | 396    |                  |
| 5   | Z2    | 2882   |                  |
| 6   | R3    | 76     |                  |
| 7   | A4    | 269    |                  |
| 8   | E5    | 171    |                  |
| 9   | L6    | 124    |                  |
| 10  | F7    | 178    |                  |
| 11  | D8    | 115    |                  |
| 12  | E9    | 200    |                  |
| 13  | aA    | 60     |                  |
| 14  | MB    | 119    |                  |
| 15  | UC    | 219    |                  |
| 16  | WD    | 78     |                  |
| 17  | XE    | 65     |                  |
| 18  | RF    | 109    |                  |
| 19  | FG    | 134    |                  |
| 20  | VH    | 85     |                  |
| 21  | TI    | 105    |                  |
| 22  | fJ    | 93     |                  |
| 23  | HK    | 101    |                  |
| 24  | OL    | 88     |                  |
| 25  | MM    | 118    |                  |
| 26  | iN    | 1590   |                  |
| 27  | PO    | 118    |                  |
| 28  | SP    | 91     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | BQ    | 132    |                  |
| 30  | GR    | 177    |                  |
| 31  | GS    | 157    |                  |
| 32  | CT    | 241    |                  |
| 33  | KU    | 129    |                  |
| 34  | NV    | 71     |                  |
| 35  | YW    | 59     |                  |
| 36  | IX    | 142    |                  |
| 37  | JY    | 103    |                  |
| 38  | QZ    | 91     |                  |
| 39  | Ba    | 44     |                  |
| 40  | Qb    | 103    |                  |
| 41  | Nc    | 116    |                  |
| 42  | Kd    | 146    |                  |
| 43  | Je    | 122    |                  |
| 44  | Af    | 212    |                  |
| 45  | Lg    | 137    |                  |
| 46  | dh    | 65     |                  |
| 47  | Oi    | 130    |                  |
| 48  | Pj    | 89     |                  |
| 49  | bk    | 51     |                  |
| 50  | Cl    | 274    |                  |
| 51  | Dm    | 213    |                  |
| 52  | Sn    | 116    |                  |
| 53  | To    | 88     |                  |

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| Mol | Chain | Length | Quality of chain                                                   |
|-----|-------|--------|--------------------------------------------------------------------|
| 54  | ep    | 38     | <div><div></div><div>79%</div><div>21%</div></div>                 |
| 55  | C1    | 166    | <div><div>17%</div><div>22%</div><div>7%</div><div>70%</div></div> |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 142686 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Methyl-accepting chemotaxis protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | B     | 368      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2871  | 1784 | 507 | 571 | 9 |         |       |

- Molecule 2 is a protein called Large ribosomal subunit protein bL12.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 2   | D     | 25       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 127   | 76 | 25 | 26 |         |       |

- Molecule 3 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | F     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 965   | 601 | 188 | 175 | 1 |         |       |

- Molecule 4 is a protein called Elongation factor Tu.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | H     | 386      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2918  | 1820 | 505 | 578 | 15 |         |       |

- Molecule 5 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 5   | Z2    | 2729     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 58553 | 26138 | 10749 | 18937 | 2729 |         |       |

- Molecule 6 is a protein called Small ribosomal subunit protein bS18.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 6   | R3    | 56       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 457   | 290 | 80 | 87 |         |       |

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | A4    | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1816  | 1147 | 327 | 335 | 7 |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | E5    | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1151  | 716 | 218 | 211 | 6 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | L6    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 583 | 193 | 165 | 5 |         |       |

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | F7    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1362  | 873 | 237 | 246 | 6 |         |       |

- Molecule 11 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 11  | D8    | 115      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2446  | 1093 | 436 | 802 | 115 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference    |
|-------|---------|----------|--------|-----------|--------------|
| D8    | 83      | U        | -      | insertion | GB 930356181 |
| D8    | 88      | A        | C      | variant   | GB 930356181 |

- Molecule 12 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | E9    | 199      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 966 | 282 | 284 | 5 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein bL32.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 13  | aA    | 53       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 442   | 264 | 100 | 75 | 3 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | MB    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 947   | 587 | 188 | 164 | 8 |         |       |

- Molecule 15 is a protein called Large ribosomal subunit protein bL25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | UC    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 760   | 485 | 138 | 136 | 1 |         |       |

- Molecule 16 is a protein called Large ribosomal subunit protein bL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | WD    | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 618   | 383 | 131 | 101 | 3 |         |       |

- Molecule 17 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | XE    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 502   | 307 | 99 | 95 | 1 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | RF    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 521 | 159 | 151 | 3 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein bS6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | FG    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 849   | 535 | 154 | 158 | 2 |         |       |

- Molecule 20 is a protein called Large ribosomal subunit protein bL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | VH    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 626   | 389 | 124 | 110 | 3 |         |       |

- Molecule 21 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 21  | TI    | 102      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 784   | 487 | 149 | 148 |  |         |       |

- Molecule 22 is a protein called Large ribosomal subunit protein bL31B.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | fJ    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 493   | 313 | 85 | 94 | 1 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | HK    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 498 | 162 | 144 | 7 |         |       |

- Molecule 24 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | OL    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 427 | 137 | 128 | 2 |         |       |

- Molecule 25 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | MM    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 907   | 560 | 182 | 162 | 3 |         |       |

- Molecule 26 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 26  | iN    | 1503     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32246 | 14388 | 5917 | 10438 | 1503 |         |       |

- Molecule 27 is a protein called Large ribosomal subunit protein bL20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | PO    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 935   | 586 | 199 | 148 | 2 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | SP    | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 614   | 390 | 116 | 105 | 3 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | BQ    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 974   | 602 | 179 | 187 | 6 |         |       |

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | GR    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1357  | 848 | 248 | 259 | 2 |         |       |

- Molecule 31 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | GS    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1200  | 744 | 233 | 216 | 7 |         |       |

- Molecule 32 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | CT    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1613  | 1013 | 302 | 291 | 7 |         |       |

- Molecule 33 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | KU    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 842   | 521 | 163 | 157 | 1 |         |       |

- Molecule 34 is a protein called Small ribosomal subunit protein bS21.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | NV    | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 472   | 299 | 95 | 77 | 1 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | YW    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 272 | 88 | 76 | 2 |         |       |

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | IX    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 198 | 197 | 3 |         |       |

- Molecule 37 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | JY    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 793   | 492 | 151 | 147 | 3 |         |       |

- Molecule 38 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | QZ    | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 632   | 395 | 119 | 116 | 2 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein bL34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | Ba    | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 369   | 227 | 89 | 51 | 2 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein bL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | Qb    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 524 | 153 | 148 | 2 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 41  | Nc    | 113      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 852   | 530 | 170 | 152 |         |       |

- Molecule 42 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | Kd    | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1062  | 656 | 206 | 197 | 3 |         |       |

- Molecule 43 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | Je    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 937   | 585 | 181 | 166 | 5 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Af    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1548  | 954 | 292 | 296 | 6 |         |       |

- Molecule 45 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Lg    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1093  | 697 | 210 | 179 | 7 |         |       |

- Molecule 46 is a protein called Large ribosomal subunit protein bL35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 46  | dh    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 519   | 326 | 107 | 82 | 4 |         |       |

- Molecule 47 is a protein called Large ribosomal subunit protein bL19.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 47  | Oi    | 115      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 917   | 572 | 184 | 161 |         |       |

- Molecule 48 is a protein called Small ribosomal subunit protein bS16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Pj    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 409 | 126 | 111 | 2 |         |       |

- Molecule 49 is a protein called Large ribosomal subunit protein bL33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | bk    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 394   | 254 | 68 | 69 | 3 |         |       |

- Molecule 50 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | Cl    | 272      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2107  | 1305 | 432 | 364 | 6 |         |       |

- Molecule 51 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | Dm    | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1689  | 1058 | 318 | 310 | 3 |         |       |

- Molecule 52 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | Sn    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 446 | 126 | 124 | 2 |         |       |

- Molecule 53 is a protein called Small ribosomal subunit protein bS20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | To    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 684   | 415 | 146 | 121 | 2 |         |       |

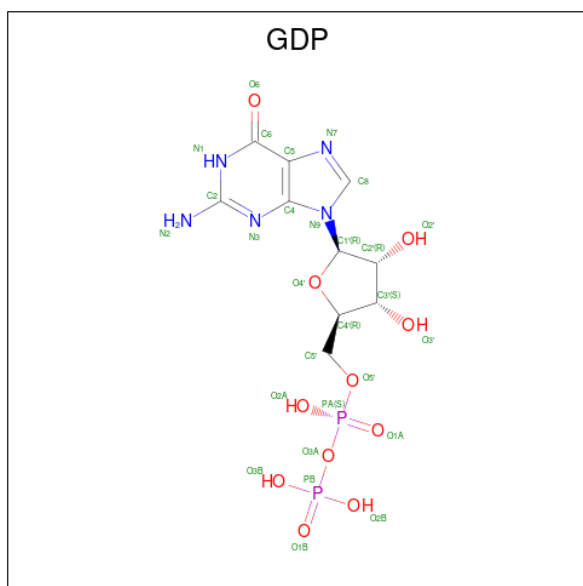
- Molecule 54 is a protein called Large ribosomal subunit protein bL36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | ep    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 298   | 182 | 66 | 46 | 4 |         |       |

- Molecule 55 is a protein called Large ribosomal subunit protein bL9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | C1    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 374   | 244 | 64 | 65 | 1 |         |       |

- Molecule 56 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 56  | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

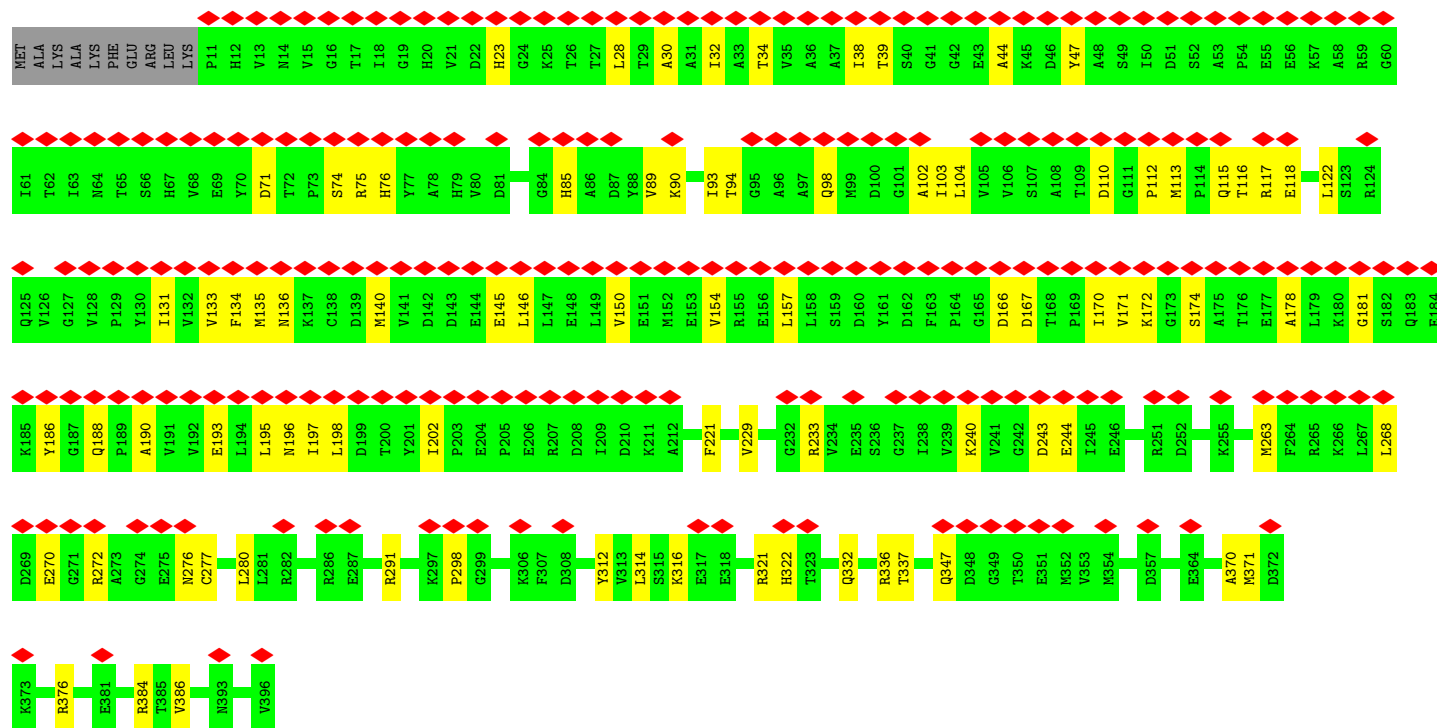
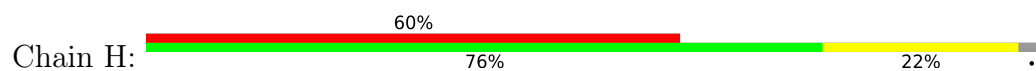
- Molecule 58 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 58  | Z2    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

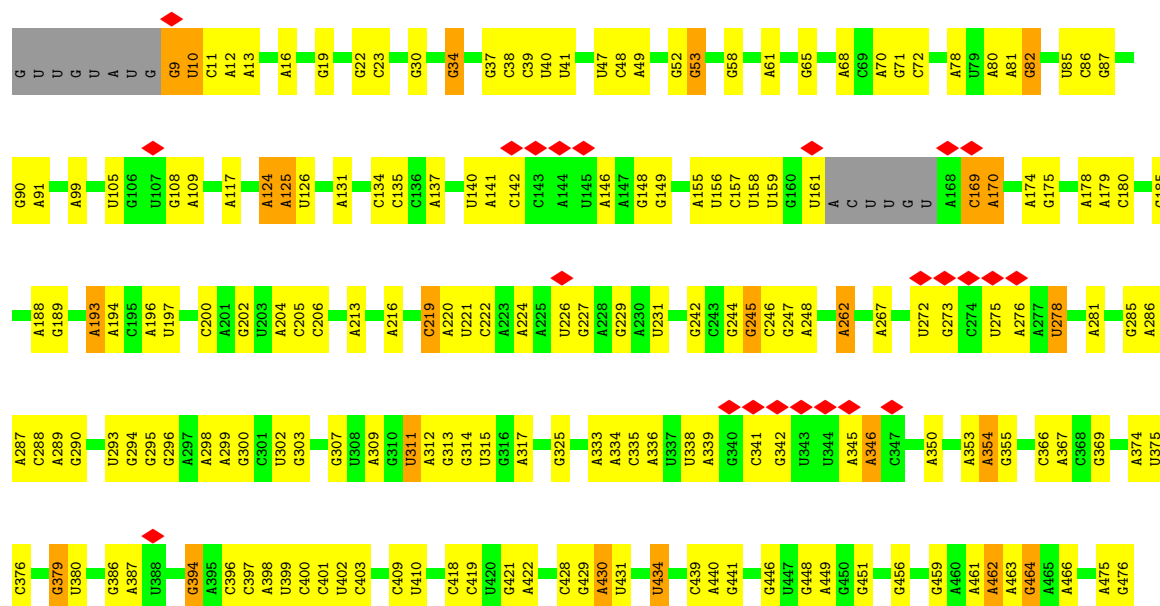




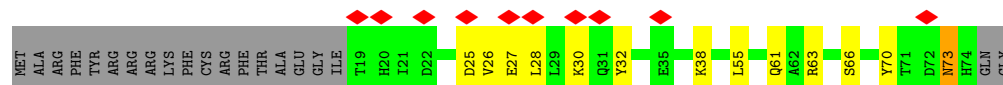
• Molecule 4: Elongation factor Tu

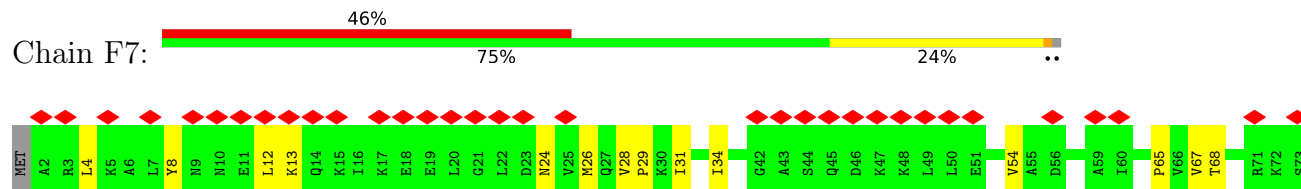


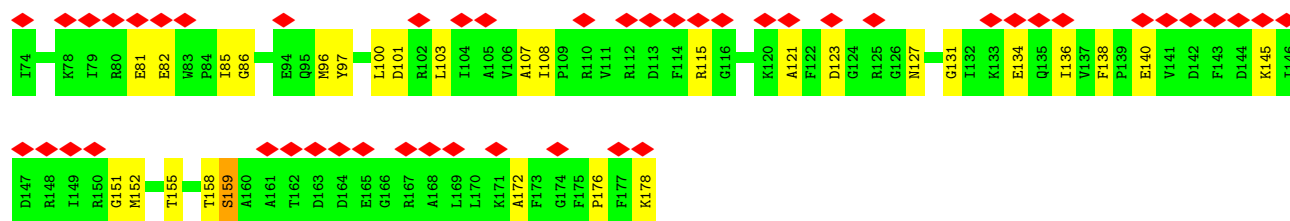
• Molecule 5: 23S rRNA



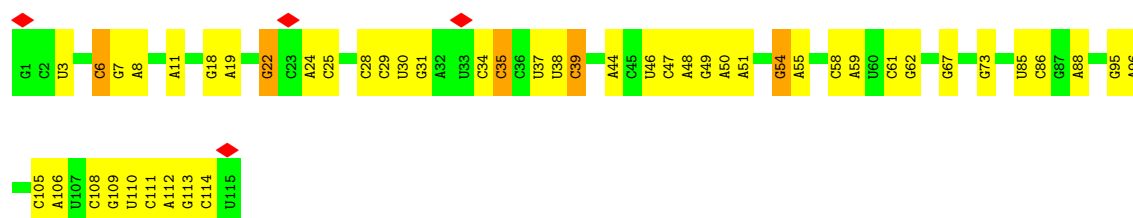




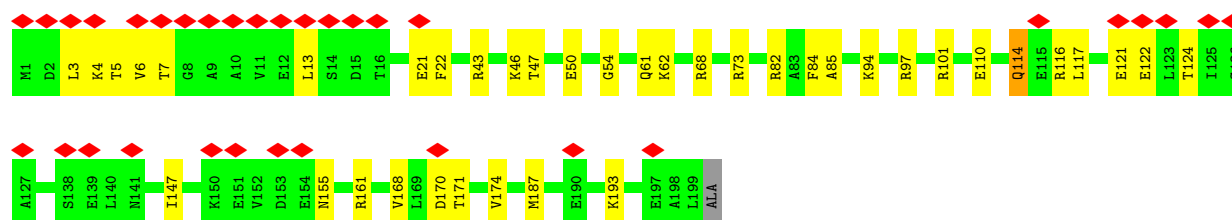
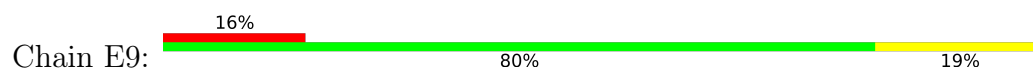




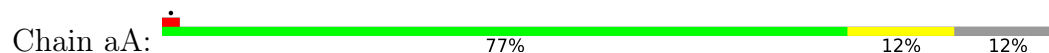
• Molecule 11: 5S rRNA



• Molecule 12: Large ribosomal subunit protein uL4



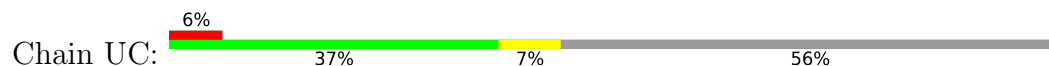
• Molecule 13: Large ribosomal subunit protein bL32

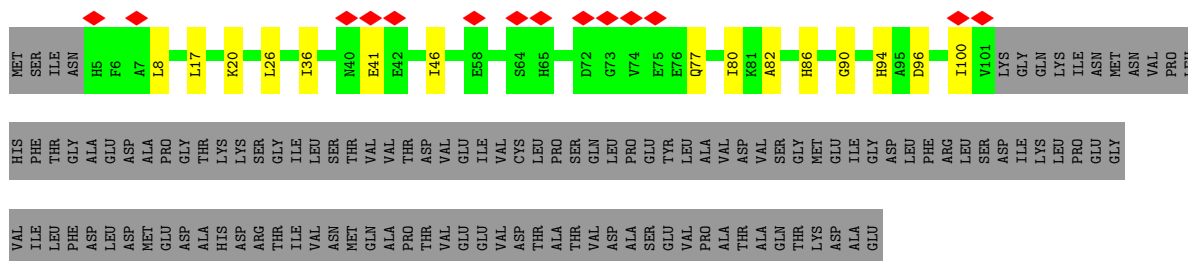


• Molecule 14: Large ribosomal subunit protein bL17

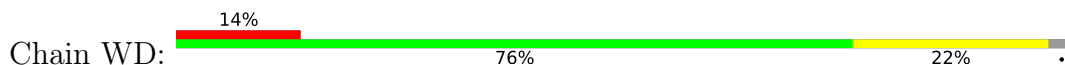


• Molecule 15: Large ribosomal subunit protein bL25

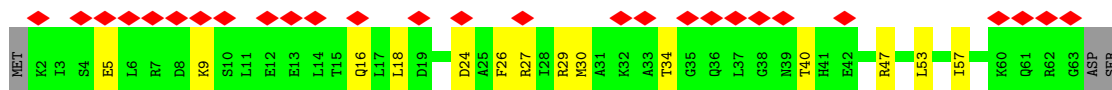
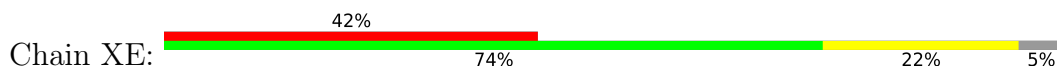




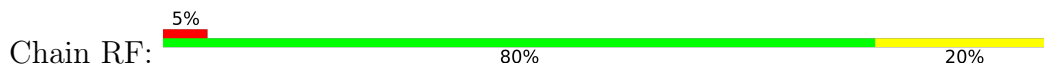
- Molecule 16: Large ribosomal subunit protein bL28



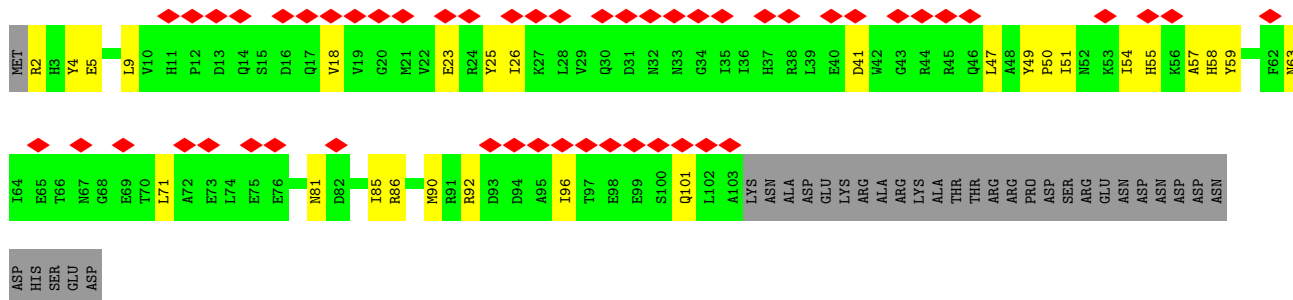
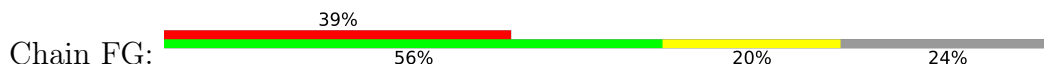
- Molecule 17: Large ribosomal subunit protein uL29



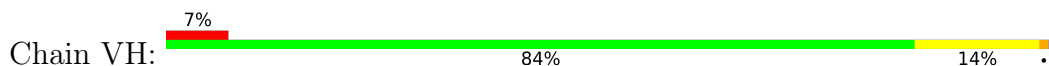
- Molecule 18: Large ribosomal subunit protein uL22



- Molecule 19: Small ribosomal subunit protein bS6

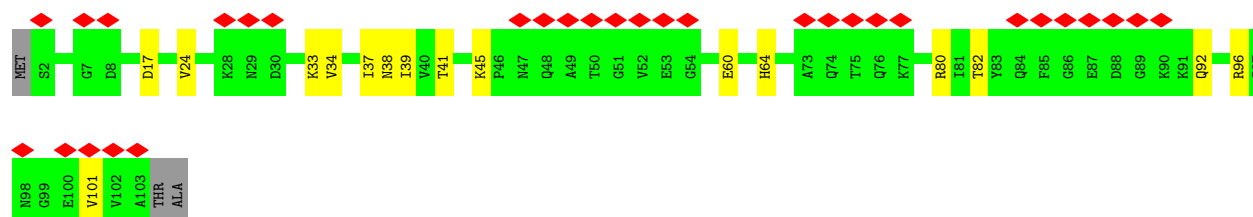
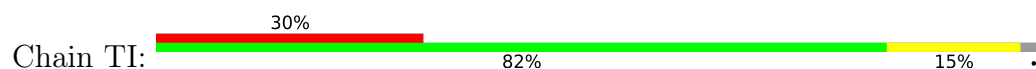


- Molecule 20: Large ribosomal subunit protein bL27

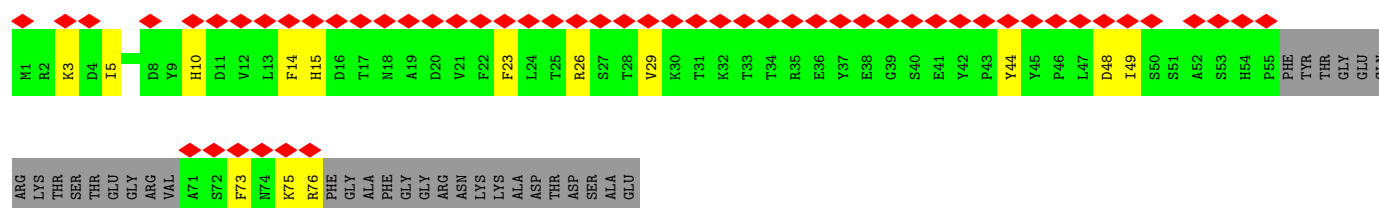




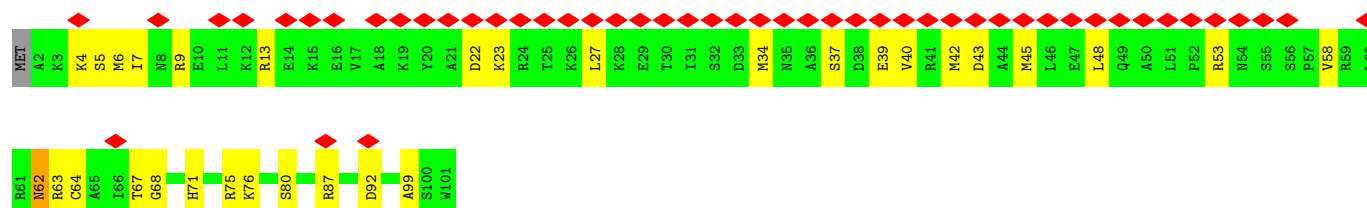
- Molecule 21: Large ribosomal subunit protein uL24



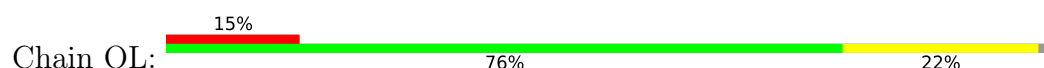
- Molecule 22: Large ribosomal subunit protein bL31B



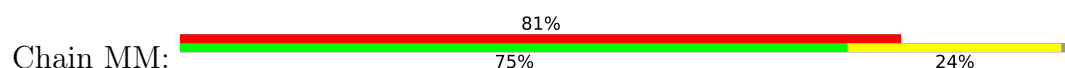
- Molecule 23: Small ribosomal subunit protein uS14

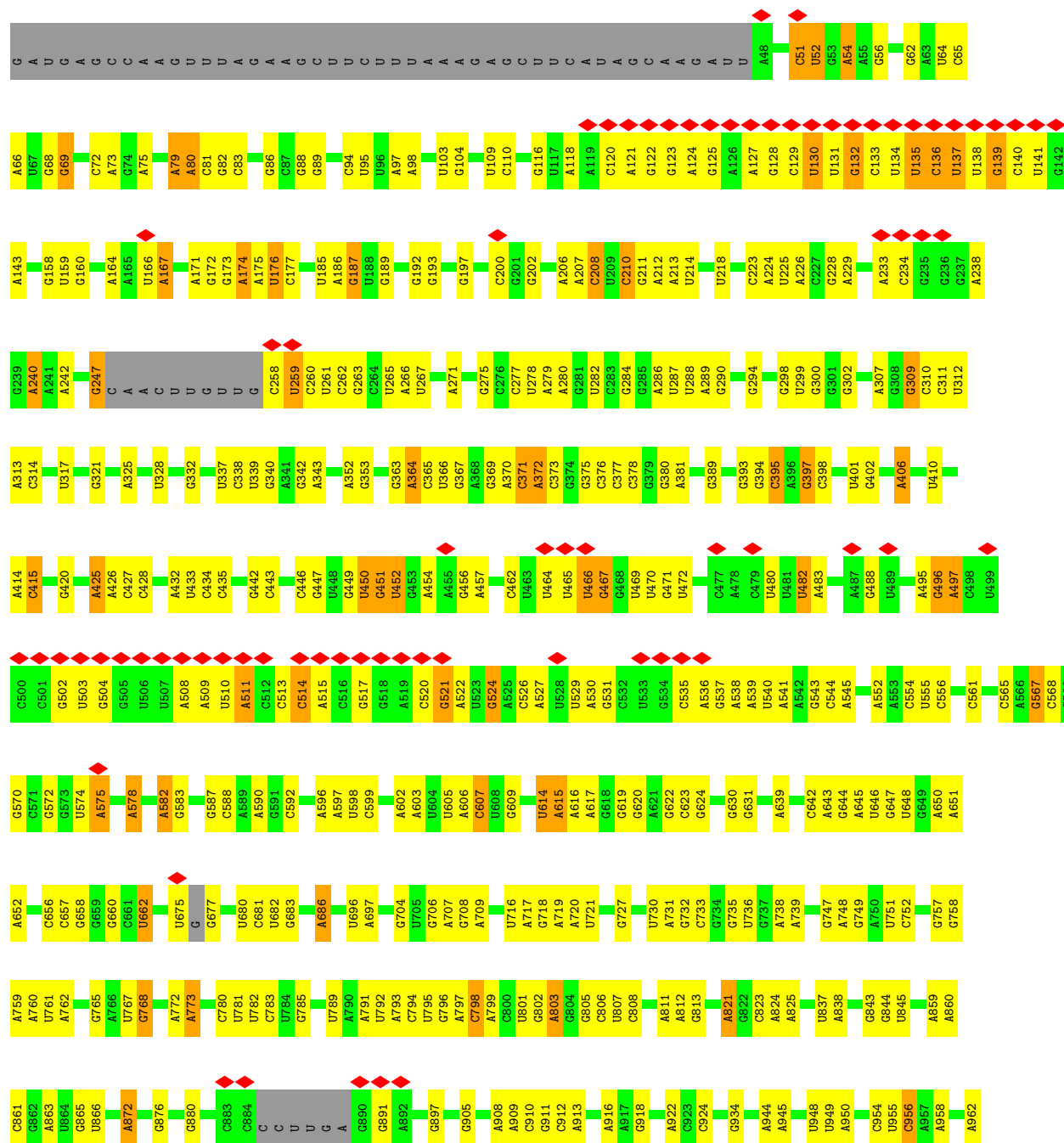


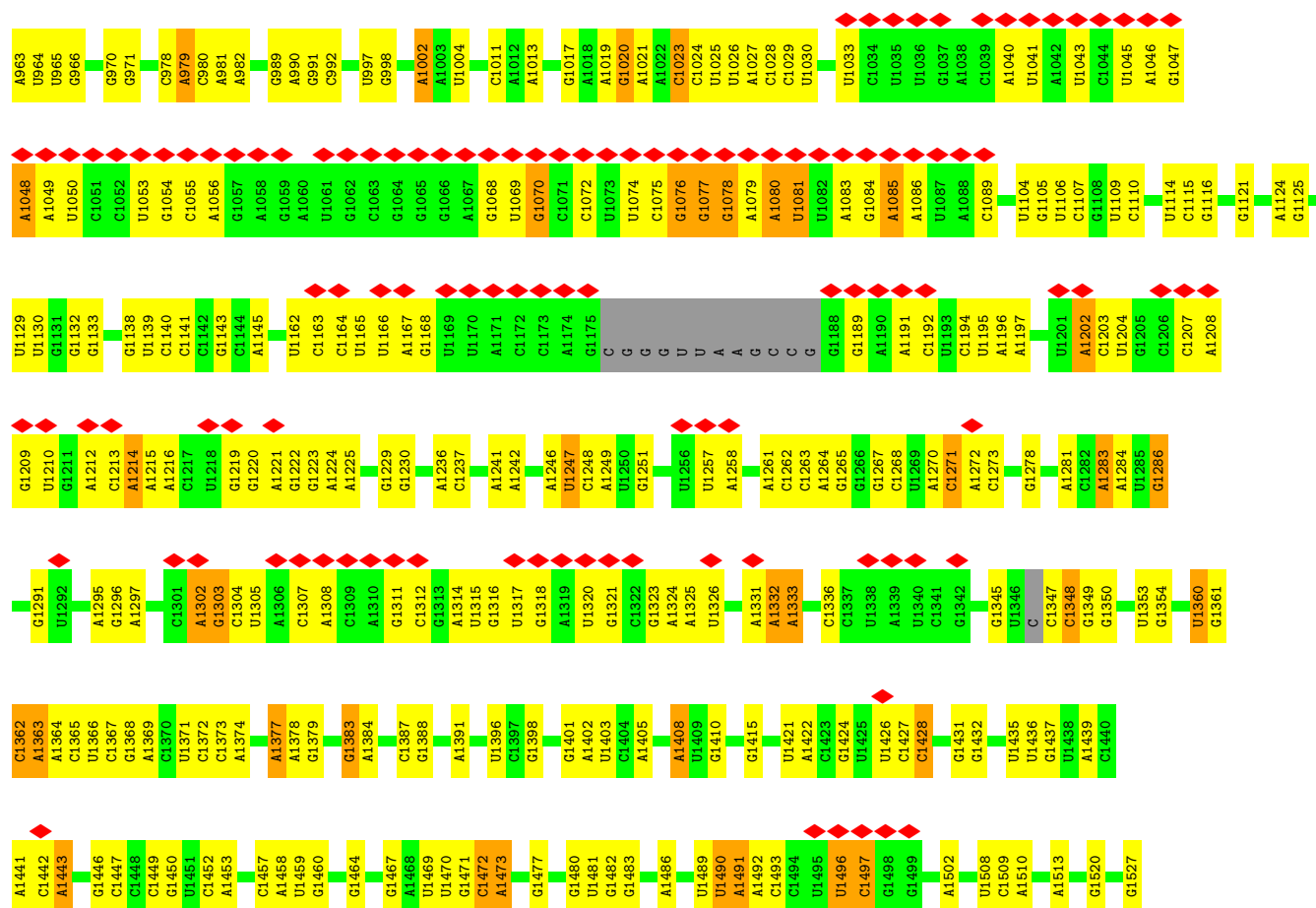
- Molecule 24: Small ribosomal subunit protein uS15



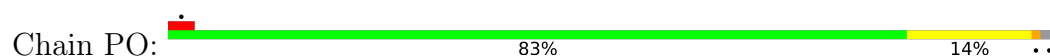
- Molecule 25: Small ribosomal subunit protein uS13



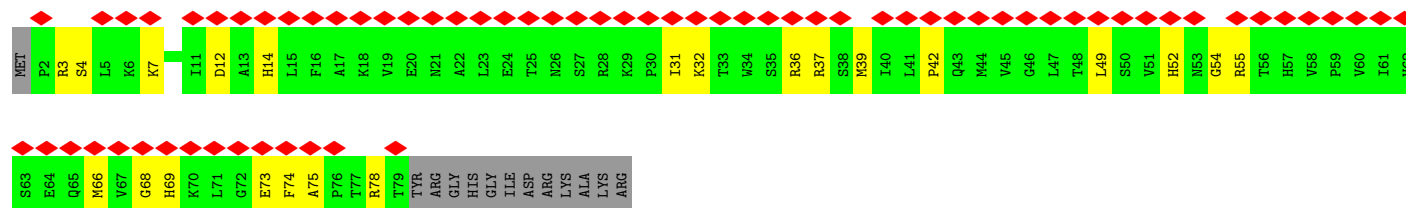
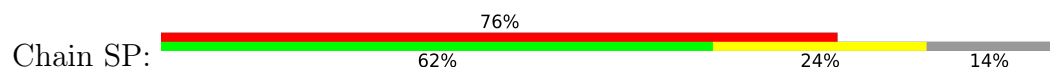




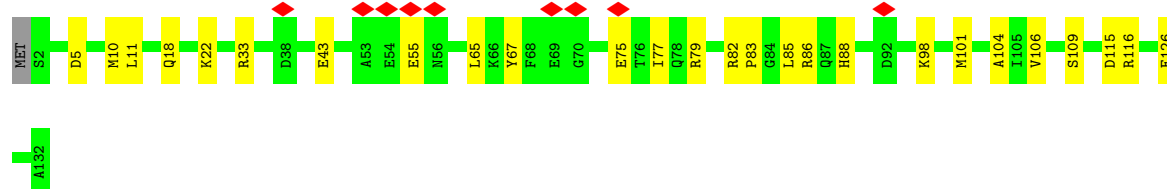
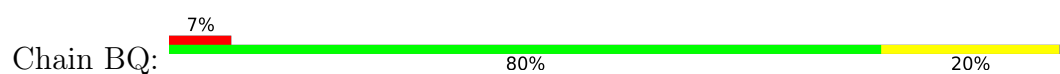
- Molecule 27: Large ribosomal subunit protein bL20



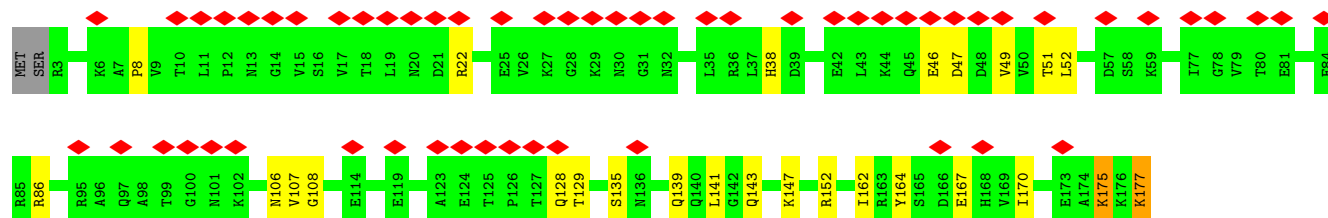
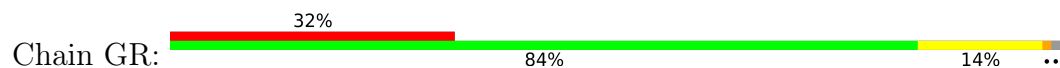
- Molecule 28: Small ribosomal subunit protein uS19



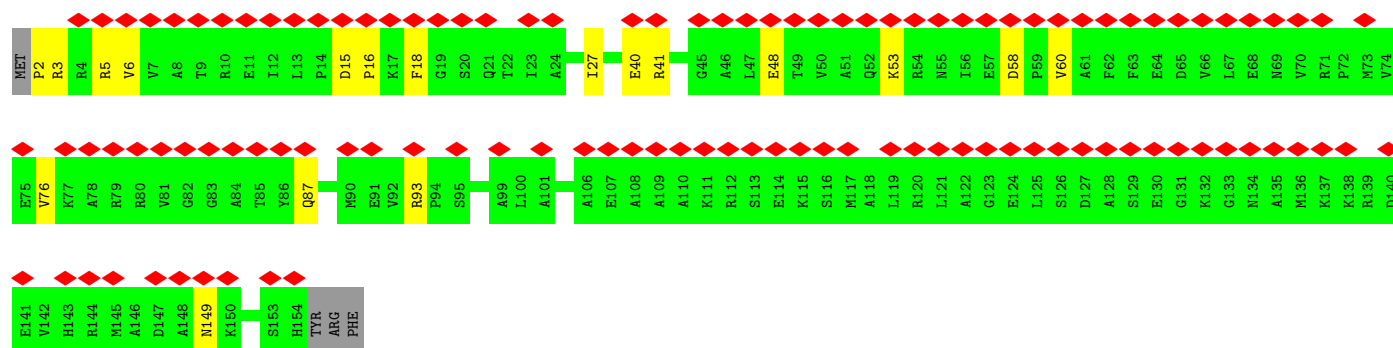
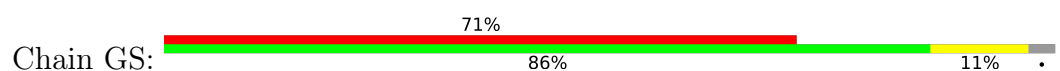
- Molecule 29: Small ribosomal subunit protein uS8



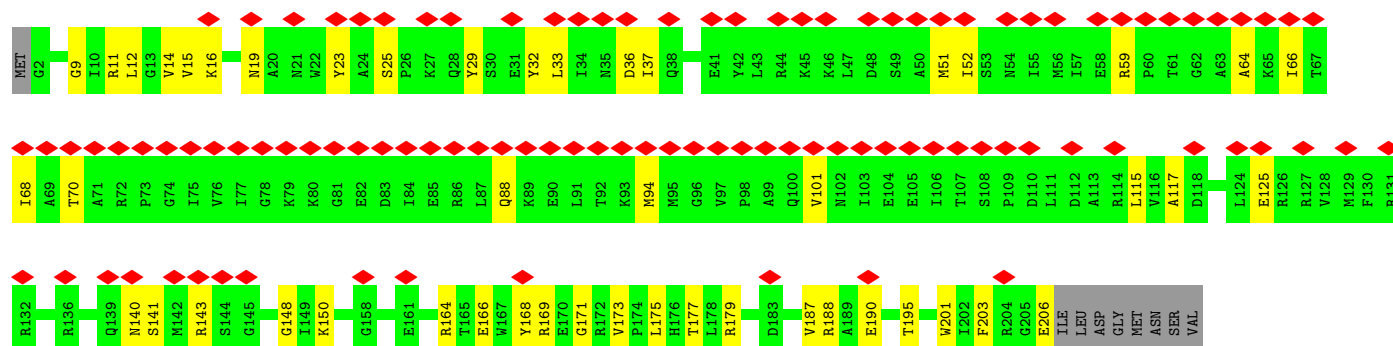
- Molecule 30: Large ribosomal subunit protein uL6



- Molecule 31: Small ribosomal subunit protein uS7



- Molecule 32: Small ribosomal subunit protein uS3



TYR ASN ASP VAL LYS GLU GLU GLN THR ARG ALA VAL LYS ARG ARG GLY ARG GLY ARG GLY ASN ARG ASN ARG SER ASP ARG GLY

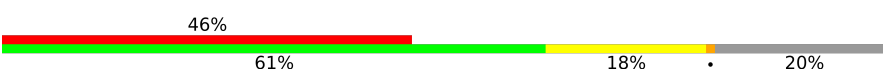
- Molecule 33: Small ribosomal subunit protein uS11

Chain KU: 

MET ALA LYS ASP THR ARG SER ARG LYS VAL THR ARG ARG S15 V16 E18 G19 I20 H24 A25 N29 T30 I31 T34 T35 D36 R37 Q38 G39 N40 A41 T46 R56 K57 F61 A62 A63 Q64 V65 E68 K72 A73 A74 Q75 E76 Y77 G78 V79 K80 N81

I82 D83 V84 L85 V86 K87 G88 P89 R93 E94 R98 A99 L100 G101 A102 L103 G104 Y105 K106 V107 N108 S109 I110 D112 P115 H118 N119 G120 V129

- Molecule 34: Small ribosomal subunit protein bS21

Chain NV: 

MET P2 A3 V4 K5 V6 K7 E8 N9 E10 P11 V12 D13 I14 A15 I16 R17 R18 F19 K20 R21 A22 C23 E24 K25 A26 G27 V28 D31 V32 R33 K34 R35 E39 K40 P41 R45 K54 R55 Y56 K57 K58 LYS LEU GLN ARG GLU THR ILE ARG THR THR ARG MET TYR

- Molecule 35: Large ribosomal subunit protein uL30

Chain YW: 

MET K2 K5 L9 K24 E38 D39 T40 T43 M46 W47 M48 N51 K55 V56 E57 GLU ALA

- Molecule 36: Large ribosomal subunit protein uL13

Chain IX: 

H1 P8 V11 W15 F16 V17 V18 D19 L25 L28 Q31 R35 T42 T45 V48 T54 V55 N58 T62 K73 Y80 T84 N88 F89 V100 V105 L109 P113 K120 K123 E133 A134 Q135 Q136 P137 K138

E139 L140 D141 I142

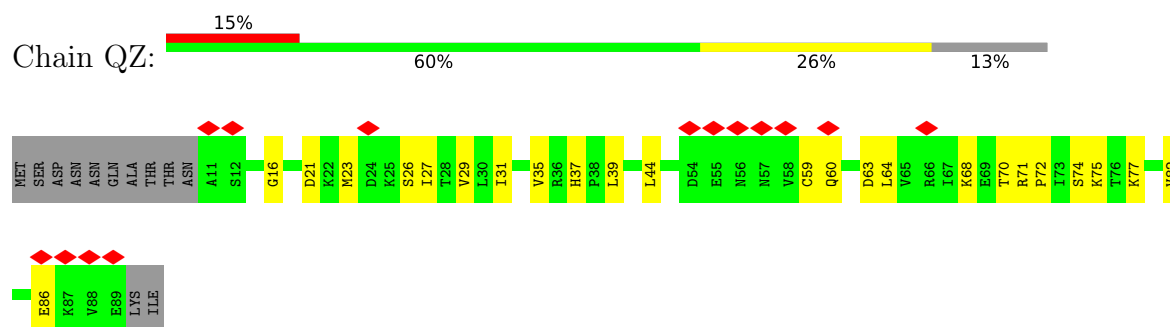
- Molecule 37: Small ribosomal subunit protein uS10

Chain JY: 

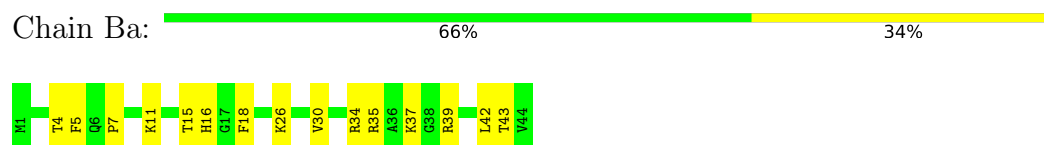
MET ALA ASN Q4 R5 I6 I7 R9 L10 K11 S12 F13 D14 H15 R16 L17 I18 D19 Q20 S21 A22 Q23 E24 T25 V26 D27 T28 A29 K30 R31 T32 G33 A34 Q35 V36 C37 G38 P39 V40 P43 T44 R45 T46 E47 N50 V51 L52 V57 N58 K59 R62 E66 T67 R68

T69 H70 K71 R72 M73 V74 D76 I76 W77 Q78 T80 D81 K82 T83 V84 D85 A86 L87 K88 R89 L90 D91 L92 L93 A94 G95 V96 D97 V98 Q99 I100 A101 L102 G103

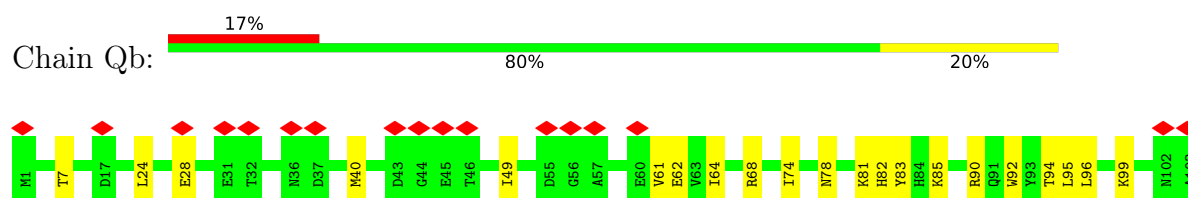
- Molecule 38: Small ribosomal subunit protein uS17



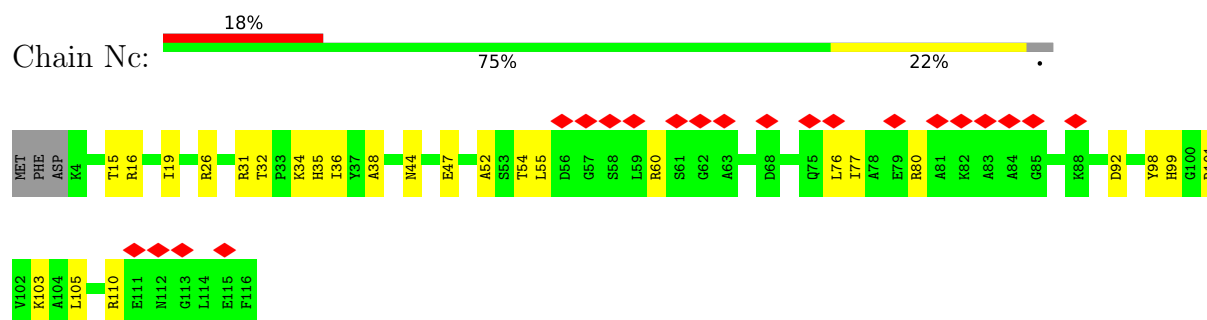
- Molecule 39: Large ribosomal subunit protein bL34



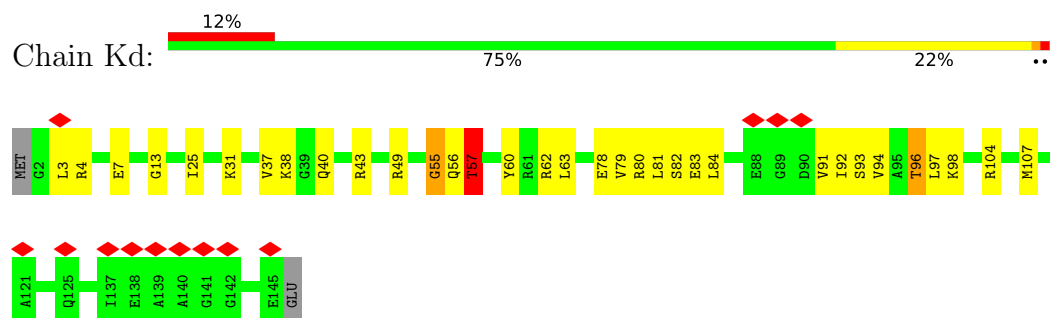
- Molecule 40: Large ribosomal subunit protein bL21



- Molecule 41: Large ribosomal subunit protein uL18



- Molecule 42: Large ribosomal subunit protein uL15



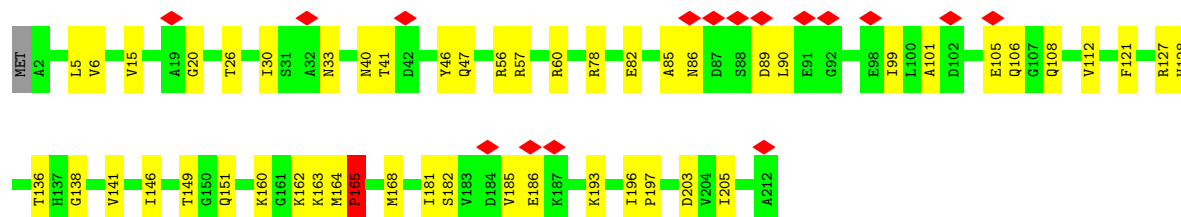
- Molecule 43: Large ribosomal subunit protein uL14

Chain Je: 



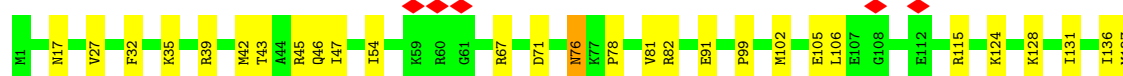
- Molecule 44: Large ribosomal subunit protein uL3

Chain Af: 



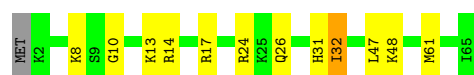
- Molecule 45: Large ribosomal subunit protein uL16

Chain Lg: 



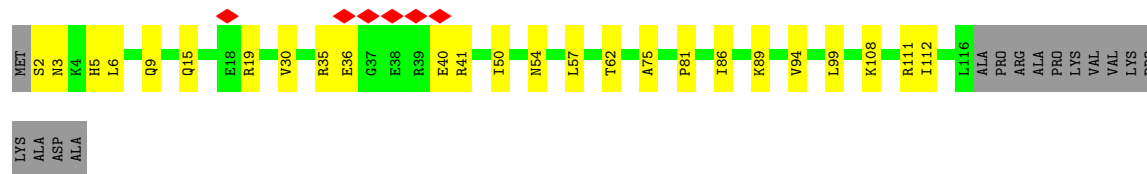
- Molecule 46: Large ribosomal subunit protein bL35

Chain dh: 



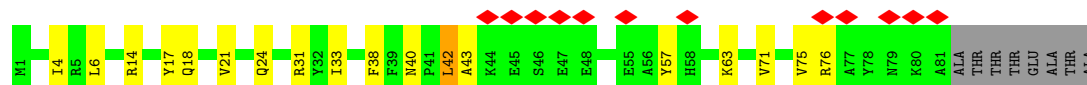
- Molecule 47: Large ribosomal subunit protein bL19

Chain Oi: 

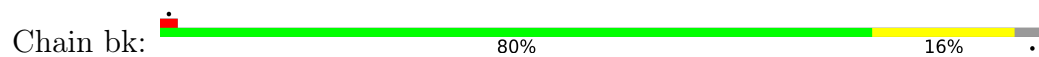


- Molecule 48: Small ribosomal subunit protein bS16

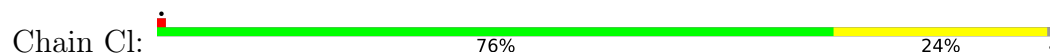
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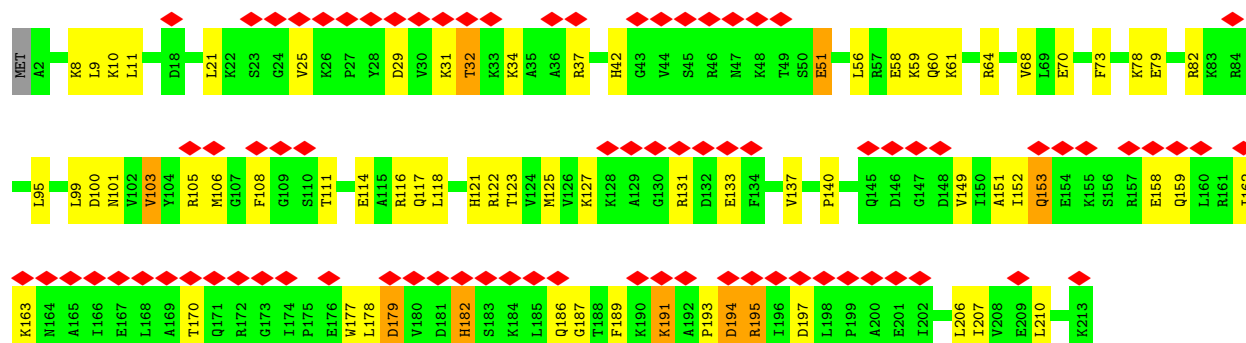
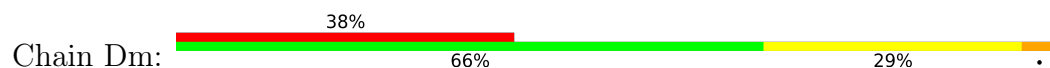
- Molecule 49: Large ribosomal subunit protein bL33



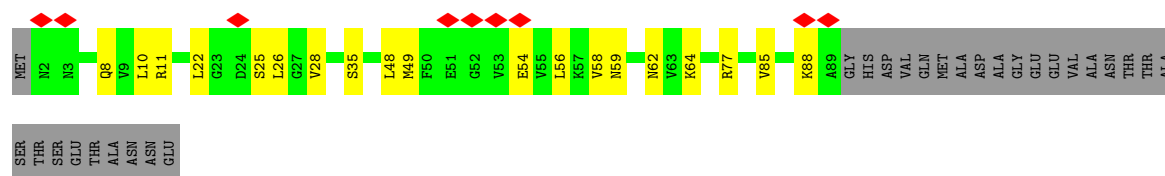
- Molecule 50: Large ribosomal subunit protein uL2



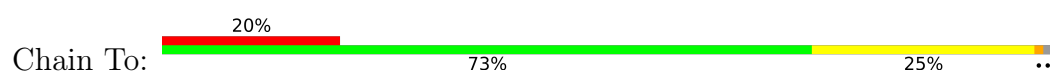
- Molecule 51: Small ribosomal subunit protein uS4

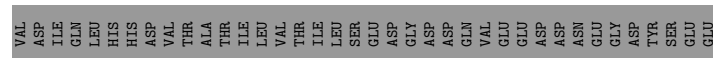


- Molecule 52: Large ribosomal subunit protein uL23



- Molecule 53: Small ribosomal subunit protein bS20





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 12151                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 900                                     | Depositor |
| Maximum defocus (nm)                 | 2400                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.156                                   | Depositor |
| Minimum map value                    | -0.070                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.004                                   | Depositor |
| Recommended contour level            | 0.0189                                  | Depositor |
| Map size (Å)                         | 390.41998, 390.41998, 390.41998         | wwPDB     |
| Map dimensions                       | 540, 540, 540                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.723, 0.723, 0.723                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP

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   | B     | 0.25         | 0/2914      | 0.48        | 1/3952 (0.0%) |
| 2   | D     | 0.08         | 0/126       | 0.19        | 0/173         |
| 3   | F     | 0.16         | 0/978       | 0.37        | 0/1311        |
| 4   | H     | 0.18         | 0/2968      | 0.41        | 0/4026        |
| 5   | Z2    | 0.24         | 0/65580     | 0.32        | 0/102277      |
| 6   | R3    | 0.16         | 0/465       | 0.31        | 0/629         |
| 7   | A4    | 0.16         | 0/1848      | 0.35        | 0/2494        |
| 8   | E5    | 0.18         | 0/1163      | 0.37        | 0/1564        |
| 9   | L6    | 0.19         | 0/959       | 0.44        | 0/1282        |
| 10  | F7    | 0.16         | 0/1383      | 0.33        | 0/1858        |
| 11  | D8    | 0.18         | 0/2733      | 0.26        | 0/4256        |
| 12  | E9    | 0.20         | 0/1559      | 0.36        | 0/2103        |
| 13  | aA    | 0.20         | 0/450       | 0.33        | 0/596         |
| 14  | MB    | 0.22         | 0/961       | 0.32        | 0/1282        |
| 15  | UC    | 0.17         | 0/774       | 0.33        | 0/1043        |
| 16  | WD    | 0.20         | 0/628       | 0.33        | 0/841         |
| 17  | XE    | 0.14         | 0/503       | 0.34        | 0/670         |
| 18  | RF    | 0.20         | 0/840       | 0.32        | 0/1125        |
| 19  | FG    | 0.13         | 0/864       | 0.28        | 0/1169        |
| 20  | VH    | 0.22         | 0/635       | 0.38        | 0/847         |
| 21  | TI    | 0.16         | 0/790       | 0.36        | 0/1057        |
| 22  | fJ    | 0.12         | 0/508       | 0.31        | 0/690         |
| 23  | HK    | 0.14         | 0/821       | 0.28        | 0/1091        |
| 24  | OL    | 0.17         | 0/702       | 0.28        | 0/941         |
| 25  | MM    | 0.11         | 0/917       | 0.27        | 0/1236        |
| 26  | iN    | 0.19         | 0/36109     | 0.28        | 0/56319       |
| 27  | PO    | 0.21         | 0/947       | 0.34        | 0/1261        |
| 28  | SP    | 0.11         | 0/628       | 0.26        | 0/847         |
| 29  | BQ    | 0.17         | 0/982       | 0.28        | 0/1318        |
| 30  | GR    | 0.15         | 0/1377      | 0.33        | 0/1861        |
| 31  | GS    | 0.12         | 0/1219      | 0.26        | 0/1634        |
| 32  | CT    | 0.15         | 0/1637      | 0.38        | 0/2200        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 33  | KU    | 0.13         | 0/857           | 0.28        | 0/1158          |
| 34  | NV    | 0.13         | 0/478           | 0.31        | 0/632           |
| 35  | YW    | 0.19         | 0/442           | 0.32        | 0/590           |
| 36  | IX    | 0.21         | 0/1134          | 0.34        | 0/1529          |
| 37  | JY    | 0.16         | 0/803           | 0.40        | 0/1084          |
| 38  | QZ    | 0.17         | 0/638           | 0.32        | 0/858           |
| 39  | Ba    | 0.26         | 0/373           | 0.37        | 0/489           |
| 40  | Qb    | 0.20         | 0/839           | 0.34        | 0/1127          |
| 41  | Nc    | 0.18         | 0/863           | 0.31        | 0/1158          |
| 42  | Kd    | 0.40         | 1/1073 (0.1%)   | 0.54        | 3/1429 (0.2%)   |
| 43  | Je    | 0.20         | 0/946           | 0.34        | 0/1271          |
| 44  | Af    | 0.33         | 1/1566 (0.1%)   | 0.52        | 3/2103 (0.1%)   |
| 45  | Lg    | 0.26         | 0/1112          | 0.45        | 0/1483          |
| 46  | dh    | 0.26         | 0/524           | 0.48        | 0/686           |
| 47  | Oi    | 0.23         | 0/927           | 0.41        | 0/1239          |
| 48  | Pj    | 0.22         | 0/660           | 0.41        | 0/887           |
| 49  | bk    | 0.22         | 0/401           | 0.37        | 0/534           |
| 50  | Cl    | 0.24         | 0/2147          | 0.40        | 0/2883          |
| 51  | Dm    | 0.19         | 0/1713          | 0.50        | 0/2296          |
| 52  | Sn    | 0.21         | 0/705           | 0.42        | 0/939           |
| 53  | To    | 0.19         | 0/688           | 0.50        | 0/916           |
| 54  | ep    | 0.26         | 0/300           | 0.38        | 0/395           |
| 55  | C1    | 0.21         | 0/379           | 0.51        | 0/511           |
| All | All   | 0.22         | 2/154536 (0.0%) | 0.33        | 7/230150 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 44  | Af    | 165 | PRO  | CG-CD | -8.05 | 1.23        | 1.50     |
| 42  | Kd    | 55  | GLY  | C-O   | -5.02 | 1.17        | 1.23     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 44  | Af    | 165 | PRO  | N-CD-CG  | -11.81 | 85.49       | 103.20   |
| 44  | Af    | 165 | PRO  | CA-CB-CG | -10.19 | 85.14       | 104.50   |
| 44  | Af    | 165 | PRO  | N-CA-CB  | -6.16  | 96.91       | 103.38   |
| 1   | B     | 7   | SER  | N-CA-C   | -6.12  | 107.64      | 114.62   |
| 42  | Kd    | 56  | GLN  | N-CA-CB  | 5.79   | 118.48      | 109.97   |
| 42  | Kd    | 57  | THR  | CA-C-N   | 5.25   | 125.19      | 119.78   |
| 42  | Kd    | 57  | THR  | C-N-CA   | 5.25   | 125.19      | 119.78   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 2871  | 0        | 2815     | 56      | 0            |
| 2   | D     | 127   | 0        | 75       | 1       | 0            |
| 3   | F     | 965   | 0        | 1009     | 29      | 0            |
| 4   | H     | 2918  | 0        | 2868     | 57      | 0            |
| 5   | Z2    | 58553 | 0        | 29435    | 655     | 0            |
| 6   | R3    | 457   | 0        | 466      | 12      | 0            |
| 7   | A4    | 1816  | 0        | 1843     | 25      | 0            |
| 8   | E5    | 1151  | 0        | 1205     | 32      | 0            |
| 9   | L6    | 946   | 0        | 1008     | 26      | 0            |
| 10  | F7    | 1362  | 0        | 1402     | 31      | 0            |
| 11  | D8    | 2446  | 0        | 1241     | 34      | 0            |
| 12  | E9    | 1537  | 0        | 1590     | 31      | 0            |
| 13  | aA    | 442   | 0        | 432      | 5       | 0            |
| 14  | MB    | 947   | 0        | 988      | 9       | 0            |
| 15  | UC    | 760   | 0        | 774      | 9       | 0            |
| 16  | WD    | 618   | 0        | 637      | 13      | 0            |
| 17  | XE    | 502   | 0        | 527      | 9       | 0            |
| 18  | RF    | 834   | 0        | 898      | 17      | 0            |
| 19  | FG    | 849   | 0        | 838      | 19      | 0            |
| 20  | VH    | 626   | 0        | 629      | 11      | 0            |
| 21  | TI    | 784   | 0        | 820      | 13      | 0            |
| 22  | fJ    | 493   | 0        | 441      | 9       | 0            |
| 23  | HK    | 811   | 0        | 845      | 29      | 0            |
| 24  | OL    | 694   | 0        | 710      | 15      | 0            |
| 25  | MM    | 907   | 0        | 955      | 21      | 0            |
| 26  | iN    | 32246 | 0        | 16223    | 430     | 0            |
| 27  | PO    | 935   | 0        | 999      | 15      | 0            |
| 28  | SP    | 614   | 0        | 643      | 15      | 0            |
| 29  | BQ    | 974   | 0        | 1009     | 19      | 0            |
| 30  | GR    | 1357  | 0        | 1397     | 17      | 0            |
| 31  | GS    | 1200  | 0        | 1231     | 12      | 0            |
| 32  | CT    | 1613  | 0        | 1677     | 31      | 0            |
| 33  | KU    | 842   | 0        | 850      | 20      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 34  | NV    | 472    | 0        | 520      | 9       | 0            |
| 35  | YW    | 438    | 0        | 476      | 7       | 0            |
| 36  | IX    | 1108   | 0        | 1145     | 21      | 0            |
| 37  | JY    | 793    | 0        | 821      | 25      | 0            |
| 38  | QZ    | 632    | 0        | 676      | 17      | 0            |
| 39  | Ba    | 369    | 0        | 418      | 14      | 0            |
| 40  | Qb    | 827    | 0        | 862      | 15      | 0            |
| 41  | Nc    | 852    | 0        | 880      | 18      | 0            |
| 42  | Kd    | 1062   | 0        | 1123     | 32      | 0            |
| 43  | Je    | 937    | 0        | 1003     | 18      | 0            |
| 44  | Af    | 1548   | 0        | 1574     | 35      | 0            |
| 45  | Lg    | 1093   | 0        | 1188     | 21      | 0            |
| 46  | dh    | 519    | 0        | 581      | 9       | 0            |
| 47  | Oi    | 917    | 0        | 969      | 21      | 0            |
| 48  | Pj    | 648    | 0        | 661      | 13      | 0            |
| 49  | bk    | 394    | 0        | 412      | 4       | 0            |
| 50  | Cl    | 2107   | 0        | 2195     | 53      | 0            |
| 51  | Dm    | 1689   | 0        | 1745     | 45      | 0            |
| 52  | Sn    | 698    | 0        | 750      | 14      | 0            |
| 53  | To    | 684    | 0        | 727      | 16      | 0            |
| 54  | ep    | 298    | 0        | 334      | 6       | 0            |
| 55  | C1    | 374    | 0        | 406      | 5       | 0            |
| 56  | H     | 28     | 0        | 12       | 1       | 0            |
| 57  | H     | 1      | 0        | 0        | 0       | 0            |
| 58  | Z2    | 1      | 0        | 0        | 1       | 0            |
| All | All   | 142686 | 0        | 97958    | 1862    | 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 8.

All (1862) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:Af:127:ARG:HA  | 44:Af:168:MET:HE3 | 1.56                     | 0.86              |
| 14:MB:37:THR:HG22 | 14:MB:39:PRO:HD2  | 1.59                     | 0.84              |
| 45:Lg:102:MET:H   | 45:Lg:102:MET:HE2 | 1.43                     | 0.83              |
| 5:Z2:142:C:O2     | 5:Z2:149:G:N2     | 2.11                     | 0.82              |
| 23:HK:58:VAL:HG21 | 26:iN:1361:G:H4'  | 1.62                     | 0.82              |
| 42:Kd:57:THR:CG2  | 42:Kd:62:ARG:HG2  | 2.09                     | 0.82              |
| 5:Z2:655:A:H4'    | 5:Z2:656:C:H5'    | 1.62                     | 0.81              |
| 5:Z2:570:G:N7     | 27:PO:6:ARG:NH2   | 2.28                     | 0.79              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:TI:34:VAL:HB    | 21:TI:37:ILE:HD11 | 1.64                     | 0.79              |
| 1:B:288:ASP:OD2    | 4:H:321:ARG:NH2   | 2.16                     | 0.79              |
| 3:F:97:LYS:NZ      | 26:iN:1223:G:OP2  | 2.15                     | 0.78              |
| 26:iN:1026:U:O2    | 26:iN:1267:G:N2   | 2.16                     | 0.78              |
| 5:Z2:671:U:O2'     | 39:Ba:5:PHE:O     | 2.01                     | 0.78              |
| 26:iN:167:A:H61    | 26:iN:282:U:H3    | 1.32                     | 0.78              |
| 33:KU:34:ILE:HD11  | 33:KU:74:ALA:HB3  | 1.65                     | 0.78              |
| 5:Z2:278:U:O4      | 5:Z2:336:A:N6     | 2.17                     | 0.77              |
| 5:Z2:193:A:H5''    | 42:Kd:49:ARG:HH12 | 1.49                     | 0.77              |
| 5:Z2:1020:G:H1     | 5:Z2:1103:U:H3    | 1.32                     | 0.77              |
| 32:CT:14:VAL:HG22  | 32:CT:15:VAL:HG13 | 1.66                     | 0.77              |
| 5:Z2:2031:C:OP1    | 13:aA:12:ARG:NH2  | 2.16                     | 0.76              |
| 37:JY:7:ARG:NH1    | 37:JY:73:MET:SD   | 2.58                     | 0.76              |
| 5:Z2:451:G:N7      | 39:Ba:39:ARG:NH2  | 2.34                     | 0.76              |
| 25:MM:23:PHE:HB3   | 25:MM:66:GLU:HB3  | 1.65                     | 0.76              |
| 26:iN:1490:U:H3    | 26:iN:1502:A:H61  | 1.33                     | 0.76              |
| 42:Kd:57:THR:HG23  | 42:Kd:62:ARG:HG2  | 1.67                     | 0.76              |
| 26:iN:1249:A:O2'   | 32:CT:188:ARG:NH1 | 2.19                     | 0.76              |
| 26:iN:717:A:H2'    | 26:iN:718:G:C8    | 2.21                     | 0.76              |
| 5:Z2:2303:A:O2'    | 5:Z2:2305:A:N7    | 2.18                     | 0.75              |
| 35:YW:48:ASN:O     | 35:YW:51:ASN:ND2  | 2.20                     | 0.75              |
| 51:Dm:194:ASP:N    | 51:Dm:194:ASP:OD1 | 2.19                     | 0.75              |
| 4:H:347:GLN:N      | 4:H:347:GLN:OE1   | 2.20                     | 0.75              |
| 5:Z2:866:G:O6      | 5:Z2:879:U:O4     | 2.05                     | 0.74              |
| 1:B:177:SER:O      | 5:Z2:2585:A:N6    | 2.21                     | 0.74              |
| 48:Pj:4:ILE:HG12   | 48:Pj:21:VAL:HG22 | 1.70                     | 0.74              |
| 26:iN:708:G:H22    | 26:iN:785:G:H1    | 1.34                     | 0.74              |
| 26:iN:630:G:OP1    | 29:BQ:86:ARG:NH1  | 2.19                     | 0.74              |
| 32:CT:179:ARG:NH1  | 32:CT:206:GLU:OE1 | 2.21                     | 0.74              |
| 5:Z2:52:G:H5''     | 5:Z2:53:G:H5'     | 1.69                     | 0.73              |
| 5:Z2:1417:A:H2'    | 5:Z2:1418:A:C8    | 2.24                     | 0.73              |
| 5:Z2:142:C:N3      | 5:Z2:149:G:N1     | 2.31                     | 0.73              |
| 5:Z2:68:A:OP2      | 17:XE:47:ARG:NH2  | 2.21                     | 0.73              |
| 14:MB:24:MET:HE1   | 14:MB:40:LYS:HD2  | 1.70                     | 0.73              |
| 50:Cl:146:LEU:HD11 | 50:Cl:154:MET:HE3 | 1.71                     | 0.73              |
| 5:Z2:2053:G:H1     | 5:Z2:2426:U:H3    | 1.37                     | 0.72              |
| 4:H:193:GLU:O      | 4:H:197:ILE:HD12  | 1.90                     | 0.72              |
| 5:Z2:219:C:H5      | 5:Z2:229:G:H21    | 1.37                     | 0.72              |
| 52:Sn:54:GLU:HB2   | 52:Sn:88:LYS:HG3  | 1.71                     | 0.72              |
| 4:H:47:TYR:OH      | 56:H:401:GDP:O1A  | 2.08                     | 0.72              |
| 5:Z2:272:U:H3      | 5:Z2:342:G:H1     | 1.37                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2311:A:H2'   | 5:Z2:2312:A:C8     | 2.25                     | 0.71              |
| 26:iN:1167:A:H4'  | 37:JY:38:GLY:HA3   | 1.71                     | 0.71              |
| 26:iN:1045:U:O2   | 26:iN:1084:G:N2    | 2.23                     | 0.71              |
| 8:E5:16:LEU:HD21  | 8:E5:44:VAL:HB     | 1.72                     | 0.71              |
| 6:R3:63:ARG:HD3   | 6:R3:70:TYR:HA     | 1.72                     | 0.71              |
| 17:XE:5:GLU:O     | 17:XE:9:LYS:NZ     | 2.24                     | 0.71              |
| 26:iN:1263:C:H2'  | 26:iN:1264:A:H8    | 1.56                     | 0.71              |
| 26:iN:1132:G:H21  | 26:iN:1212:A:H62   | 1.38                     | 0.70              |
| 5:Z2:1885:A:H8    | 5:Z2:1888:C:H41    | 1.38                     | 0.70              |
| 5:Z2:1925:U:OP1   | 5:Z2:2587:U:O2'    | 2.09                     | 0.70              |
| 5:Z2:169:C:O2'    | 5:Z2:170:A:OP1     | 2.10                     | 0.70              |
| 26:iN:446:C:H5''  | 51:Dm:140:PRO:HD2  | 1.74                     | 0.70              |
| 4:H:32:ILE:HG23   | 4:H:195:LEU:HD21   | 1.72                     | 0.69              |
| 5:Z2:2663:C:H5'   | 44:Af:197:PRO:HA   | 1.74                     | 0.69              |
| 37:JY:45:ARG:NH2  | 37:JY:47:GLU:OE2   | 2.24                     | 0.69              |
| 50:Cl:21:HIS:NE2  | 50:Cl:199:GLU:OE2  | 2.25                     | 0.69              |
| 5:Z2:1775:A:OP2   | 50:Cl:221:ARG:NH1  | 2.25                     | 0.69              |
| 5:Z2:2011:C:OP2   | 58:Z2:2901:HOH:O   | 2.10                     | 0.69              |
| 26:iN:768:G:OP2   | 26:iN:876:G:N2     | 2.25                     | 0.69              |
| 25:MM:65:THR:OG1  | 25:MM:66:GLU:OE2   | 2.11                     | 0.69              |
| 5:Z2:866:G:H1     | 5:Z2:879:U:H3      | 1.39                     | 0.69              |
| 5:Z2:1899:A:C2    | 26:iN:1537:A:H2'   | 2.27                     | 0.69              |
| 8:E5:102:GLN:HE21 | 8:E5:129:LEU:HD12  | 1.57                     | 0.69              |
| 26:iN:762:A:H5'   | 33:KU:119:ASN:HB2  | 1.73                     | 0.69              |
| 26:iN:1263:C:H2'  | 26:iN:1264:A:C8    | 2.28                     | 0.69              |
| 50:Cl:133:LYS:HB3 | 50:Cl:186:VAL:HG22 | 1.75                     | 0.68              |
| 30:GR:164:TYR:HB2 | 30:GR:167:GLU:HB2  | 1.75                     | 0.68              |
| 47:Oi:19:ARG:HD2  | 47:Oi:86:ILE:HD12  | 1.74                     | 0.68              |
| 5:Z2:1585:A:H5''  | 5:Z2:1586:A:H5'    | 1.73                     | 0.68              |
| 6:R3:73:ASN:C     | 6:R3:73:ASN:HD22   | 2.02                     | 0.68              |
| 9:L6:18:LYS:NZ    | 26:iN:954:C:OP2    | 2.25                     | 0.68              |
| 26:iN:514:C:H2'   | 26:iN:515:A:H8     | 1.59                     | 0.68              |
| 45:Lg:42:MET:HE2  | 45:Lg:47:ILE:HD13  | 1.75                     | 0.68              |
| 50:Cl:21:HIS:HB2  | 50:Cl:24:LEU:HD23  | 1.75                     | 0.68              |
| 24:OL:11:ILE:HG21 | 24:OL:21:THR:HG22  | 1.76                     | 0.68              |
| 26:iN:990:A:H2'   | 26:iN:991:G:C8     | 2.28                     | 0.68              |
| 5:Z2:477:G:H4'    | 18:RF:6:LYS:HB2    | 1.76                     | 0.68              |
| 5:Z2:836:C:H2'    | 5:Z2:837:A:H8      | 1.59                     | 0.67              |
| 26:iN:757:G:H2'   | 26:iN:758:G:C8     | 2.30                     | 0.67              |
| 4:H:28:LEU:O      | 4:H:32:ILE:HD12    | 1.94                     | 0.67              |
| 26:iN:721:U:H3    | 26:iN:757:G:H22    | 1.41                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:iN:1311:G:N2    | 26:iN:1314:A:OP2   | 2.22                     | 0.67              |
| 45:Lg:78:PRO:HG2   | 45:Lg:81:VAL:HG21  | 1.77                     | 0.67              |
| 5:Z2:2274:U:H2'    | 5:Z2:2275:G:C8     | 2.30                     | 0.67              |
| 11:D8:6:C:O3'      | 41:Nc:26:ARG:NH2   | 2.28                     | 0.66              |
| 26:iN:1115:C:H2'   | 26:iN:1116:G:H8    | 1.60                     | 0.66              |
| 7:A4:20:HIS:HB3    | 7:A4:48:LEU:HD21   | 1.77                     | 0.66              |
| 9:L6:46:ASN:HB2    | 26:iN:572:G:O6     | 1.96                     | 0.66              |
| 30:GR:135:SER:HB3  | 30:GR:141:LEU:HB2  | 1.78                     | 0.66              |
| 25:MM:64:MET:HG2   | 25:MM:69:LEU:HB2   | 1.78                     | 0.66              |
| 7:A4:56:ASN:O      | 7:A4:60:ASN:ND2    | 2.20                     | 0.66              |
| 23:HK:87:ARG:HD2   | 32:CT:37:ILE:HD12  | 1.78                     | 0.66              |
| 41:Nc:44:ASN:ND2   | 41:Nc:47:GLU:OE2   | 2.27                     | 0.66              |
| 5:Z2:552:U:O3'     | 42:Kd:38:LYS:NZ    | 2.29                     | 0.65              |
| 5:Z2:833:U:H2'     | 5:Z2:834:A:H8      | 1.60                     | 0.65              |
| 5:Z2:866:G:C6      | 5:Z2:879:U:O4      | 2.50                     | 0.65              |
| 5:Z2:1788:A:H2'    | 5:Z2:1789:A:C8     | 2.31                     | 0.65              |
| 16:WD:7:VAL:HG23   | 16:WD:8:THR:HG23   | 1.79                     | 0.65              |
| 26:iN:302:G:OP1    | 53:To:75:ARG:NH2   | 2.27                     | 0.65              |
| 26:iN:733:C:OP1    | 33:KU:29:ASN:ND2   | 2.29                     | 0.65              |
| 26:iN:123:G:H1     | 26:iN:138:U:H3     | 1.41                     | 0.65              |
| 5:Z2:189:G:O2'     | 5:Z2:662:A:N1      | 2.29                     | 0.65              |
| 7:A4:168:VAL:HG21  | 7:A4:178:ILE:HD11  | 1.78                     | 0.65              |
| 26:iN:1467:G:O3'   | 43:Je:49:ARG:NH2   | 2.30                     | 0.65              |
| 44:Af:112:VAL:HG11 | 44:Af:196:ILE:HD12 | 1.79                     | 0.65              |
| 1:B:130:ARG:NH2    | 5:Z2:1928:C:OP2    | 2.22                     | 0.65              |
| 5:Z2:915:A:O2'     | 35:YW:24:LYS:NZ    | 2.28                     | 0.65              |
| 32:CT:59:ARG:HA    | 32:CT:64:ALA:HA    | 1.79                     | 0.65              |
| 40:Qb:62:GLU:HB3   | 40:Qb:99:LYS:HE3   | 1.79                     | 0.65              |
| 3:F:19:LEU:HD12    | 3:F:61:LEU:HD21    | 1.79                     | 0.65              |
| 26:iN:544:C:H2'    | 26:iN:545:A:C8     | 2.31                     | 0.65              |
| 32:CT:11:ARG:NH2   | 32:CT:177:THR:O    | 2.28                     | 0.65              |
| 51:Dm:9:LEU:HD13   | 51:Dm:32:THR:HB    | 1.78                     | 0.64              |
| 26:iN:466:U:H2'    | 26:iN:467:G:C8     | 2.32                     | 0.64              |
| 44:Af:26:THR:HG21  | 44:Af:196:ILE:CG1  | 2.27                     | 0.64              |
| 5:Z2:1014:C:OP2    | 45:Lg:128:LYS:NZ   | 2.31                     | 0.64              |
| 5:Z2:2823:G:N2     | 5:Z2:2826:A:OP2    | 2.28                     | 0.64              |
| 26:iN:129:C:H4'    | 26:iN:130:U:H2'    | 1.80                     | 0.64              |
| 4:H:270:GLU:OE2    | 4:H:272:ARG:NH1    | 2.30                     | 0.64              |
| 25:MM:66:GLU:OE2   | 25:MM:66:GLU:N     | 2.23                     | 0.64              |
| 4:H:85:HIS:NE2     | 4:H:118:GLU:OE1    | 2.24                     | 0.64              |
| 5:Z2:836:C:H2'     | 5:Z2:837:A:C8      | 2.33                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:Z2:1459:G:O2'    | 5:Z2:1500:G:O6    | 2.16                     | 0.64              |
| 26:iN:247:G:H21    | 26:iN:509:A:H61   | 1.46                     | 0.64              |
| 26:iN:284:G:H1     | 26:iN:328:U:H3    | 1.46                     | 0.64              |
| 26:iN:312:U:H2'    | 26:iN:313:A:C8    | 2.31                     | 0.64              |
| 26:iN:1023:C:OP1   | 26:iN:1268:C:N4   | 2.31                     | 0.64              |
| 5:Z2:844:G:O2'     | 5:Z2:901:G:O6     | 2.14                     | 0.64              |
| 5:Z2:2287:G:H22    | 5:Z2:2295:U:H3    | 1.46                     | 0.64              |
| 26:iN:380:G:H2'    | 26:iN:381:A:C8    | 2.33                     | 0.64              |
| 5:Z2:1707:G:O2'    | 5:Z2:1725:A:N6    | 2.30                     | 0.63              |
| 18:RF:29:ILE:HD12  | 18:RF:69:LEU:HB2  | 1.81                     | 0.63              |
| 5:Z2:863:A:N6      | 5:Z2:885:A:N7     | 2.45                     | 0.63              |
| 7:A4:172:ASP:HB2   | 7:A4:196:SER:HB3  | 1.81                     | 0.63              |
| 26:iN:1207:C:H2'   | 26:iN:1208:A:H8   | 1.63                     | 0.63              |
| 5:Z2:1062:U:H4'    | 5:Z2:1063:C:H5'   | 1.79                     | 0.63              |
| 37:JY:46:ILE:HG12  | 37:JY:68:ARG:HG2  | 1.81                     | 0.63              |
| 51:Dm:125:MET:HE2  | 51:Dm:153:GLN:HA  | 1.80                     | 0.63              |
| 5:Z2:957:A:H5''    | 40:Qb:81:LYS:HD2  | 1.79                     | 0.63              |
| 8:E5:87:HIS:HB3    | 29:BQ:101:MET:HE1 | 1.81                     | 0.63              |
| 12:E9:117:LEU:HD11 | 12:E9:187:MET:HE3 | 1.80                     | 0.63              |
| 43:Je:97:ARG:HB3   | 43:Je:97:ARG:HH11 | 1.63                     | 0.63              |
| 45:Lg:35:LYS:HA    | 45:Lg:102:MET:HA  | 1.81                     | 0.63              |
| 5:Z2:872:U:OP1     | 25:MM:92:ARG:NH2  | 2.32                     | 0.63              |
| 5:Z2:2226:U:H2'    | 5:Z2:2227:U:C6    | 2.33                     | 0.63              |
| 26:iN:544:C:H2'    | 26:iN:545:A:H8    | 1.63                     | 0.63              |
| 25:MM:17:ILE:O     | 25:MM:20:THR:OG1  | 2.17                     | 0.62              |
| 8:E5:28:LYS:HD3    | 26:iN:1125:G:H5'  | 1.81                     | 0.62              |
| 10:F7:12:LEU:HD22  | 10:F7:172:ALA:HB1 | 1.81                     | 0.62              |
| 8:E5:60:GLU:OE1    | 32:CT:168:TYR:OH  | 2.14                     | 0.62              |
| 9:L6:12:ARG:HB3    | 26:iN:605:U:H1'   | 1.81                     | 0.62              |
| 5:Z2:1089:U:H2'    | 5:Z2:1090:A:H8    | 1.63                     | 0.62              |
| 15:UC:17:LEU:HD22  | 15:UC:26:LEU:HD12 | 1.81                     | 0.62              |
| 26:iN:1368:G:H2'   | 26:iN:1369:A:C8   | 2.34                     | 0.62              |
| 44:Af:127:ARG:NH1  | 44:Af:164:MET:O   | 2.32                     | 0.62              |
| 29:BQ:43:GLU:OE2   | 29:BQ:116:ARG:NH1 | 2.33                     | 0.62              |
| 50:Cl:117:MET:HE3  | 50:Cl:118:SER:H   | 1.65                     | 0.62              |
| 5:Z2:1012:A:N6     | 5:Z2:1109:G:H2'   | 2.15                     | 0.62              |
| 5:Z2:2196:A:H2'    | 5:Z2:2197:C:C6    | 2.34                     | 0.62              |
| 24:OL:20:ASP:OD1   | 24:OL:21:THR:N    | 2.30                     | 0.62              |
| 29:BQ:75:GLU:OE2   | 29:BQ:98:LYS:NZ   | 2.23                     | 0.62              |
| 5:Z2:285:G:OP1     | 21:TI:82:THR:OG1  | 2.15                     | 0.61              |
| 5:Z2:866:G:O6      | 5:Z2:879:U:C4     | 2.53                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2581:A:H5''  | 50:Cl:234:GLY:HA3  | 1.82                     | 0.61              |
| 5:Z2:380:U:H5''   | 16:WD:32:ASN:HB2   | 1.82                     | 0.61              |
| 26:iN:289:A:N1    | 26:iN:321:G:O2'    | 2.32                     | 0.61              |
| 26:iN:340:G:N2    | 26:iN:343:A:OP2    | 2.29                     | 0.61              |
| 26:iN:462:C:OP1   | 26:iN:556:C:O2'    | 2.17                     | 0.61              |
| 26:iN:759:A:H2'   | 26:iN:760:A:C8     | 2.35                     | 0.61              |
| 31:GS:87:GLN:O    | 31:GS:149:ASN:ND2  | 2.32                     | 0.61              |
| 8:E5:39:THR:HG22  | 8:E5:57:LYS:HG2    | 1.81                     | 0.61              |
| 26:iN:192:G:H2'   | 26:iN:193:G:C8     | 2.34                     | 0.61              |
| 26:iN:1320:U:H2'  | 26:iN:1321:G:C8    | 2.36                     | 0.61              |
| 26:iN:1332:A:H2'  | 26:iN:1333:A:C8    | 2.35                     | 0.61              |
| 26:iN:719:A:H1'   | 33:KU:118:HIS:CD2  | 2.35                     | 0.61              |
| 35:YW:43:THR:HA   | 35:YW:46:MET:HE3   | 1.82                     | 0.61              |
| 45:Lg:76:ASN:HB2  | 45:Lg:91:GLU:HG3   | 1.80                     | 0.61              |
| 12:E9:193:LYS:HE2 | 12:E9:193:LYS:HA   | 1.82                     | 0.61              |
| 1:B:212:ILE:HB    | 1:B:235:THR:HG22   | 1.82                     | 0.61              |
| 26:iN:79:A:H2'    | 26:iN:80:A:C8      | 2.35                     | 0.61              |
| 26:iN:934:G:O2'   | 26:iN:950:A:N6     | 2.33                     | 0.61              |
| 8:E5:99:VAL:HB    | 8:E5:116:MET:HE3   | 1.83                     | 0.61              |
| 43:Je:25:LEU:HD12 | 43:Je:38:ILE:HG22  | 1.83                     | 0.61              |
| 46:dh:31:HIS:ND1  | 46:dh:32:ILE:HG12  | 2.15                     | 0.60              |
| 26:iN:990:A:H2'   | 26:iN:991:G:H8     | 1.65                     | 0.60              |
| 28:SP:69:HIS:HB3  | 28:SP:73:GLU:HG3   | 1.83                     | 0.60              |
| 35:YW:9:LEU:HD21  | 35:YW:55:LYS:HB2   | 1.82                     | 0.60              |
| 1:B:137:GLU:HG3   | 1:B:144:VAL:HB     | 1.84                     | 0.60              |
| 3:F:9:ARG:HH12    | 26:iN:1194:C:P     | 2.24                     | 0.60              |
| 5:Z2:1012:A:H2'   | 5:Z2:1013:A:C8     | 2.37                     | 0.60              |
| 29:BQ:11:LEU:HD22 | 29:BQ:77:ILE:HD11  | 1.83                     | 0.60              |
| 31:GS:87:GLN:HB3  | 31:GS:149:ASN:HD21 | 1.66                     | 0.60              |
| 5:Z2:1780:A:H2'   | 5:Z2:1781:C:C6     | 2.37                     | 0.60              |
| 36:IX:19:ASP:OD2  | 36:IX:58:ASN:ND2   | 2.33                     | 0.60              |
| 5:Z2:561:U:H2'    | 5:Z2:562:G:C8      | 2.37                     | 0.60              |
| 5:Z2:1453:A:H2'   | 5:Z2:1454:A:C8     | 2.36                     | 0.60              |
| 5:Z2:1782:U:H2'   | 5:Z2:1783:C:H6     | 1.67                     | 0.60              |
| 5:Z2:2038:A:H4'   | 44:Af:151:GLN:O    | 2.01                     | 0.60              |
| 5:Z2:727:G:H2'    | 5:Z2:728:U:C6      | 2.37                     | 0.60              |
| 11:D8:46:U:OP2    | 41:Nc:31:ARG:NH2   | 2.35                     | 0.60              |
| 26:iN:496:G:N2    | 26:iN:521:G:O2'    | 2.35                     | 0.60              |
| 5:Z2:272:U:H2'    | 5:Z2:273:G:H8      | 1.67                     | 0.60              |
| 5:Z2:2190:G:H4'   | 50:Cl:150:LYS:HG3  | 1.82                     | 0.60              |
| 5:Z2:749:A:H2     | 50:Cl:218:PRO:HG3  | 1.67                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2842:U:H5''  | 47:Oi:6:LEU:CD2    | 2.32                     | 0.59              |
| 11:D8:58:C:H2'    | 11:D8:59:A:C8      | 2.37                     | 0.59              |
| 24:OL:15:GLN:NE2  | 24:OL:20:ASP:OD1   | 2.35                     | 0.59              |
| 26:iN:1353:U:H2'  | 26:iN:1354:G:H8    | 1.67                     | 0.59              |
| 44:Af:26:THR:HG21 | 44:Af:196:ILE:HG13 | 1.84                     | 0.59              |
| 1:B:316:ASP:OD1   | 1:B:316:ASP:N      | 2.34                     | 0.59              |
| 4:H:244:GLU:HG3   | 4:H:298:PRO:HG2    | 1.83                     | 0.59              |
| 20:VH:48:GLY:HA3  | 20:VH:81:MET:HG3   | 1.84                     | 0.59              |
| 5:Z2:1401:C:O2'   | 5:Z2:1575:G:O2'    | 2.19                     | 0.59              |
| 7:A4:102:LEU:H    | 7:A4:105:MET:HE3   | 1.67                     | 0.59              |
| 44:Af:41:THR:OG1  | 44:Af:47:GLN:NE2   | 2.35                     | 0.59              |
| 39:Ba:35:ARG:HG3  | 39:Ba:42:LEU:HD21  | 1.83                     | 0.59              |
| 47:Oi:35:ARG:HG2  | 47:Oi:40:GLU:HG2   | 1.84                     | 0.59              |
| 49:bk:35:PHE:HB2  | 49:bk:42:HIS:CE1   | 2.38                     | 0.59              |
| 1:B:291:ARG:O     | 1:B:295:GLN:HG2    | 2.02                     | 0.59              |
| 5:Z2:1089:U:H2'   | 5:Z2:1090:A:C8     | 2.38                     | 0.59              |
| 5:Z2:1356:U:O2'   | 5:Z2:2196:A:N3     | 2.30                     | 0.59              |
| 8:E5:110:VAL:O    | 8:E5:117:ARG:NH1   | 2.35                     | 0.59              |
| 22:fJ:15:HIS:HB3  | 22:fJ:44:TYR:HE1   | 1.66                     | 0.59              |
| 5:Z2:1580:A:O2'   | 5:Z2:1581:A:OP1    | 2.20                     | 0.59              |
| 5:Z2:2574:C:H2'   | 5:Z2:2575:G:C8     | 2.37                     | 0.59              |
| 14:MB:33:LEU:HD13 | 14:MB:114:GLU:HG3  | 1.83                     | 0.59              |
| 5:Z2:1160:G:H4'   | 5:Z2:1161:U:H3'    | 1.83                     | 0.59              |
| 17:XE:29:ARG:NH1  | 52:Sn:10:LEU:O     | 2.35                     | 0.59              |
| 18:RF:29:ILE:HD11 | 18:RF:55:ILE:HD12  | 1.85                     | 0.59              |
| 26:iN:75:A:O2'    | 26:iN:339:U:OP1    | 2.17                     | 0.59              |
| 5:Z2:246:C:O2     | 46:dh:13:LYS:NZ    | 2.36                     | 0.59              |
| 5:Z2:272:U:H2'    | 5:Z2:273:G:C8      | 2.37                     | 0.59              |
| 5:Z2:2011:C:H2'   | 5:Z2:2012:A:C8     | 2.38                     | 0.59              |
| 5:Z2:2537:U:H2'   | 5:Z2:2538:U:C6     | 2.37                     | 0.59              |
| 5:Z2:2057:A:H2'   | 5:Z2:2058:C:C6     | 2.37                     | 0.59              |
| 26:iN:535:C:H2'   | 26:iN:536:A:C8     | 2.38                     | 0.59              |
| 26:iN:1483:G:H5'' | 53:To:33:LYS:HE2   | 1.85                     | 0.59              |
| 33:KU:30:THR:HG21 | 33:KU:63:ALA:HB2   | 1.85                     | 0.59              |
| 5:Z2:562:G:O2'    | 5:Z2:1238:A:OP1    | 2.21                     | 0.58              |
| 5:Z2:792:U:P      | 42:Kd:38:LYS:HD2   | 2.43                     | 0.58              |
| 11:D8:3:U:OP1     | 11:D8:59:A:O2'     | 2.21                     | 0.58              |
| 3:F:13:SER:HB3    | 3:F:68:GLY:HA3     | 1.85                     | 0.58              |
| 3:F:26:ILE:HG12   | 3:F:61:LEU:HD12    | 1.85                     | 0.58              |
| 4:H:263:MET:HG2   | 4:H:277:CYS:HA     | 1.85                     | 0.58              |
| 19:FG:18:VAL:HG11 | 19:FG:58:HIS:CE1   | 2.38                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:MM:83:LEU:HG    | 28:SP:74:PHE:HE1   | 1.68                     | 0.58              |
| 26:iN:64:U:H2'     | 26:iN:65:C:C6      | 2.38                     | 0.58              |
| 26:iN:1130:U:H3    | 26:iN:1143:G:H22   | 1.49                     | 0.58              |
| 26:iN:1363:A:H5''  | 28:SP:3:ARG:HH12   | 1.69                     | 0.58              |
| 3:F:104:ARG:NH1    | 3:F:105:ASP:O      | 2.36                     | 0.58              |
| 4:H:134:PHE:HE2    | 4:H:136:ASN:HB3    | 1.68                     | 0.58              |
| 4:H:190:ALA:HA     | 4:H:193:GLU:OE2    | 2.03                     | 0.58              |
| 28:SP:36:ARG:NH2   | 28:SP:75:ALA:O     | 2.36                     | 0.58              |
| 50:Cl:69:ARG:NH2   | 50:Cl:127:GLY:O    | 2.26                     | 0.58              |
| 5:Z2:2668:G:OP1    | 43:Je:78:ARG:NH1   | 2.36                     | 0.58              |
| 19:FG:41:ASP:OD1   | 19:FG:58:HIS:NE2   | 2.35                     | 0.58              |
| 41:Nc:76:LEU:HD11  | 41:Nc:80:ARG:HH21  | 1.69                     | 0.58              |
| 4:H:316:LYS:HE2    | 4:H:322:HIS:HA     | 1.86                     | 0.58              |
| 5:Z2:2216:U:H2'    | 5:Z2:2217:G:C8     | 2.39                     | 0.58              |
| 26:iN:278:U:H2'    | 26:iN:279:A:C8     | 2.39                     | 0.58              |
| 32:CT:94:MET:HE2   | 32:CT:94:MET:O     | 2.04                     | 0.58              |
| 5:Z2:798:U:H2'     | 5:Z2:799:C:C6      | 2.39                     | 0.58              |
| 26:iN:79:A:H2'     | 26:iN:80:A:H8      | 1.68                     | 0.58              |
| 3:F:32:PRO:HG2     | 3:F:35:GLU:HB3     | 1.85                     | 0.58              |
| 4:H:178:ALA:O      | 4:H:188:GLN:NE2    | 2.36                     | 0.58              |
| 5:Z2:244:G:OP2     | 5:Z2:246:C:N4      | 2.36                     | 0.58              |
| 5:Z2:446:G:N2      | 5:Z2:449:A:OP2     | 2.31                     | 0.58              |
| 5:Z2:593:A:H2'     | 5:Z2:594:A:C8      | 2.38                     | 0.58              |
| 26:iN:497:A:H2     | 26:iN:521:G:H21    | 1.50                     | 0.58              |
| 30:GR:8:PRO:HB3    | 30:GR:51:THR:HG22  | 1.85                     | 0.58              |
| 3:F:16:ARG:NH2     | 26:iN:1192:C:O2    | 2.37                     | 0.58              |
| 5:Z2:82:G:H22      | 5:Z2:117:A:H2      | 1.52                     | 0.58              |
| 5:Z2:1681:U:H5''   | 5:Z2:1682:C:H5     | 1.67                     | 0.58              |
| 5:Z2:2009:C:H5'    | 5:Z2:2600:U:H4'    | 1.84                     | 0.58              |
| 8:E5:100:TYR:OH    | 8:E5:102:GLN:OE1   | 2.22                     | 0.57              |
| 41:Nc:98:TYR:OH    | 41:Nc:110:ARG:NH2  | 2.37                     | 0.57              |
| 45:Lg:54:ILE:HG21  | 45:Lg:106:LEU:HD11 | 1.86                     | 0.57              |
| 51:Dm:127:LYS:HG2  | 51:Dm:149:VAL:HB   | 1.85                     | 0.57              |
| 4:H:112:PRO:C      | 4:H:113:MET:HE2    | 2.29                     | 0.57              |
| 5:Z2:749:A:H5''    | 50:Cl:209:GLY:HA3  | 1.86                     | 0.57              |
| 23:HK:5:SER:HB3    | 26:iN:1261:A:H5''  | 1.85                     | 0.57              |
| 26:iN:1080:A:O2'   | 26:iN:1081:U:OP1   | 2.22                     | 0.57              |
| 50:Cl:130:LEU:HD12 | 50:Cl:192:ILE:HD11 | 1.86                     | 0.57              |
| 5:Z2:1633:G:H5''   | 5:Z2:1634:C:H5'    | 1.86                     | 0.57              |
| 11:D8:35:C:O2      | 41:Nc:99:HIS:NE2   | 2.28                     | 0.57              |
| 26:iN:706:G:H2'    | 26:iN:707:A:C8     | 2.39                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:NV:4:VAL:HG21   | 34:NV:19:PHE:HA   | 1.86                     | 0.57              |
| 5:Z2:1325:G:H1'    | 52:Sn:59:ASN:HB3  | 1.86                     | 0.57              |
| 5:Z2:2311:A:H2'    | 5:Z2:2312:A:H8    | 1.70                     | 0.57              |
| 9:L6:4:THR:OG1     | 29:BQ:82:ARG:NH2  | 2.37                     | 0.57              |
| 5:Z2:1299:C:O2'    | 5:Z2:1376:A:N3    | 2.37                     | 0.57              |
| 5:Z2:1782:U:H2'    | 5:Z2:1783:C:C6    | 2.39                     | 0.57              |
| 5:Z2:2760:G:H5''   | 5:Z2:2761:A:H5'   | 1.86                     | 0.57              |
| 48:Pj:71:VAL:O     | 48:Pj:75:VAL:HG23 | 2.03                     | 0.57              |
| 4:H:174:SER:N      | 4:H:186:TYR:O     | 2.37                     | 0.57              |
| 5:Z2:644:G:O2'     | 12:E9:94:LYS:O    | 2.22                     | 0.57              |
| 5:Z2:1403:A:O2'    | 5:Z2:1405:G:N7    | 2.34                     | 0.57              |
| 5:Z2:1556:G:H5'    | 50:Cl:60:GLN:HA   | 1.86                     | 0.57              |
| 15:UC:80:ILE:HG12  | 45:Lg:137:MET:HE1 | 1.87                     | 0.57              |
| 44:Af:146:ILE:HD11 | 44:Af:165:PRO:HD3 | 1.86                     | 0.57              |
| 5:Z2:248:A:OP1     | 46:dh:8:LYS:HE2   | 2.04                     | 0.57              |
| 5:Z2:287:A:OP2     | 21:TI:80:ARG:NH1  | 2.38                     | 0.57              |
| 10:F7:67:VAL:O     | 11:D8:39:C:N4     | 2.35                     | 0.57              |
| 26:iN:1537:A:O2'   | 26:iN:1538:A:OP1  | 2.14                     | 0.57              |
| 26:iN:81:C:H2'     | 26:iN:82:G:H8     | 1.70                     | 0.57              |
| 28:SP:12:ASP:OD2   | 28:SP:14:HIS:ND1  | 2.38                     | 0.57              |
| 5:Z2:816:G:O2'     | 42:Kd:40:GLN:OE1  | 2.23                     | 0.57              |
| 5:Z2:818:A:H2'     | 5:Z2:819:G:C8     | 2.39                     | 0.57              |
| 5:Z2:767:A:C2      | 50:Cl:225:MET:HG2 | 2.40                     | 0.57              |
| 16:WD:31:PRO:HB2   | 16:WD:33:LEU:HG   | 1.86                     | 0.57              |
| 26:iN:482:U:H5''   | 51:Dm:122:ARG:HD3 | 1.86                     | 0.57              |
| 45:Lg:17:ASN:HD21  | 45:Lg:39:ARG:HB2  | 1.70                     | 0.57              |
| 5:Z2:566:C:H2'     | 5:Z2:567:A:C8     | 2.40                     | 0.56              |
| 26:iN:602:A:H4'    | 26:iN:603:A:H3'   | 1.87                     | 0.56              |
| 26:iN:1362:C:O2    | 28:SP:37:ARG:NH1  | 2.37                     | 0.56              |
| 26:iN:1408:A:O2'   | 26:iN:1410:G:N7   | 2.30                     | 0.56              |
| 26:iN:1502:A:OP1   | 53:To:34:ARG:NH2  | 2.38                     | 0.56              |
| 51:Dm:79:GLU:OE2   | 51:Dm:82:ARG:NH2  | 2.38                     | 0.56              |
| 4:H:75:ARG:NH2     | 4:H:202:ILE:O     | 2.38                     | 0.56              |
| 5:Z2:749:A:H5''    | 50:Cl:209:GLY:CA  | 2.35                     | 0.56              |
| 5:Z2:1413:G:H2'    | 5:Z2:1414:G:H8    | 1.71                     | 0.56              |
| 5:Z2:2190:G:OP2    | 50:Cl:147:LYS:NZ  | 2.39                     | 0.56              |
| 19:FG:51:ILE:O     | 19:FG:54:ILE:HG12 | 2.05                     | 0.56              |
| 26:iN:772:A:H2'    | 26:iN:773:A:C8    | 2.40                     | 0.56              |
| 26:iN:1558:A:H2'   | 26:iN:1559:G:C8   | 2.41                     | 0.56              |
| 32:CT:23:TYR:HD2   | 37:JY:12:SER:HA   | 1.69                     | 0.56              |
| 32:CT:25:SER:O     | 32:CT:29:TYR:N    | 2.37                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:iN:1401:G:H2'  | 26:iN:1402:A:C8   | 2.41                     | 0.56              |
| 26:iN:1508:U:H2'  | 26:iN:1509:C:C6   | 2.41                     | 0.56              |
| 5:Z2:451:G:OP2    | 39:Ba:37:LYS:NZ   | 2.37                     | 0.56              |
| 5:Z2:1875:A:H2'   | 5:Z2:1876:A:C8    | 2.41                     | 0.56              |
| 5:Z2:2530:A:H2'   | 5:Z2:2531:U:C6    | 2.41                     | 0.56              |
| 8:E5:57:LYS:HE2   | 26:iN:1125:G:N7   | 2.21                     | 0.56              |
| 23:HK:64:CYS:HB2  | 23:HK:80:SER:HB3  | 1.87                     | 0.56              |
| 26:iN:598:U:H2'   | 26:iN:599:C:C6    | 2.41                     | 0.56              |
| 26:iN:735:G:O6    | 33:KU:57:LYS:NZ   | 2.38                     | 0.56              |
| 1:B:60:ILE:O      | 1:B:64:ILE:HG23   | 2.05                     | 0.56              |
| 11:D8:25:C:OP1    | 41:Nc:35:HIS:NE2  | 2.35                     | 0.56              |
| 26:iN:471:G:OP2   | 51:Dm:10:LYS:NZ   | 2.33                     | 0.56              |
| 26:iN:514:C:H2'   | 26:iN:515:A:C8    | 2.39                     | 0.56              |
| 5:Z2:47:U:H2'     | 5:Z2:48:C:C6      | 2.41                     | 0.56              |
| 5:Z2:993:A:N3     | 5:Z2:1138:C:O2'   | 2.38                     | 0.56              |
| 5:Z2:2328:A:N3    | 5:Z2:2364:A:H2'   | 2.20                     | 0.56              |
| 24:OL:20:ASP:HA   | 26:iN:794:C:H4'   | 1.88                     | 0.56              |
| 5:Z2:578:U:H2'    | 5:Z2:579:U:C6     | 2.40                     | 0.56              |
| 12:E9:46:LYS:HB3  | 12:E9:50:GLU:HB2  | 1.88                     | 0.56              |
| 26:iN:1115:C:H2'  | 26:iN:1116:G:C8   | 2.41                     | 0.56              |
| 15:UC:86:HIS:HB3  | 15:UC:90:GLY:H    | 1.70                     | 0.56              |
| 16:WD:7:VAL:HG12  | 16:WD:71:LEU:HD21 | 1.86                     | 0.56              |
| 26:iN:813:G:H4'   | 26:iN:1558:A:H4'  | 1.88                     | 0.56              |
| 26:iN:1449:C:H2'  | 26:iN:1450:G:C8   | 2.41                     | 0.56              |
| 48:Pj:6:LEU:HB3   | 48:Pj:17:TYR:HB3  | 1.87                     | 0.56              |
| 1:B:220:SER:HB3   | 5:Z2:2540:G:O3'   | 2.06                     | 0.56              |
| 4:H:134:PHE:HD1   | 4:H:171:VAL:HG13  | 1.71                     | 0.56              |
| 5:Z2:688:U:H2'    | 5:Z2:689:G:O4'    | 2.06                     | 0.56              |
| 5:Z2:1341:C:H2'   | 5:Z2:1342:G:O4'   | 2.06                     | 0.56              |
| 26:iN:623:C:H2'   | 26:iN:624:G:O4'   | 2.06                     | 0.56              |
| 5:Z2:2234:G:OP1   | 45:Lg:82:ARG:NH1  | 2.39                     | 0.55              |
| 26:iN:588:C:H5'   | 51:Dm:70:GLU:HB2  | 1.88                     | 0.55              |
| 32:CT:148:GLY:HA2 | 32:CT:171:GLY:HA3 | 1.87                     | 0.55              |
| 42:Kd:80:ARG:HB2  | 42:Kd:83:GLU:HG3  | 1.88                     | 0.55              |
| 5:Z2:2831:U:OP2   | 5:Z2:2832:G:O2'   | 2.21                     | 0.55              |
| 18:RF:51:LEU:O    | 18:RF:55:ILE:HG12 | 2.06                     | 0.55              |
| 23:HK:34:MET:HE1  | 26:iN:1318:G:H5'  | 1.88                     | 0.55              |
| 26:iN:278:U:H2'   | 26:iN:279:A:H8    | 1.72                     | 0.55              |
| 26:iN:1472:C:H2'  | 26:iN:1473:A:C8   | 2.41                     | 0.55              |
| 48:Pj:18:GLN:HA   | 48:Pj:38:PHE:HA   | 1.89                     | 0.55              |
| 10:F7:8:TYR:HA    | 10:F7:12:LEU:HB2  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:Qb:68:ARG:HD3  | 40:Qb:92:TRP:CE2  | 2.41                     | 0.55              |
| 5:Z2:579:U:H2'    | 5:Z2:580:C:C6     | 2.41                     | 0.55              |
| 5:Z2:2842:U:H5''  | 47:Oi:6:LEU:HD21  | 1.89                     | 0.55              |
| 26:iN:158:G:H1'   | 26:iN:397:G:H5'   | 1.88                     | 0.55              |
| 26:iN:792:U:H2'   | 26:iN:793:A:H8    | 1.72                     | 0.55              |
| 26:iN:795:U:H2'   | 26:iN:796:G:O4'   | 2.07                     | 0.55              |
| 5:Z2:866:G:N1     | 5:Z2:879:U:N3     | 2.50                     | 0.55              |
| 5:Z2:1276:G:H2'   | 5:Z2:1277:C:C6    | 2.41                     | 0.55              |
| 5:Z2:1485:G:H5''  | 50:Cl:95:LYS:NZ   | 2.21                     | 0.55              |
| 26:iN:539:A:H2'   | 26:iN:540:U:C5    | 2.41                     | 0.55              |
| 5:Z2:583:U:H2'    | 5:Z2:584:A:H8     | 1.72                     | 0.55              |
| 5:Z2:811:U:O2'    | 42:Kd:55:GLY:HA3  | 2.07                     | 0.55              |
| 5:Z2:2811:U:H5''  | 47:Oi:54:ASN:O    | 2.06                     | 0.55              |
| 26:iN:261:U:H2'   | 26:iN:262:C:C6    | 2.42                     | 0.55              |
| 26:iN:342:G:H2'   | 26:iN:343:A:C8    | 2.42                     | 0.55              |
| 10:F7:103:LEU:HA  | 10:F7:107:ALA:HB3 | 1.89                     | 0.55              |
| 11:D8:11:A:N1     | 11:D8:67:G:O2'    | 2.38                     | 0.55              |
| 26:iN:299:U:H2'   | 26:iN:300:G:H8    | 1.70                     | 0.55              |
| 26:iN:353:G:H5''  | 48:Pj:31:ARG:HB2  | 1.88                     | 0.55              |
| 26:iN:1368:G:H2'  | 26:iN:1369:A:H8   | 1.72                     | 0.55              |
| 32:CT:125:GLU:OE2 | 32:CT:190:GLU:N   | 2.39                     | 0.55              |
| 48:Pj:14:ARG:HG2  | 48:Pj:42:LEU:HD11 | 1.89                     | 0.55              |
| 48:Pj:40:ASN:HB3  | 48:Pj:43:ALA:HB2  | 1.88                     | 0.55              |
| 5:Z2:833:U:H2'    | 5:Z2:834:A:C8     | 2.42                     | 0.55              |
| 5:Z2:1232:G:OP1   | 12:E9:43:ARG:NH1  | 2.39                     | 0.55              |
| 5:Z2:2206:G:OP1   | 50:Cl:171:TYR:OH  | 2.22                     | 0.55              |
| 7:A4:8:LYS:H      | 7:A4:8:LYS:HD3    | 1.71                     | 0.55              |
| 26:iN:780:C:H2'   | 26:iN:781:U:H6    | 1.72                     | 0.55              |
| 43:Je:7:MET:HE1   | 43:Je:44:LYS:HG3  | 1.89                     | 0.55              |
| 5:Z2:1447:A:H2'   | 5:Z2:1448:G:C8    | 2.42                     | 0.55              |
| 5:Z2:2814:G:N2    | 5:Z2:2833:U:O2    | 2.39                     | 0.55              |
| 16:WD:6:GLN:HB3   | 16:WD:71:LEU:HD11 | 1.89                     | 0.55              |
| 26:iN:103:U:H2'   | 26:iN:104:G:C8    | 2.42                     | 0.55              |
| 26:iN:622:G:H2'   | 26:iN:623:C:C6    | 2.42                     | 0.55              |
| 26:iN:780:C:H2'   | 26:iN:781:U:C6    | 2.41                     | 0.55              |
| 4:H:110:ASP:C     | 4:H:113:MET:HE3   | 2.31                     | 0.54              |
| 7:A4:122:LEU:HD23 | 7:A4:146:MET:HB2  | 1.88                     | 0.54              |
| 3:F:63:ILE:HG21   | 3:F:77:ILE:HG12   | 1.90                     | 0.54              |
| 5:Z2:216:A:N3     | 5:Z2:231:U:O2'    | 2.33                     | 0.54              |
| 5:Z2:624:U:H2'    | 5:Z2:625:C:C6     | 2.42                     | 0.54              |
| 5:Z2:932:C:H2'    | 5:Z2:933:G:H8     | 1.71                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2050:C:H2'    | 5:Z2:2051:C:C6     | 2.42                     | 0.54              |
| 13:aA:15:MET:O     | 13:aA:18:SER:OG    | 2.23                     | 0.54              |
| 26:iN:132:G:H1'    | 26:iN:133:C:C5     | 2.42                     | 0.54              |
| 32:CT:52:ILE:HG22  | 32:CT:70:THR:HB    | 1.88                     | 0.54              |
| 55:C1:8:ARG:HG2    | 55:C1:14:LYS:HA    | 1.90                     | 0.54              |
| 5:Z2:1589:G:OP2    | 52:Sn:62:ASN:ND2   | 2.40                     | 0.54              |
| 26:iN:718:G:H21    | 33:KU:118:HIS:HB2  | 1.72                     | 0.54              |
| 26:iN:1496:U:H5''  | 26:iN:1497:C:H5    | 1.72                     | 0.54              |
| 40:Qb:78:ASN:HB2   | 40:Qb:83:TYR:HB3   | 1.89                     | 0.54              |
| 5:Z2:1453:A:H2'    | 5:Z2:1454:A:H8     | 1.71                     | 0.54              |
| 5:Z2:2564:G:N2     | 5:Z2:2564:G:OP2    | 2.35                     | 0.54              |
| 29:BQ:22:LYS:O     | 29:BQ:67:TYR:OH    | 2.19                     | 0.54              |
| 44:Af:26:THR:HG21  | 44:Af:196:ILE:HG12 | 1.89                     | 0.54              |
| 5:Z2:583:U:H2'     | 5:Z2:584:A:C8      | 2.43                     | 0.54              |
| 5:Z2:984:A:H2'     | 5:Z2:985:A:C8      | 2.42                     | 0.54              |
| 5:Z2:1555:G:OP2    | 50:Cl:83:TYR:OH    | 2.25                     | 0.54              |
| 5:Z2:2457:U:O2'    | 5:Z2:2458:C:OP1    | 2.25                     | 0.54              |
| 21:TI:33:LYS:HD2   | 21:TI:60:GLU:HG2   | 1.89                     | 0.54              |
| 26:iN:1324:A:H4'   | 26:iN:1326:U:H5    | 1.73                     | 0.54              |
| 51:Dm:179:ASP:OD1  | 51:Dm:179:ASP:N    | 2.40                     | 0.54              |
| 4:H:193:GLU:O      | 4:H:196:ASN:N      | 2.41                     | 0.54              |
| 5:Z2:976:C:H4'     | 40:Qb:74:ILE:HD13  | 1.90                     | 0.54              |
| 26:iN:103:U:H2'    | 26:iN:104:G:H8     | 1.73                     | 0.54              |
| 26:iN:352:A:O2'    | 26:iN:650:A:N1     | 2.40                     | 0.54              |
| 26:iN:517:G:P      | 48:Pj:76:ARG:HH12  | 2.30                     | 0.54              |
| 26:iN:656:C:H2'    | 26:iN:657:C:C6     | 2.43                     | 0.54              |
| 51:Dm:99:LEU:O     | 51:Dm:103:VAL:HG13 | 2.08                     | 0.54              |
| 26:iN:758:G:H2'    | 26:iN:759:A:C8     | 2.42                     | 0.54              |
| 1:B:285:ASP:HB3    | 1:B:288:ASP:HB2    | 1.89                     | 0.54              |
| 5:Z2:563:G:OP1     | 5:Z2:1239:U:O2'    | 2.18                     | 0.54              |
| 5:Z2:1780:A:H2'    | 5:Z2:1781:C:H6     | 1.70                     | 0.54              |
| 5:Z2:2229:G:H2'    | 5:Z2:2230:A:H8     | 1.73                     | 0.54              |
| 26:iN:696:U:O4     | 26:iN:796:G:O2'    | 2.22                     | 0.54              |
| 32:CT:140:ASN:HA   | 32:CT:143:ARG:HH12 | 1.72                     | 0.54              |
| 5:Z2:124:A:H5'     | 5:Z2:125:A:H8      | 1.73                     | 0.54              |
| 5:Z2:841:G:H2'     | 5:Z2:842:G:C8      | 2.42                     | 0.54              |
| 44:Af:5:LEU:HD13   | 44:Af:30:ILE:HD12  | 1.90                     | 0.54              |
| 5:Z2:2522:C:H5'    | 54:ep:3:VAL:HG21   | 1.90                     | 0.54              |
| 19:FG:23:GLU:HA    | 19:FG:26:ILE:HB    | 1.90                     | 0.54              |
| 32:CT:164:ARG:NH1  | 32:CT:166:GLU:OE2  | 2.41                     | 0.54              |
| 32:CT:188:ARG:HH21 | 32:CT:195:THR:HG21 | 1.73                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:dh:8:LYS:HG3   | 46:dh:61:MET:HG2   | 1.90                     | 0.54              |
| 1:B:94:MET:HE2    | 1:B:96:LEU:HB2     | 1.89                     | 0.53              |
| 8:E5:126:LYS:HE2  | 8:E5:126:LYS:HA    | 1.89                     | 0.53              |
| 12:E9:7:THR:OG1   | 12:E9:121:GLU:OE2  | 2.20                     | 0.53              |
| 25:MM:102:THR:OG1 | 26:iN:1270:A:OP1   | 2.22                     | 0.53              |
| 5:Z2:2036:C:H4'   | 44:Af:146:ILE:HD12 | 1.91                     | 0.53              |
| 20:VH:11:ARG:HH11 | 20:VH:14:ARG:HH11  | 1.55                     | 0.53              |
| 26:iN:389:G:OP1   | 47:Oi:41:ARG:NH1   | 2.38                     | 0.53              |
| 26:iN:1353:U:H2'  | 26:iN:1354:G:C8    | 2.43                     | 0.53              |
| 26:iN:1422:A:OP1  | 31:GS:93:ARG:NH2   | 2.31                     | 0.53              |
| 30:GR:170:ILE:H   | 30:GR:170:ILE:HD12 | 1.73                     | 0.53              |
| 5:Z2:660:A:N3     | 5:Z2:2426:U:O2'    | 2.37                     | 0.53              |
| 5:Z2:1581:A:H2'   | 5:Z2:1582:A:C8     | 2.43                     | 0.53              |
| 5:Z2:39:C:N4      | 5:Z2:430:A:OP2     | 2.41                     | 0.53              |
| 5:Z2:262:A:N1     | 5:Z2:410:U:O2'     | 2.37                     | 0.53              |
| 5:Z2:1286:A:OP2   | 5:Z2:1595:U:O2'    | 2.26                     | 0.53              |
| 5:Z2:2229:G:H2'   | 5:Z2:2230:A:C8     | 2.44                     | 0.53              |
| 5:Z2:2356:A:H2'   | 5:Z2:2357:C:C6     | 2.43                     | 0.53              |
| 5:Z2:2632:C:H2'   | 5:Z2:2633:U:H6     | 1.73                     | 0.53              |
| 23:HK:42:MET:SD   | 23:HK:43:ASP:N     | 2.82                     | 0.53              |
| 24:OL:63:ARG:NH1  | 24:OL:67:ASP:OD1   | 2.40                     | 0.53              |
| 25:MM:90:ARG:HB2  | 25:MM:97:VAL:HG12  | 1.90                     | 0.53              |
| 39:Ba:11:LYS:O    | 39:Ba:15:THR:HG22  | 2.09                     | 0.53              |
| 5:Z2:1293:G:H4'   | 39:Ba:7:PRO:HG2    | 1.91                     | 0.53              |
| 5:Z2:2457:U:HO2'  | 5:Z2:2458:C:P      | 2.32                     | 0.53              |
| 7:A4:70:ASN:ND2   | 7:A4:164:ASP:OD2   | 2.41                     | 0.53              |
| 26:iN:1020:G:OP2  | 26:iN:1403:U:O2'   | 2.25                     | 0.53              |
| 26:iN:1207:C:H2'  | 26:iN:1208:A:C8    | 2.42                     | 0.53              |
| 1:B:125:THR:HB    | 1:B:136:ILE:HB     | 1.90                     | 0.53              |
| 4:H:23:HIS:O      | 4:H:136:ASN:ND2    | 2.38                     | 0.53              |
| 5:Z2:1795:A:H2'   | 5:Z2:1796:A:C8     | 2.44                     | 0.53              |
| 5:Z2:2661:A:H2'   | 5:Z2:2662:A:C8     | 2.44                     | 0.53              |
| 8:E5:155:PRO:HG3  | 29:BQ:101:MET:HE2  | 1.89                     | 0.53              |
| 26:iN:1220:G:H2'  | 26:iN:1221:A:H8    | 1.73                     | 0.53              |
| 3:F:25:SER:OG     | 3:F:60:ASP:OD1     | 2.24                     | 0.53              |
| 5:Z2:178:A:H2'    | 5:Z2:179:A:C8      | 2.43                     | 0.53              |
| 21:TI:17:ASP:OD2  | 21:TI:38:ASN:N     | 2.32                     | 0.53              |
| 26:iN:962:A:H2'   | 26:iN:963:A:C8     | 2.43                     | 0.53              |
| 1:B:312:LYS:HB3   | 1:B:321:THR:HG23   | 1.90                     | 0.53              |
| 5:Z2:23:C:H5''    | 13:aA:14:ASP:HB2   | 1.90                     | 0.53              |
| 5:Z2:1426:U:H2'   | 5:Z2:1427:C:C6     | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Z2:1996:G:H5''  | 18:RF:42:LYS:HB2  | 1.90                     | 0.53              |
| 5:Z2:2573:A:H2'   | 5:Z2:2574:C:C6    | 2.44                     | 0.53              |
| 8:E5:93:ARG:NH2   | 8:E5:95:GLY:O     | 2.37                     | 0.53              |
| 19:FG:18:VAL:HG11 | 19:FG:58:HIS:HE1  | 1.73                     | 0.53              |
| 1:B:334:ALA:O     | 1:B:338:ILE:HG12  | 2.09                     | 0.53              |
| 1:B:353:PRO:HB2   | 1:B:356:MET:HE3   | 1.90                     | 0.53              |
| 4:H:117:ARG:HD2   | 4:H:157:LEU:HD21  | 1.91                     | 0.53              |
| 5:Z2:1794:A:H8    | 5:Z2:1794:A:OP1   | 1.92                     | 0.53              |
| 9:L6:8:ILE:HD12   | 38:QZ:44:LEU:HD21 | 1.91                     | 0.53              |
| 26:iN:1552:A:H2'  | 26:iN:1553:G:C8   | 2.43                     | 0.53              |
| 32:CT:33:LEU:O    | 32:CT:37:ILE:HG12 | 2.09                     | 0.53              |
| 1:B:23:THR:OG1    | 1:B:77:LEU:O      | 2.23                     | 0.53              |
| 5:Z2:397:C:H2'    | 5:Z2:398:A:C8     | 2.44                     | 0.53              |
| 5:Z2:2796:C:H5''  | 44:Af:57:ARG:NH1  | 2.23                     | 0.53              |
| 16:WD:3:ARG:HG3   | 16:WD:33:LEU:HD12 | 1.91                     | 0.53              |
| 24:OL:11:ILE:HG23 | 24:OL:26:VAL:HG21 | 1.90                     | 0.53              |
| 26:iN:1077:G:H2'  | 26:iN:1078:G:C8   | 2.44                     | 0.53              |
| 39:Ba:30:VAL:O    | 39:Ba:34:ARG:HG2  | 2.09                     | 0.53              |
| 4:H:197:ILE:HD12  | 4:H:197:ILE:H     | 1.74                     | 0.52              |
| 26:iN:81:C:H2'    | 26:iN:82:G:C8     | 2.44                     | 0.52              |
| 44:Af:33:ASN:HB2  | 44:Af:99:ILE:HB   | 1.91                     | 0.52              |
| 44:Af:56:ARG:HH21 | 44:Af:60:ARG:HG3  | 1.74                     | 0.52              |
| 50:Cl:123:PRO:HB2 | 50:Cl:125:ARG:HD3 | 1.91                     | 0.52              |
| 51:Dm:32:THR:C    | 51:Dm:34:LYS:H    | 2.17                     | 0.52              |
| 51:Dm:78:LYS:HB2  | 51:Dm:78:LYS:NZ   | 2.23                     | 0.52              |
| 5:Z2:867:G:H2'    | 5:Z2:868:G:C8     | 2.45                     | 0.52              |
| 10:F7:96:MET:HG3  | 10:F7:97:TYR:N    | 2.24                     | 0.52              |
| 5:Z2:2550:G:H2'   | 5:Z2:2551:A:C8    | 2.44                     | 0.52              |
| 18:RF:12:ILE:HD12 | 18:RF:42:LYS:HE2  | 1.89                     | 0.52              |
| 26:iN:135:U:H2'   | 26:iN:136:C:C6    | 2.44                     | 0.52              |
| 26:iN:1481:U:H2'  | 26:iN:1482:G:C8   | 2.44                     | 0.52              |
| 1:B:71:TYR:HE1    | 1:B:93:ARG:CZ     | 2.23                     | 0.52              |
| 7:A4:75:VAL:HB    | 7:A4:168:VAL:HG12 | 1.90                     | 0.52              |
| 8:E5:25:ARG:HD3   | 8:E5:36:PHE:HB3   | 1.91                     | 0.52              |
| 26:iN:123:G:H2'   | 26:iN:124:A:C8    | 2.44                     | 0.52              |
| 49:bk:5:ILE:HG21  | 49:bk:21:LYS:HD3  | 1.91                     | 0.52              |
| 1:B:62:ASP:N      | 1:B:62:ASP:OD1    | 2.42                     | 0.52              |
| 3:F:112:LYS:NZ    | 3:F:116:LEU:O     | 2.42                     | 0.52              |
| 5:Z2:289:A:H2'    | 5:Z2:290:G:H8     | 1.75                     | 0.52              |
| 5:Z2:1552:C:H2'   | 5:Z2:1553:C:C6    | 2.44                     | 0.52              |
| 6:R3:25:ASP:HB3   | 6:R3:28:LEU:HB3   | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:iN:1106:U:H2'   | 26:iN:1107:C:C6    | 2.44                     | 0.52              |
| 47:Oi:15:GLN:O     | 47:Oi:57:LEU:HD13  | 2.09                     | 0.52              |
| 5:Z2:1182:U:H2'    | 5:Z2:1183:U:C6     | 2.45                     | 0.52              |
| 5:Z2:2574:C:H2'    | 5:Z2:2575:G:H8     | 1.73                     | 0.52              |
| 23:HK:9:ARG:NH1    | 26:iN:1025:U:OP1   | 2.34                     | 0.52              |
| 26:iN:1283:A:H2    | 26:iN:1286:G:N3    | 2.08                     | 0.52              |
| 43:Je:86:LEU:HB2   | 43:Je:94:ILE:HD11  | 1.92                     | 0.52              |
| 5:Z2:1556:G:OP2    | 50:Cl:28:ARG:NH2   | 2.36                     | 0.52              |
| 26:iN:309:G:H3'    | 38:QZ:75:LYS:HB2   | 1.90                     | 0.52              |
| 26:iN:480:U:O2'    | 51:Dm:121:HIS:ND1  | 2.31                     | 0.52              |
| 26:iN:1163:C:H2'   | 26:iN:1164:C:H6    | 1.74                     | 0.52              |
| 39:Ba:18:PHE:HA    | 39:Ba:43:THR:HG21  | 1.92                     | 0.52              |
| 1:B:151:ASN:OD1    | 1:B:153:LYS:HG3    | 2.10                     | 0.52              |
| 9:L6:58:THR:OG1    | 26:iN:406:A:OP1    | 2.25                     | 0.52              |
| 26:iN:68:G:H2'     | 26:iN:69:G:C8      | 2.45                     | 0.52              |
| 26:iN:575:A:N6     | 26:iN:1251:G:O2'   | 2.43                     | 0.52              |
| 28:SP:66:MET:HG2   | 28:SP:74:PHE:CZ    | 2.45                     | 0.52              |
| 35:YW:38:GLU:HG3   | 35:YW:40:THR:HG23  | 1.92                     | 0.52              |
| 38:QZ:74:SER:OG    | 38:QZ:75:LYS:N     | 2.41                     | 0.52              |
| 5:Z2:1295:G:OP2    | 5:Z2:1295:G:N2     | 2.32                     | 0.52              |
| 12:E9:3:LEU:HD23   | 12:E9:13:LEU:HD12  | 1.91                     | 0.52              |
| 33:KU:120:GLY:H    | 34:NV:35:ARG:HH22  | 1.57                     | 0.52              |
| 51:Dm:177:TRP:CE2  | 51:Dm:193:PRO:HB3  | 2.45                     | 0.52              |
| 12:E9:122:GLU:HG2  | 12:E9:124:THR:HG23 | 1.91                     | 0.52              |
| 26:iN:597:A:H2'    | 26:iN:598:U:C6     | 2.45                     | 0.52              |
| 26:iN:1165:U:C2    | 26:iN:1166:U:C5    | 2.97                     | 0.52              |
| 45:Lg:39:ARG:HB3   | 45:Lg:99:PRO:HD3   | 1.91                     | 0.52              |
| 50:Cl:137:LEU:HD22 | 50:Cl:166:GLY:HA2  | 1.91                     | 0.52              |
| 3:F:40:GLU:OE1     | 3:F:43:ARG:NH1     | 2.43                     | 0.51              |
| 5:Z2:565:U:H2'     | 5:Z2:566:C:C6      | 2.45                     | 0.51              |
| 23:HK:9:ARG:HH21   | 26:iN:1262:C:P     | 2.33                     | 0.51              |
| 3:F:10:ARG:HG3     | 3:F:11:LYS:H       | 1.75                     | 0.51              |
| 3:F:65:VAL:HB      | 3:F:73:GLN:HG2     | 1.92                     | 0.51              |
| 5:Z2:932:C:H2'     | 5:Z2:933:G:C8      | 2.45                     | 0.51              |
| 5:Z2:2256:A:H2'    | 5:Z2:2257:A:C8     | 2.46                     | 0.51              |
| 11:D8:37:U:O2'     | 11:D8:44:A:N1      | 2.39                     | 0.51              |
| 26:iN:420:G:H5''   | 48:Pj:24:GLN:HG2   | 1.91                     | 0.51              |
| 26:iN:427:C:H2'    | 26:iN:428:C:H6     | 1.75                     | 0.51              |
| 37:JY:9:ARG:HB2    | 37:JY:99:GLN:HB2   | 1.91                     | 0.51              |
| 5:Z2:350:A:O2'     | 5:Z2:353:A:N1      | 2.41                     | 0.51              |
| 5:Z2:695:G:H2'     | 5:Z2:696:C:C6      | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:A4:28:TRP:CZ3    | 7:A4:30:PRO:HA     | 2.45                     | 0.51              |
| 26:iN:524:G:O2'    | 26:iN:526:C:N4     | 2.43                     | 0.51              |
| 26:iN:1377:A:H2'   | 26:iN:1378:A:C8    | 2.45                     | 0.51              |
| 32:CT:51:MET:HB3   | 32:CT:115:LEU:HD22 | 1.92                     | 0.51              |
| 47:Oi:30:VAL:HG22  | 47:Oi:86:ILE:HG12  | 1.91                     | 0.51              |
| 3:F:20:ALA:O       | 3:F:60:ASP:N       | 2.37                     | 0.51              |
| 5:Z2:334:A:H2'     | 5:Z2:335:C:C6      | 2.46                     | 0.51              |
| 11:D8:111:C:H2'    | 11:D8:112:A:H8     | 1.75                     | 0.51              |
| 20:VH:11:ARG:NH1   | 20:VH:14:ARG:HH11  | 2.09                     | 0.51              |
| 24:OL:23:SER:OG    | 24:OL:25:GLU:OE2   | 2.28                     | 0.51              |
| 26:iN:258:C:H2'    | 26:iN:259:U:C6     | 2.45                     | 0.51              |
| 38:QZ:64:LEU:HB2   | 38:QZ:86:GLU:HB3   | 1.93                     | 0.51              |
| 5:Z2:1670:G:H2'    | 5:Z2:1671:U:C6     | 2.45                     | 0.51              |
| 5:Z2:2274:U:H2'    | 5:Z2:2275:G:H8     | 1.73                     | 0.51              |
| 10:F7:145:LYS:H    | 10:F7:145:LYS:HD3  | 1.75                     | 0.51              |
| 12:E9:147:ILE:HB   | 12:E9:168:VAL:HG22 | 1.93                     | 0.51              |
| 25:MM:89:ILE:HA    | 25:MM:92:ARG:HD3   | 1.93                     | 0.51              |
| 26:iN:271:A:H4'    | 48:Pj:63:LYS:HD3   | 1.90                     | 0.51              |
| 26:iN:955:U:H2'    | 26:iN:956:C:C6     | 2.46                     | 0.51              |
| 26:iN:1481:U:H2'   | 26:iN:1482:G:H8    | 1.75                     | 0.51              |
| 26:iN:1576:A:O2'   | 26:iN:1577:U:OP1   | 2.29                     | 0.51              |
| 42:Kd:4:ARG:HB2    | 42:Kd:7:GLU:OE1    | 2.11                     | 0.51              |
| 1:B:41:LEU:HA      | 1:B:44:VAL:HG12    | 1.92                     | 0.51              |
| 4:H:181:GLY:HA2    | 4:H:188:GLN:NE2    | 2.26                     | 0.51              |
| 5:Z2:517:U:H2'     | 5:Z2:518:A:C8      | 2.46                     | 0.51              |
| 5:Z2:1250:G:O2'    | 5:Z2:1998:G:O6     | 2.28                     | 0.51              |
| 5:Z2:1422:U:H2'    | 5:Z2:1423:A:H8     | 1.75                     | 0.51              |
| 5:Z2:1592:C:O2'    | 5:Z2:1598:A:N1     | 2.39                     | 0.51              |
| 11:D8:34:C:H2'     | 11:D8:35:C:H6      | 1.75                     | 0.51              |
| 5:Z2:624:U:H2'     | 5:Z2:625:C:H6      | 1.76                     | 0.51              |
| 5:Z2:2060:U:H2'    | 5:Z2:2061:U:C6     | 2.45                     | 0.51              |
| 5:Z2:2573:A:H2'    | 5:Z2:2574:C:H6     | 1.75                     | 0.51              |
| 5:Z2:2683:A:H2'    | 5:Z2:2684:C:C6     | 2.46                     | 0.51              |
| 19:FG:9:LEU:HD11   | 19:FG:59:TYR:CZ    | 2.46                     | 0.51              |
| 21:TI:82:THR:HB    | 21:TI:96:ARG:HE    | 1.76                     | 0.51              |
| 5:Z2:739:C:O2'     | 5:Z2:1256:A:N1     | 2.43                     | 0.51              |
| 9:L6:4:THR:HG21    | 29:BQ:85:LEU:HD13  | 1.91                     | 0.51              |
| 10:F7:8:TYR:OH     | 10:F7:29:PRO:O     | 2.28                     | 0.51              |
| 10:F7:108:ILE:HG21 | 10:F7:176:PRO:HG2  | 1.92                     | 0.51              |
| 26:iN:1441:A:H4'   | 26:iN:1442:C:H5''  | 1.92                     | 0.51              |
| 37:JY:57:VAL:HG22  | 37:JY:58:ASN:H     | 1.75                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:Af:101:ALA:HB3 | 44:Af:185:VAL:HG22 | 1.93                     | 0.51              |
| 1:B:98:THR:OG1    | 1:B:101:ARG:NH1    | 2.44                     | 0.51              |
| 5:Z2:1300:A:H2'   | 5:Z2:1301:G:C8     | 2.45                     | 0.51              |
| 8:E5:97:SER:OG    | 8:E5:135:SER:O     | 2.27                     | 0.51              |
| 26:iN:582:A:H2'   | 26:iN:583:G:C8     | 2.46                     | 0.51              |
| 26:iN:717:A:H2'   | 26:iN:718:G:H8     | 1.73                     | 0.51              |
| 37:JY:72:ARG:HG2  | 37:JY:72:ARG:HH11  | 1.76                     | 0.51              |
| 51:Dm:158:GLU:OE1 | 51:Dm:158:GLU:N    | 2.41                     | 0.51              |
| 1:B:82:ILE:HG12   | 1:B:91:LEU:HD21    | 1.93                     | 0.51              |
| 3:F:26:ILE:HG21   | 3:F:33:LEU:HD12    | 1.93                     | 0.51              |
| 5:Z2:188:A:H2'    | 5:Z2:189:G:N3      | 2.26                     | 0.51              |
| 5:Z2:887:C:H2'    | 5:Z2:888:C:C6      | 2.46                     | 0.51              |
| 5:Z2:1166:A:H2'   | 5:Z2:1167:A:C8     | 2.46                     | 0.51              |
| 5:Z2:1171:G:H5''  | 40:Qb:83:TYR:CE1   | 2.46                     | 0.51              |
| 23:HK:53:ARG:HD2  | 26:iN:1362:C:N3    | 2.26                     | 0.51              |
| 26:iN:363:G:H2'   | 26:iN:364:A:O4'    | 2.11                     | 0.51              |
| 26:iN:433:U:H2'   | 26:iN:434:C:C6     | 2.46                     | 0.51              |
| 26:iN:1246:A:H4'  | 26:iN:1247:U:H5''  | 1.92                     | 0.51              |
| 5:Z2:185:G:H5'    | 16:WD:14:VAL:HG11  | 1.93                     | 0.50              |
| 5:Z2:421:G:H2'    | 5:Z2:422:A:C8      | 2.45                     | 0.50              |
| 5:Z2:642:U:H2'    | 5:Z2:643:U:C6      | 2.46                     | 0.50              |
| 5:Z2:1031:G:O2'   | 5:Z2:1094:G:N1     | 2.36                     | 0.50              |
| 5:Z2:2200:U:H2'   | 5:Z2:2201:A:H8     | 1.76                     | 0.50              |
| 9:L6:50:ARG:HB3   | 9:L6:66:TYR:HE1    | 1.75                     | 0.50              |
| 26:iN:279:A:H2'   | 26:iN:280:A:C8     | 2.46                     | 0.50              |
| 26:iN:989:G:C2    | 26:iN:990:A:C8     | 2.99                     | 0.50              |
| 5:Z2:37:G:H2'     | 5:Z2:38:C:C6       | 2.47                     | 0.50              |
| 5:Z2:2037:U:O2    | 5:Z2:2038:A:N6     | 2.40                     | 0.50              |
| 5:Z2:2580:G:H2'   | 5:Z2:2581:A:C8     | 2.45                     | 0.50              |
| 26:iN:1048:A:C4   | 26:iN:1070:G:H1'   | 2.45                     | 0.50              |
| 42:Kd:79:VAL:HG21 | 42:Kd:97:LEU:HD13  | 1.92                     | 0.50              |
| 44:Af:47:GLN:HB3  | 44:Af:90:LEU:HD11  | 1.92                     | 0.50              |
| 49:bk:34:LYS:HB2  | 49:bk:45:PHE:CD1   | 2.46                     | 0.50              |
| 51:Dm:8:LYS:HB3   | 51:Dm:21:LEU:HB3   | 1.93                     | 0.50              |
| 4:H:134:PHE:CE2   | 4:H:136:ASN:HB3    | 2.46                     | 0.50              |
| 5:Z2:380:U:OP2    | 16:WD:10:LYS:NZ    | 2.45                     | 0.50              |
| 5:Z2:724:A:H1'    | 5:Z2:725:C:H5      | 1.76                     | 0.50              |
| 25:MM:49:ASP:OD1  | 25:MM:50:ASP:N     | 2.44                     | 0.50              |
| 27:PO:74:LEU:HA   | 27:PO:78:ARG:HH21  | 1.76                     | 0.50              |
| 47:Oi:6:LEU:HD22  | 47:Oi:6:LEU:H      | 1.76                     | 0.50              |
| 1:B:55:ARG:O      | 1:B:59:THR:HG22    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2670:U:H2'   | 5:Z2:2671:G:O4'    | 2.11                     | 0.50              |
| 26:iN:136:C:O2'   | 26:iN:137:U:OP2    | 2.26                     | 0.50              |
| 26:iN:1046:A:N6   | 26:iN:1083:A:H61   | 2.09                     | 0.50              |
| 5:Z2:1378:U:H2'   | 5:Z2:1379:A:O4'    | 2.11                     | 0.50              |
| 5:Z2:1431:C:H2'   | 5:Z2:1432:U:C6     | 2.47                     | 0.50              |
| 26:iN:614:U:H5''  | 26:iN:863:A:C5     | 2.47                     | 0.50              |
| 26:iN:1189:G:N2   | 26:iN:1191:A:H62   | 2.10                     | 0.50              |
| 26:iN:1471:G:H2'  | 26:iN:1472:C:C6    | 2.45                     | 0.50              |
| 26:iN:1508:U:H2'  | 26:iN:1509:C:H6    | 1.76                     | 0.50              |
| 5:Z2:12:A:H2'     | 5:Z2:13:A:C8       | 2.47                     | 0.50              |
| 5:Z2:1413:G:H2'   | 5:Z2:1414:G:C8     | 2.47                     | 0.50              |
| 18:RF:81:THR:HG21 | 18:RF:97:SER:HB2   | 1.92                     | 0.50              |
| 26:iN:366:U:H2'   | 26:iN:367:G:O4'    | 2.12                     | 0.50              |
| 26:iN:503:U:H2'   | 26:iN:504:G:C8     | 2.47                     | 0.50              |
| 26:iN:1371:U:H2'  | 26:iN:1372:C:H6    | 1.76                     | 0.50              |
| 27:PO:83:MET:HE3  | 27:PO:113:ALA:HB2  | 1.94                     | 0.50              |
| 1:B:47:ARG:HH11   | 1:B:47:ARG:HG3     | 1.75                     | 0.50              |
| 5:Z2:245:G:O5'    | 5:Z2:246:C:H5''    | 2.11                     | 0.50              |
| 5:Z2:677:C:H5''   | 50:Cl:39:LYS:HB2   | 1.93                     | 0.50              |
| 5:Z2:932:C:H1'    | 5:Z2:968:A:C8      | 2.46                     | 0.50              |
| 5:Z2:977:G:OP1    | 27:PO:50:ARG:NH1   | 2.33                     | 0.50              |
| 5:Z2:1300:A:H2'   | 5:Z2:1301:G:H8     | 1.76                     | 0.50              |
| 5:Z2:1370:U:H2'   | 5:Z2:1371:U:C6     | 2.47                     | 0.50              |
| 10:F7:13:LYS:HG3  | 10:F7:28:VAL:HG11  | 1.93                     | 0.50              |
| 15:UC:82:ALA:HB3  | 15:UC:96:ASP:HB2   | 1.94                     | 0.50              |
| 26:iN:414:A:H2'   | 26:iN:415:C:O4'    | 2.12                     | 0.50              |
| 30:GR:143:GLN:HG3 | 30:GR:147:LYS:HD3  | 1.93                     | 0.50              |
| 37:JY:6:ILE:HG22  | 37:JY:102:LEU:HA   | 1.92                     | 0.50              |
| 43:Je:97:ARG:HB3  | 43:Je:97:ARG:NH1   | 2.27                     | 0.50              |
| 44:Af:46:TYR:OH   | 44:Af:82:GLU:OE2   | 2.28                     | 0.50              |
| 5:Z2:34:G:N2      | 5:Z2:495:G:H1'     | 2.27                     | 0.50              |
| 5:Z2:1918:A:H2'   | 5:Z2:1919:G:O4'    | 2.12                     | 0.50              |
| 5:Z2:2444:A:H2'   | 5:Z2:2445:C:C6     | 2.46                     | 0.50              |
| 9:L6:21:VAL:HG21  | 26:iN:596:A:H5''   | 1.94                     | 0.50              |
| 12:E9:21:GLU:HG3  | 12:E9:22:PHE:N     | 2.27                     | 0.50              |
| 26:iN:185:U:H2'   | 26:iN:186:A:C8     | 2.46                     | 0.50              |
| 41:Nc:32:THR:O    | 41:Nc:101:ARG:NH2  | 2.44                     | 0.50              |
| 1:B:312:LYS:HD2   | 1:B:330:VAL:HG12   | 1.94                     | 0.50              |
| 5:Z2:1580:A:H2'   | 5:Z2:1581:A:C8     | 2.47                     | 0.50              |
| 41:Nc:38:ALA:HB2  | 41:Nc:105:LEU:HD11 | 1.94                     | 0.50              |
| 5:Z2:402:U:H2'    | 5:Z2:403:C:C6      | 2.47                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:1602:A:C2    | 18:RF:93:ALA:HB2   | 2.47                     | 0.49              |
| 5:Z2:1785:G:H1'   | 50:Cl:154:MET:HE1  | 1.93                     | 0.49              |
| 21:TI:24:VAL:HG22 | 21:TI:34:VAL:HG22  | 1.94                     | 0.49              |
| 26:iN:495:A:H3'   | 26:iN:496:G:C5'    | 2.42                     | 0.49              |
| 26:iN:1558:A:H2'  | 26:iN:1559:G:H8    | 1.76                     | 0.49              |
| 51:Dm:118:LEU:O   | 51:Dm:123:THR:OG1  | 2.29                     | 0.49              |
| 5:Z2:1416:G:H2'   | 5:Z2:1417:A:C8     | 2.47                     | 0.49              |
| 5:Z2:1890:G:O2'   | 5:Z2:1914:A:N1     | 2.42                     | 0.49              |
| 5:Z2:2058:C:H2'   | 5:Z2:2059:C:H6     | 1.76                     | 0.49              |
| 5:Z2:2073:U:H2'   | 5:Z2:2074:A:H8     | 1.77                     | 0.49              |
| 5:Z2:2200:U:H2'   | 5:Z2:2201:A:C8     | 2.47                     | 0.49              |
| 7:A4:59:LEU:O     | 7:A4:63:ASN:ND2    | 2.44                     | 0.49              |
| 12:E9:170:ASP:OD1 | 12:E9:171:THR:N    | 2.45                     | 0.49              |
| 26:iN:139:G:H5''  | 26:iN:140:C:C5     | 2.47                     | 0.49              |
| 26:iN:520:C:H2'   | 26:iN:521:G:C4     | 2.46                     | 0.49              |
| 45:Lg:32:PHE:CE2  | 45:Lg:131:ILE:HG23 | 2.47                     | 0.49              |
| 5:Z2:197:U:H4'    | 16:WD:22:ASN:HB3   | 1.94                     | 0.49              |
| 5:Z2:1681:U:H5''  | 5:Z2:1682:C:C5     | 2.46                     | 0.49              |
| 5:Z2:2528:G:H2'   | 5:Z2:2529:U:O4'    | 2.12                     | 0.49              |
| 5:Z2:2771:C:H2'   | 5:Z2:2772:C:C6     | 2.47                     | 0.49              |
| 26:iN:88:G:H2'    | 26:iN:89:G:C8      | 2.47                     | 0.49              |
| 26:iN:371:C:H4'   | 26:iN:372:A:H5''   | 1.94                     | 0.49              |
| 26:iN:393:G:H2'   | 26:iN:394:G:C8     | 2.47                     | 0.49              |
| 1:B:212:ILE:HG22  | 1:B:219:ILE:HG22   | 1.94                     | 0.49              |
| 7:A4:127:GLU:HA   | 7:A4:127:GLU:OE1   | 2.12                     | 0.49              |
| 4:H:188:GLN:OE1   | 4:H:188:GLN:N      | 2.45                     | 0.49              |
| 5:Z2:10:U:H2'     | 5:Z2:11:C:C6       | 2.47                     | 0.49              |
| 5:Z2:867:G:H2'    | 5:Z2:868:G:H8      | 1.76                     | 0.49              |
| 5:Z2:2368:C:H2'   | 5:Z2:2369:U:C6     | 2.47                     | 0.49              |
| 5:Z2:2780:C:O2'   | 13:aA:26:GLU:OE1   | 2.24                     | 0.49              |
| 23:HK:75:ARG:HG2  | 26:iN:1302:A:N6    | 2.27                     | 0.49              |
| 26:iN:51:C:H4'    | 26:iN:52:U:OP2     | 2.13                     | 0.49              |
| 32:CT:15:VAL:HG11 | 32:CT:179:ARG:HA   | 1.94                     | 0.49              |
| 48:Pj:57:TYR:CZ   | 48:Pj:75:VAL:HG21  | 2.47                     | 0.49              |
| 5:Z2:10:U:H2'     | 5:Z2:11:C:H6       | 1.77                     | 0.49              |
| 5:Z2:71:G:H2'     | 5:Z2:72:C:C6       | 2.47                     | 0.49              |
| 12:E9:54:GLY:HA3  | 12:E9:73:ARG:HG2   | 1.94                     | 0.49              |
| 26:iN:287:U:O4    | 26:iN:950:A:H1'    | 2.12                     | 0.49              |
| 36:IX:15:TRP:HB3  | 36:IX:137:PRO:HB3  | 1.94                     | 0.49              |
| 36:IX:73:LYS:HE3  | 36:IX:88:ASN:HD21  | 1.78                     | 0.49              |
| 5:Z2:795:U:C4     | 42:Kd:31:LYS:O     | 2.66                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:1012:A:H61   | 5:Z2:1109:G:H2'    | 1.76                     | 0.49              |
| 5:Z2:1343:A:H2    | 5:Z2:1356:U:H3     | 1.61                     | 0.49              |
| 5:Z2:2196:A:O2'   | 5:Z2:2197:C:OP1    | 2.29                     | 0.49              |
| 5:Z2:2450:C:O2    | 45:Lg:124:LYS:NZ   | 2.32                     | 0.49              |
| 6:R3:61:GLN:NE2   | 26:iN:780:C:OP1    | 2.46                     | 0.49              |
| 26:iN:120:C:H2'   | 26:iN:121:A:C8     | 2.48                     | 0.49              |
| 26:iN:1296:G:H2'  | 26:iN:1297:A:C8    | 2.46                     | 0.49              |
| 5:Z2:584:A:H2'    | 5:Z2:585:G:H8      | 1.77                     | 0.49              |
| 26:iN:1164:C:H2'  | 26:iN:1165:U:H6    | 1.77                     | 0.49              |
| 55:C1:1:MET:HE3   | 55:C1:23:PRO:HA    | 1.93                     | 0.49              |
| 1:B:37:LEU:O      | 1:B:41:LEU:HG      | 2.12                     | 0.49              |
| 1:B:71:TYR:CE2    | 1:B:91:LEU:HD13    | 2.48                     | 0.49              |
| 1:B:205:GLU:OE2   | 1:B:205:GLU:N      | 2.45                     | 0.49              |
| 7:A4:84:ILE:H     | 7:A4:84:ILE:HD12   | 1.76                     | 0.49              |
| 26:iN:88:G:H2'    | 26:iN:89:G:H8      | 1.77                     | 0.49              |
| 26:iN:682:U:H2'   | 26:iN:683:G:H8     | 1.77                     | 0.49              |
| 26:iN:1457:C:H2'  | 26:iN:1458:A:C8    | 2.48                     | 0.49              |
| 5:Z2:463:A:O2'    | 21:TI:41:THR:O     | 2.30                     | 0.49              |
| 5:Z2:667:G:H5'    | 39:Ba:26:LYS:HG3   | 1.94                     | 0.49              |
| 5:Z2:834:A:H2'    | 5:Z2:835:C:C6      | 2.48                     | 0.49              |
| 5:Z2:868:G:H22    | 5:Z2:876:G:H22     | 1.61                     | 0.49              |
| 5:Z2:2610:G:N2    | 5:Z2:2760:G:OP2    | 2.44                     | 0.49              |
| 26:iN:567:G:H2'   | 26:iN:568:C:C6     | 2.47                     | 0.49              |
| 26:iN:1373:C:C2   | 26:iN:1374:A:C8    | 3.01                     | 0.49              |
| 42:Kd:82:SER:HB3  | 42:Kd:116:GLY:HA3  | 1.95                     | 0.49              |
| 50:Cl:94:LEU:HD11 | 50:Cl:104:ILE:HD13 | 1.94                     | 0.49              |
| 53:To:68:HIS:CE1  | 53:To:70:ASN:OD1   | 2.64                     | 0.49              |
| 1:B:296:GLY:O     | 1:B:368:ARG:NH1    | 2.41                     | 0.48              |
| 5:Z2:927:A:OP1    | 42:Kd:37:VAL:HG22  | 2.13                     | 0.48              |
| 5:Z2:1501:A:H3'   | 5:Z2:1502:G:H8     | 1.78                     | 0.48              |
| 5:Z2:2438:G:H2'   | 5:Z2:2439:C:C6     | 2.49                     | 0.48              |
| 6:R3:25:ASP:OD1   | 19:FG:101:GLN:NE2  | 2.35                     | 0.48              |
| 25:MM:85:CYS:SG   | 25:MM:88:GLY:N     | 2.86                     | 0.48              |
| 26:iN:736:U:O2'   | 26:iN:738:A:N7     | 2.36                     | 0.48              |
| 26:iN:1567:U:H2'  | 26:iN:1568:G:H8    | 1.78                     | 0.48              |
| 38:QZ:27:ILE:HG21 | 38:QZ:59:CYS:SG    | 2.53                     | 0.48              |
| 45:Lg:102:MET:HE2 | 45:Lg:102:MET:N    | 2.19                     | 0.48              |
| 51:Dm:59:LYS:HD3  | 51:Dm:210:LEU:HD23 | 1.94                     | 0.48              |
| 1:B:63:LYS:HB3    | 1:B:63:LYS:HE3     | 1.55                     | 0.48              |
| 4:H:312:TYR:CE2   | 4:H:314:LEU:HD23   | 2.48                     | 0.48              |
| 5:Z2:293:U:H2'    | 5:Z2:294:G:O4'     | 2.12                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z2:466:A:H5''    | 21:TI:45:LYS:HD2   | 1.95                     | 0.48              |
| 5:Z2:1480:A:N3     | 5:Z2:1565:C:O2'    | 2.39                     | 0.48              |
| 30:GR:107:VAL:HG23 | 30:GR:108:GLY:H    | 1.79                     | 0.48              |
| 47:Oi:2:SER:N      | 47:Oi:9:GLN:OE1    | 2.45                     | 0.48              |
| 51:Dm:106:MET:HG3  | 51:Dm:178:LEU:HD13 | 1.95                     | 0.48              |
| 5:Z2:943:A:H2'     | 5:Z2:944:A:C8      | 2.48                     | 0.48              |
| 5:Z2:1349:A:OP2    | 16:WD:2:SER:OG     | 2.31                     | 0.48              |
| 5:Z2:2196:A:H2'    | 5:Z2:2197:C:H6     | 1.78                     | 0.48              |
| 5:Z2:2428:G:OP1    | 12:E9:68:ARG:NH1   | 2.36                     | 0.48              |
| 11:D8:22:G:N7      | 11:D8:54:G:H2'     | 2.28                     | 0.48              |
| 53:To:51:TYR:CZ    | 53:To:55:ILE:HD11  | 2.48                     | 0.48              |
| 5:Z2:1460:U:H2'    | 5:Z2:1461:A:H8     | 1.79                     | 0.48              |
| 5:Z2:2073:U:H2'    | 5:Z2:2074:A:C8     | 2.47                     | 0.48              |
| 8:E5:34:ARG:HD3    | 26:iN:62:G:O2'     | 2.13                     | 0.48              |
| 19:FG:5:GLU:OE1    | 19:FG:92:ARG:NE    | 2.39                     | 0.48              |
| 26:iN:299:U:H2'    | 26:iN:300:G:C8     | 2.47                     | 0.48              |
| 26:iN:1046:A:H2'   | 26:iN:1047:G:C8    | 2.48                     | 0.48              |
| 26:iN:1295:A:H2'   | 26:iN:1296:G:C8    | 2.49                     | 0.48              |
| 26:iN:1372:C:H2'   | 26:iN:1373:C:H6    | 1.78                     | 0.48              |
| 38:QZ:74:SER:HB3   | 38:QZ:77:LYS:HB3   | 1.96                     | 0.48              |
| 5:Z2:158:U:H2'     | 5:Z2:159:U:C6      | 2.48                     | 0.48              |
| 5:Z2:625:C:H2'     | 5:Z2:626:U:C6      | 2.48                     | 0.48              |
| 5:Z2:633:G:H4'     | 5:Z2:2334:G:H5'    | 1.96                     | 0.48              |
| 5:Z2:1280:G:OP1    | 5:Z2:2692:G:O2'    | 2.24                     | 0.48              |
| 5:Z2:1855:G:H3'    | 5:Z2:1856:U:H5''   | 1.94                     | 0.48              |
| 10:F7:68:THR:N     | 10:F7:86:GLY:O     | 2.43                     | 0.48              |
| 20:VH:31:ILE:HD13  | 20:VH:61:ALA:HB2   | 1.96                     | 0.48              |
| 26:iN:427:C:H2'    | 26:iN:428:C:C6     | 2.48                     | 0.48              |
| 26:iN:1214:A:H2'   | 26:iN:1215:A:C8    | 2.48                     | 0.48              |
| 27:PO:109:LEU:HD22 | 40:Qb:40:MET:HE1   | 1.94                     | 0.48              |
| 28:SP:4:SER:HB2    | 28:SP:7:LYS:HG3    | 1.95                     | 0.48              |
| 44:Af:20:GLY:HA2   | 47:Oi:81:PRO:HG2   | 1.96                     | 0.48              |
| 3:F:10:ARG:CG      | 3:F:11:LYS:H       | 2.26                     | 0.48              |
| 26:iN:260:C:H2'    | 26:iN:261:U:C6     | 2.49                     | 0.48              |
| 37:JY:52:LEU:H     | 37:JY:52:LEU:HD12  | 1.78                     | 0.48              |
| 50:Cl:232:HIS:NE2  | 50:Cl:244:PRO:HA   | 2.29                     | 0.48              |
| 5:Z2:769:G:H5'     | 5:Z2:770:G:OP1     | 2.14                     | 0.48              |
| 5:Z2:837:A:H2'     | 5:Z2:838:U:C6      | 2.48                     | 0.48              |
| 5:Z2:1940:G:O2'    | 5:Z2:1942:U:O4     | 2.31                     | 0.48              |
| 6:R3:38:LYS:HG2    | 26:iN:762:A:C2     | 2.49                     | 0.48              |
| 7:A4:84:ILE:HG21   | 7:A4:216:SER:HA    | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:OL:11:ILE:O    | 24:OL:15:GLN:HG2  | 2.14                     | 0.48              |
| 26:iN:1452:C:H2'  | 26:iN:1453:A:H8   | 1.78                     | 0.48              |
| 53:To:79:LEU:O    | 53:To:83:ILE:HG13 | 2.14                     | 0.48              |
| 3:F:82:THR:HG23   | 3:F:96:LEU:HD23   | 1.95                     | 0.48              |
| 4:H:291:ARG:NH1   | 4:H:337:THR:O     | 2.46                     | 0.48              |
| 5:Z2:242:G:O2'    | 5:Z2:367:A:N1     | 2.44                     | 0.48              |
| 5:Z2:459:G:H4'    | 5:Z2:485:A:N1     | 2.29                     | 0.48              |
| 8:E5:111:ILE:HG13 | 8:E5:111:ILE:O    | 2.13                     | 0.48              |
| 8:E5:120:LEU:HD13 | 8:E5:128:VAL:HG11 | 1.96                     | 0.48              |
| 11:D8:18:G:H2'    | 11:D8:19:A:H8     | 1.79                     | 0.48              |
| 11:D8:113:G:H2'   | 11:D8:114:C:C6    | 2.49                     | 0.48              |
| 26:iN:395:C:H4'   | 26:iN:397:G:OP1   | 2.14                     | 0.48              |
| 42:Kd:98:LYS:NZ   | 42:Kd:107:MET:O   | 2.45                     | 0.48              |
| 4:H:371:MET:HE2   | 4:H:371:MET:HB3   | 1.75                     | 0.48              |
| 5:Z2:798:U:H2'    | 5:Z2:799:C:H6     | 1.77                     | 0.48              |
| 5:Z2:1165:C:H2'   | 5:Z2:1166:A:C8    | 2.48                     | 0.48              |
| 5:Z2:2207:G:H4'   | 5:Z2:2209:C:C2    | 2.48                     | 0.48              |
| 9:L6:46:ASN:ND2   | 9:L6:89:ASP:OD2   | 2.41                     | 0.48              |
| 11:D8:18:G:H2'    | 11:D8:19:A:C8     | 2.49                     | 0.48              |
| 26:iN:289:A:C2    | 26:iN:325:A:C5    | 3.02                     | 0.48              |
| 28:SP:39:MET:HE3  | 28:SP:68:GLY:HA2  | 1.94                     | 0.48              |
| 1:B:301:LEU:HG    | 1:B:303:VAL:HG22  | 1.95                     | 0.48              |
| 5:Z2:2194:U:H3    | 5:Z2:2199:A:H61   | 1.61                     | 0.48              |
| 8:E5:109:GLY:H    | 8:E5:127:ASP:HB3  | 1.79                     | 0.48              |
| 11:D8:111:C:H2'   | 11:D8:112:A:C8    | 2.49                     | 0.48              |
| 26:iN:401:U:H2'   | 26:iN:402:G:C8    | 2.48                     | 0.48              |
| 26:iN:982:A:N3    | 26:iN:1421:U:O2'  | 2.37                     | 0.48              |
| 44:Af:15:VAL:HG13 | 47:Oi:15:GLN:HE22 | 1.79                     | 0.48              |
| 5:Z2:1850:U:OP1   | 5:Z2:2393:G:O2'   | 2.25                     | 0.47              |
| 8:E5:77:ILE:HD13  | 8:E5:150:ARG:HB2  | 1.96                     | 0.47              |
| 23:HK:71:HIS:ND1  | 26:iN:1020:G:OP1  | 2.38                     | 0.47              |
| 24:OL:4:ASN:OD1   | 24:OL:7:ARG:NH2   | 2.47                     | 0.47              |
| 26:iN:605:U:H5'   | 26:iN:606:A:C5    | 2.49                     | 0.47              |
| 26:iN:1017:G:OP1  | 37:JY:59:LYS:HD2  | 2.14                     | 0.47              |
| 26:iN:1162:U:H1'  | 26:iN:1224:A:C4   | 2.49                     | 0.47              |
| 26:iN:1264:A:H2'  | 26:iN:1265:G:C8   | 2.49                     | 0.47              |
| 40:Qb:82:HIS:CD2  | 42:Kd:25:ILE:HG12 | 2.49                     | 0.47              |
| 54:ep:9:LYS:HE3   | 54:ep:16:VAL:HG23 | 1.96                     | 0.47              |
| 3:F:49:PRO:HD3    | 3:F:78:ARG:HG3    | 1.95                     | 0.47              |
| 4:H:166:ASP:OD1   | 4:H:167:ASP:N     | 2.47                     | 0.47              |
| 5:Z2:1086:C:H2'   | 5:Z2:1087:A:H8    | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Z2:1253:A:H2'   | 5:Z2:1254:C:C6    | 2.49                     | 0.47              |
| 5:Z2:1698:G:H4'   | 5:Z2:2824:C:O2    | 2.14                     | 0.47              |
| 5:Z2:2261:A:OP2   | 20:VH:12:ASN:ND2  | 2.48                     | 0.47              |
| 5:Z2:2444:A:H1'   | 5:Z2:2475:U:C2    | 2.49                     | 0.47              |
| 5:Z2:2540:G:H2'   | 5:Z2:2541:C:C6    | 2.49                     | 0.47              |
| 6:R3:26:VAL:O     | 6:R3:30:LYS:HG2   | 2.14                     | 0.47              |
| 23:HK:39:GLU:HA   | 23:HK:42:MET:HE3  | 1.96                     | 0.47              |
| 26:iN:66:A:O2'    | 26:iN:615:A:N1    | 2.45                     | 0.47              |
| 26:iN:1026:U:H4'  | 26:iN:1027:A:O4'  | 2.14                     | 0.47              |
| 26:iN:1446:G:H2'  | 26:iN:1447:C:O4'  | 2.14                     | 0.47              |
| 26:iN:1549:G:OP1  | 26:iN:1552:A:H4'  | 2.14                     | 0.47              |
| 39:Ba:34:ARG:CZ   | 39:Ba:39:ARG:HD2  | 2.44                     | 0.47              |
| 50:Cl:199:GLU:OE1 | 50:Cl:199:GLU:N   | 2.45                     | 0.47              |
| 4:H:229:VAL:HG22  | 4:H:280:LEU:HG    | 1.95                     | 0.47              |
| 5:Z2:397:C:H2'    | 5:Z2:398:A:H8     | 1.79                     | 0.47              |
| 5:Z2:2023:U:H2'   | 5:Z2:2024:G:C8    | 2.49                     | 0.47              |
| 10:F7:26:MET:HG2  | 11:D8:55:A:C5     | 2.49                     | 0.47              |
| 22:fJ:48:ASP:OD1  | 22:fJ:49:ILE:N    | 2.48                     | 0.47              |
| 32:CT:9:GLY:HA2   | 32:CT:12:LEU:HG   | 1.97                     | 0.47              |
| 32:CT:66:ILE:H    | 32:CT:66:ILE:HD12 | 1.80                     | 0.47              |
| 5:Z2:564:G:O2'    | 5:Z2:2005:A:OP1   | 2.30                     | 0.47              |
| 5:Z2:2610:G:O2'   | 5:Z2:2764:A:N1    | 2.43                     | 0.47              |
| 23:HK:99:ALA:HB2  | 37:JY:66:GLU:HB3  | 1.96                     | 0.47              |
| 26:iN:380:G:H2'   | 26:iN:381:A:H8    | 1.78                     | 0.47              |
| 26:iN:686:A:N7    | 29:BQ:109:SER:HA  | 2.29                     | 0.47              |
| 26:iN:1080:A:H2'  | 26:iN:1081:U:C6   | 2.50                     | 0.47              |
| 47:Oi:36:GLU:OE2  | 47:Oi:41:ARG:NH2  | 2.44                     | 0.47              |
| 50:Cl:120:GLU:OE1 | 50:Cl:120:GLU:N   | 2.48                     | 0.47              |
| 4:H:102:ALA:HB3   | 4:H:131:ILE:HG12  | 1.96                     | 0.47              |
| 5:Z2:156:U:H2'    | 5:Z2:157:C:C6     | 2.50                     | 0.47              |
| 5:Z2:1791:A:N3    | 50:Cl:50:THR:HB   | 2.30                     | 0.47              |
| 5:Z2:1857:A:H2'   | 5:Z2:1858:A:C8    | 2.49                     | 0.47              |
| 5:Z2:2286:G:O2'   | 10:F7:121:ALA:O   | 2.32                     | 0.47              |
| 6:R3:73:ASN:O     | 6:R3:73:ASN:ND2   | 2.26                     | 0.47              |
| 11:D8:47:C:H2'    | 11:D8:48:A:C8     | 2.49                     | 0.47              |
| 11:D8:58:C:H2'    | 11:D8:59:A:H8     | 1.77                     | 0.47              |
| 26:iN:1435:U:H2'  | 26:iN:1436:U:C6   | 2.49                     | 0.47              |
| 41:Nc:31:ARG:HA   | 41:Nc:36:ILE:HA   | 1.97                     | 0.47              |
| 43:Je:4:VAL:HG13  | 43:Je:22:ILE:HA   | 1.95                     | 0.47              |
| 5:Z2:307:G:O2'    | 5:Z2:309:A:OP2    | 2.30                     | 0.47              |
| 5:Z2:674:A:H2'    | 5:Z2:675:U:C6     | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Z2:778:A:OP2    | 5:Z2:2057:A:O2'   | 2.30                     | 0.47              |
| 5:Z2:2372:G:H5''  | 5:Z2:2373:U:O4'   | 2.13                     | 0.47              |
| 5:Z2:2547:A:OP1   | 5:Z2:2631:G:O2'   | 2.27                     | 0.47              |
| 5:Z2:2683:A:H2'   | 5:Z2:2684:C:H6    | 1.80                     | 0.47              |
| 8:E5:137:ASN:ND2  | 26:iN:65:C:H5''   | 2.30                     | 0.47              |
| 9:L6:33:VAL:HG12  | 9:L6:77:HIS:HA    | 1.97                     | 0.47              |
| 9:L6:120:LYS:HE2  | 26:iN:83:C:OP1    | 2.14                     | 0.47              |
| 10:F7:115:ARG:HD2 | 25:MM:71:ARG:NH1  | 2.30                     | 0.47              |
| 14:MB:35:LYS:HB2  | 14:MB:112:TYR:CE1 | 2.50                     | 0.47              |
| 15:UC:41:GLU:N    | 15:UC:41:GLU:OE1  | 2.47                     | 0.47              |
| 26:iN:720:A:H2'   | 26:iN:721:U:H6    | 1.78                     | 0.47              |
| 30:GR:22:ARG:NH1  | 30:GR:38:HIS:O    | 2.47                     | 0.47              |
| 34:NV:21:ARG:HH12 | 34:NV:25:LYS:HE2  | 1.79                     | 0.47              |
| 37:JY:7:ARG:HG2   | 37:JY:101:ALA:HB2 | 1.95                     | 0.47              |
| 51:Dm:73:PHE:HE1  | 51:Dm:95:LEU:HD11 | 1.79                     | 0.47              |
| 52:Sn:48:LEU:HG   | 52:Sn:49:MET:HG2  | 1.96                     | 0.47              |
| 1:B:145:ALA:HB1   | 1:B:151:ASN:HD21  | 1.79                     | 0.47              |
| 5:Z2:169:C:HO2'   | 5:Z2:170:A:P      | 2.35                     | 0.47              |
| 5:Z2:286:A:N1     | 5:Z2:309:A:O2'    | 2.43                     | 0.47              |
| 5:Z2:345:A:O2'    | 5:Z2:346:A:H8     | 1.97                     | 0.47              |
| 5:Z2:567:A:H2'    | 5:Z2:568:G:C8     | 2.50                     | 0.47              |
| 5:Z2:792:U:OP2    | 42:Kd:43:ARG:NH2  | 2.48                     | 0.47              |
| 5:Z2:1672:A:H2'   | 5:Z2:1673:C:C6    | 2.50                     | 0.47              |
| 5:Z2:1927:C:O2'   | 5:Z2:1928:C:OP1   | 2.32                     | 0.47              |
| 5:Z2:2298:U:H2'   | 5:Z2:2299:U:C6    | 2.49                     | 0.47              |
| 10:F7:178:LYS:HD2 | 10:F7:178:LYS:C   | 2.40                     | 0.47              |
| 17:XE:18:LEU:HA   | 17:XE:53:LEU:HD13 | 1.96                     | 0.47              |
| 26:iN:367:G:N1    | 26:iN:370:A:OP2   | 2.47                     | 0.47              |
| 26:iN:432:A:H3'   | 26:iN:433:U:H6    | 1.80                     | 0.47              |
| 26:iN:642:C:H2'   | 26:iN:643:A:H8    | 1.80                     | 0.47              |
| 26:iN:721:U:O2    | 26:iN:821:A:O2'   | 2.32                     | 0.47              |
| 26:iN:1387:C:H2'  | 26:iN:1388:G:C8   | 2.50                     | 0.47              |
| 4:H:93:ILE:HD13   | 4:H:312:TYR:HB2   | 1.97                     | 0.47              |
| 5:Z2:1063:C:H2'   | 5:Z2:1064:C:H6    | 1.79                     | 0.47              |
| 8:E5:130:THR:O    | 26:iN:54:A:O2'    | 2.33                     | 0.47              |
| 8:E5:137:ASN:HD21 | 26:iN:65:C:H5''   | 1.80                     | 0.47              |
| 12:E9:110:GLU:O   | 12:E9:114:GLN:HG3 | 2.15                     | 0.47              |
| 27:PO:102:ASP:OD2 | 27:PO:105:THR:OG1 | 2.27                     | 0.47              |
| 36:IX:25:LEU:HA   | 36:IX:62:ILE:HD11 | 1.97                     | 0.47              |
| 5:Z2:849:G:H2'    | 5:Z2:850:C:C6     | 2.49                     | 0.47              |
| 5:Z2:1417:A:H2'   | 5:Z2:1418:A:H8    | 1.75                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z2:1558:A:H2'    | 5:Z2:1559:A:C8     | 2.50                     | 0.47              |
| 5:Z2:2261:A:H5''   | 20:VH:12:ASN:HD22  | 1.79                     | 0.47              |
| 5:Z2:2297:G:H1'    | 10:F7:155:THR:HG21 | 1.97                     | 0.47              |
| 8:E5:158:MET:HE2   | 29:BQ:98:LYS:HD2   | 1.97                     | 0.47              |
| 10:F7:34:ILE:HD11  | 10:F7:100:LEU:HD12 | 1.97                     | 0.47              |
| 23:HK:27:LEU:HD22  | 23:HK:48:LEU:HD13  | 1.95                     | 0.47              |
| 26:iN:447:G:OP2    | 51:Dm:116:ARG:NH2  | 2.44                     | 0.47              |
| 26:iN:570:G:O2'    | 26:iN:578:A:N1     | 2.39                     | 0.47              |
| 26:iN:1531:G:H2'   | 26:iN:1532:G:C8    | 2.50                     | 0.47              |
| 51:Dm:9:LEU:HD11   | 51:Dm:31:LYS:HG3   | 1.97                     | 0.47              |
| 51:Dm:159:GLN:HB3  | 51:Dm:162:ILE:HB   | 1.97                     | 0.47              |
| 4:H:145:GLU:HG2    | 4:H:146:LEU:HD22   | 1.96                     | 0.47              |
| 5:Z2:566:C:H2'     | 5:Z2:567:A:H8      | 1.79                     | 0.47              |
| 5:Z2:571:A:N1      | 5:Z2:794:G:O2'     | 2.38                     | 0.47              |
| 5:Z2:2024:G:H2'    | 5:Z2:2025:U:O4'    | 2.15                     | 0.47              |
| 5:Z2:2050:C:H2'    | 5:Z2:2051:C:H6     | 1.79                     | 0.47              |
| 5:Z2:2310:A:H2'    | 5:Z2:2311:A:C8     | 2.50                     | 0.47              |
| 5:Z2:2632:C:H2'    | 5:Z2:2633:U:C6     | 2.50                     | 0.47              |
| 25:MM:107:ARG:HE   | 25:MM:113:THR:HB   | 1.80                     | 0.47              |
| 26:iN:792:U:H2'    | 26:iN:793:A:C8     | 2.50                     | 0.47              |
| 26:iN:1459:U:H2'   | 26:iN:1460:G:H8    | 1.80                     | 0.47              |
| 5:Z2:91:A:C2       | 5:Z2:109:A:C5      | 3.04                     | 0.46              |
| 5:Z2:617:A:H2'     | 5:Z2:618:A:C8      | 2.50                     | 0.46              |
| 5:Z2:931:A:H2'     | 5:Z2:932:C:C6      | 2.50                     | 0.46              |
| 5:Z2:1899:A:C6     | 26:iN:1539:G:C8    | 3.03                     | 0.46              |
| 21:TI:39:ILE:HA    | 21:TI:60:GLU:HA    | 1.97                     | 0.46              |
| 26:iN:240:A:N3     | 26:iN:265:U:O2'    | 2.42                     | 0.46              |
| 26:iN:530:A:H2'    | 26:iN:531:G:O4'    | 2.15                     | 0.46              |
| 26:iN:624:G:N1     | 26:iN:803:A:OP2    | 2.36                     | 0.46              |
| 26:iN:651:A:H2'    | 26:iN:652:A:O4'    | 2.15                     | 0.46              |
| 26:iN:801:U:H2'    | 26:iN:802:G:O4'    | 2.14                     | 0.46              |
| 27:PO:109:LEU:HD13 | 40:Qb:49:ILE:HD13  | 1.96                     | 0.46              |
| 30:GR:46:GLU:HB2   | 30:GR:49:VAL:HG12  | 1.96                     | 0.46              |
| 51:Dm:58:GLU:HG2   | 51:Dm:206:LEU:HB2  | 1.95                     | 0.46              |
| 54:ep:2:LYS:HE2    | 54:ep:32:ARG:O     | 2.15                     | 0.46              |
| 4:H:221:PHE:HB2    | 4:H:229:VAL:HB     | 1.97                     | 0.46              |
| 5:Z2:34:G:H22      | 5:Z2:495:G:H1'     | 1.81                     | 0.46              |
| 5:Z2:91:A:N1       | 5:Z2:105:U:O2'     | 2.48                     | 0.46              |
| 5:Z2:2360:A:H2'    | 5:Z2:2361:A:C8     | 2.50                     | 0.46              |
| 26:iN:376:C:OP1    | 53:To:2:ALA:N      | 2.48                     | 0.46              |
| 51:Dm:68:VAL:HG23  | 51:Dm:73:PHE:HB2   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:254:VAL:HG12  | 1:B:258:VAL:HG23  | 1.96                     | 0.46              |
| 5:Z2:289:A:H2'    | 5:Z2:290:G:C8     | 2.50                     | 0.46              |
| 5:Z2:338:U:C2     | 5:Z2:339:A:C8     | 3.04                     | 0.46              |
| 5:Z2:2072:U:H2'   | 5:Z2:2073:U:C6    | 2.49                     | 0.46              |
| 11:D8:109:G:H2'   | 11:D8:110:U:C6    | 2.50                     | 0.46              |
| 23:HK:92:ASP:N    | 23:HK:92:ASP:OD1  | 2.48                     | 0.46              |
| 51:Dm:100:ASP:OD1 | 51:Dm:101:ASN:N   | 2.48                     | 0.46              |
| 5:Z2:1116:U:H5''  | 36:IX:84:ILE:HG12 | 1.96                     | 0.46              |
| 5:Z2:1418:A:H2'   | 5:Z2:1419:G:O4'   | 2.15                     | 0.46              |
| 5:Z2:1422:U:H2'   | 5:Z2:1423:A:C8    | 2.50                     | 0.46              |
| 26:iN:72:C:H2'    | 26:iN:73:A:C8     | 2.50                     | 0.46              |
| 42:Kd:60:TYR:O    | 46:dh:14:ARG:HD2  | 2.16                     | 0.46              |
| 4:H:263:MET:HB2   | 4:H:268:LEU:HD21  | 1.96                     | 0.46              |
| 5:Z2:224:A:C2     | 5:Z2:2390:A:H1'   | 2.50                     | 0.46              |
| 5:Z2:1208:U:H2'   | 5:Z2:1209:A:C8    | 2.50                     | 0.46              |
| 5:Z2:1392:U:H2'   | 5:Z2:1393:U:C6    | 2.49                     | 0.46              |
| 5:Z2:1839:A:H2'   | 5:Z2:1840:A:C8    | 2.50                     | 0.46              |
| 5:Z2:2728:C:O2    | 30:GR:139:GLN:NE2 | 2.44                     | 0.46              |
| 26:iN:823:C:H2'   | 26:iN:824:A:O4'   | 2.15                     | 0.46              |
| 29:BQ:18:GLN:HG2  | 29:BQ:65:LEU:HD13 | 1.96                     | 0.46              |
| 4:H:336:ARG:NH2   | 4:H:370:ALA:O     | 2.49                     | 0.46              |
| 5:Z2:379:G:H1'    | 16:WD:29:PHE:HB3  | 1.97                     | 0.46              |
| 5:Z2:400:C:H2'    | 5:Z2:401:C:C6     | 2.50                     | 0.46              |
| 5:Z2:2643:A:N7    | 30:GR:175:LYS:NZ  | 2.64                     | 0.46              |
| 24:OL:2:LEU:O     | 24:OL:7:ARG:NH1   | 2.49                     | 0.46              |
| 26:iN:135:U:H2'   | 26:iN:136:C:C5    | 2.50                     | 0.46              |
| 1:B:160:ILE:HD11  | 20:VH:3:HIS:HB3   | 1.97                     | 0.46              |
| 5:Z2:90:G:H1      | 5:Z2:108:G:HO2'   | 1.61                     | 0.46              |
| 5:Z2:637:U:O2'    | 5:Z2:638:C:OP1    | 2.26                     | 0.46              |
| 5:Z2:2051:C:H2'   | 5:Z2:2052:C:H6    | 1.80                     | 0.46              |
| 5:Z2:2288:U:C2    | 10:F7:151:GLY:HA3 | 2.50                     | 0.46              |
| 26:iN:644:G:H2'   | 26:iN:645:A:H8    | 1.80                     | 0.46              |
| 37:JY:84:VAL:O    | 37:JY:88:MET:HE1  | 2.16                     | 0.46              |
| 51:Dm:105:ARG:HA  | 51:Dm:105:ARG:HD2 | 1.76                     | 0.46              |
| 52:Sn:8:GLN:OE1   | 52:Sn:11:ARG:NH1  | 2.48                     | 0.46              |
| 1:B:332:ASP:OD1   | 1:B:332:ASP:N     | 2.43                     | 0.46              |
| 5:Z2:612:A:OP1    | 42:Kd:80:ARG:NE   | 2.36                     | 0.46              |
| 5:Z2:1265:G:H2'   | 5:Z2:1266:U:C6    | 2.51                     | 0.46              |
| 5:Z2:2766:A:H2'   | 5:Z2:2767:U:O2    | 2.16                     | 0.46              |
| 5:Z2:2786:A:O2'   | 5:Z2:2787:A:OP1   | 2.32                     | 0.46              |
| 20:VH:25:ILE:HG22 | 20:VH:67:VAL:HG11 | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:iN:912:C:H2'    | 26:iN:913:A:O4'    | 2.16                     | 0.46              |
| 26:iN:1049:A:OP2   | 26:iN:1068:G:N2    | 2.35                     | 0.46              |
| 26:iN:1261:A:H2'   | 26:iN:1262:C:H6    | 1.81                     | 0.46              |
| 45:Lg:32:PHE:HE2   | 45:Lg:131:ILE:HG23 | 1.81                     | 0.46              |
| 4:H:85:HIS:HB2     | 4:H:115:GLN:OE1    | 2.16                     | 0.46              |
| 4:H:103:ILE:HD11   | 4:H:198:LEU:HD11   | 1.97                     | 0.46              |
| 5:Z2:812:U:O2'     | 5:Z2:2054:U:C2     | 2.63                     | 0.46              |
| 5:Z2:866:G:C6      | 5:Z2:879:U:C4      | 3.04                     | 0.46              |
| 5:Z2:1629:A:H2'    | 5:Z2:1630:G:O4'    | 2.15                     | 0.46              |
| 13:aA:11:SER:O     | 13:aA:15:MET:HG3   | 2.15                     | 0.46              |
| 17:XE:26:PHE:CG    | 52:Sn:49:MET:HE1   | 2.51                     | 0.46              |
| 22:fJ:14:PHE:O     | 22:fJ:23:PHE:N     | 2.48                     | 0.46              |
| 26:iN:513:C:H2'    | 26:iN:514:C:C6     | 2.50                     | 0.46              |
| 26:iN:644:G:H2'    | 26:iN:645:A:C8     | 2.51                     | 0.46              |
| 36:IX:35:ARG:HB2   | 36:IX:54:ILE:HD11  | 1.98                     | 0.46              |
| 36:IX:80:TYR:CE2   | 44:Af:160:LYS:HG2  | 2.51                     | 0.46              |
| 36:IX:141:ASP:OD1  | 36:IX:141:ASP:N    | 2.49                     | 0.46              |
| 41:Nc:15:THR:O     | 41:Nc:19:ILE:HG12  | 2.15                     | 0.46              |
| 5:Z2:134:C:H2'     | 5:Z2:135:C:C6      | 2.51                     | 0.46              |
| 5:Z2:156:U:H2'     | 5:Z2:157:C:H6      | 1.81                     | 0.46              |
| 5:Z2:157:C:H2'     | 5:Z2:158:U:H6      | 1.82                     | 0.46              |
| 5:Z2:745:G:H2'     | 5:Z2:746:A:O4'     | 2.16                     | 0.46              |
| 5:Z2:971:C:H2'     | 5:Z2:972:A:O4'     | 2.16                     | 0.46              |
| 5:Z2:2598:U:H2'    | 5:Z2:2599:C:H6     | 1.81                     | 0.46              |
| 11:D8:46:U:H2'     | 11:D8:47:C:C6      | 2.51                     | 0.46              |
| 14:MB:103:ARG:HD2  | 14:MB:106:ASP:OD1  | 2.16                     | 0.46              |
| 17:XE:24:ASP:OD1   | 17:XE:27:ARG:NH2   | 2.42                     | 0.46              |
| 26:iN:228:G:C5     | 26:iN:229:A:C8     | 3.04                     | 0.46              |
| 26:iN:555:U:H2'    | 26:iN:556:C:C6     | 2.51                     | 0.46              |
| 26:iN:656:C:H2'    | 26:iN:657:C:H6     | 1.80                     | 0.46              |
| 26:iN:1360:U:O2'   | 26:iN:1405:A:N3    | 2.44                     | 0.46              |
| 26:iN:1383:G:H2'   | 26:iN:1384:A:C8    | 2.51                     | 0.46              |
| 27:PO:64:ARG:HD3   | 36:IX:42:THR:O     | 2.15                     | 0.46              |
| 37:JY:15:HIS:HB3   | 37:JY:70:HIS:CE1   | 2.51                     | 0.46              |
| 42:Kd:94:VAL:HG12  | 42:Kd:98:LYS:HE2   | 1.98                     | 0.46              |
| 43:Je:104:ARG:HH11 | 43:Je:107:ARG:HH21 | 1.64                     | 0.46              |
| 50:Cl:119:GLY:O    | 50:Cl:130:LEU:HD23 | 2.15                     | 0.46              |
| 55:C1:23:PRO:O     | 55:C1:27:ARG:HB3   | 2.16                     | 0.46              |
| 5:Z2:9:G:H2'       | 5:Z2:10:U:C6       | 2.51                     | 0.45              |
| 5:Z2:637:U:H2'     | 5:Z2:638:C:C6      | 2.52                     | 0.45              |
| 5:Z2:1337:A:H2'    | 5:Z2:1338:A:C8     | 2.51                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2000:A:H2'   | 5:Z2:2001:A:C8     | 2.51                     | 0.45              |
| 11:D8:85:U:H3'    | 11:D8:86:C:O2      | 2.15                     | 0.45              |
| 26:iN:213:A:H2'   | 26:iN:214:U:O4'    | 2.16                     | 0.45              |
| 26:iN:643:A:H2'   | 26:iN:644:G:H8     | 1.81                     | 0.45              |
| 44:Af:186:GLU:OE1 | 44:Af:186:GLU:N    | 2.49                     | 0.45              |
| 3:F:5:TYR:OH      | 26:iN:1192:C:O2'   | 2.31                     | 0.45              |
| 3:F:40:GLU:HG3    | 31:GS:16:PRO:HB2   | 1.98                     | 0.45              |
| 5:Z2:204:A:H2'    | 5:Z2:205:C:O4'     | 2.17                     | 0.45              |
| 5:Z2:660:A:O2'    | 12:E9:61:GLN:NE2   | 2.49                     | 0.45              |
| 5:Z2:714:G:C6     | 50:Cl:207:LYS:HB2  | 2.50                     | 0.45              |
| 5:Z2:1165:C:H2'   | 5:Z2:1166:A:H8     | 1.82                     | 0.45              |
| 5:Z2:2375:A:O2'   | 42:Kd:62:ARG:O     | 2.33                     | 0.45              |
| 5:Z2:2775:A:H2'   | 5:Z2:2776:A:C8     | 2.52                     | 0.45              |
| 5:Z2:2853:C:H2'   | 5:Z2:2854:U:C6     | 2.51                     | 0.45              |
| 12:E9:97:ARG:HD3  | 12:E9:101:ARG:HH21 | 1.82                     | 0.45              |
| 18:RF:37:THR:HG23 | 18:RF:38:TYR:CD2   | 2.51                     | 0.45              |
| 25:MM:51:ILE:HG13 | 25:MM:52:GLN:N     | 2.31                     | 0.45              |
| 26:iN:307:A:O2'   | 38:QZ:72:PRO:O     | 2.30                     | 0.45              |
| 26:iN:607:C:C4    | 38:QZ:39:LEU:HD11  | 2.52                     | 0.45              |
| 26:iN:682:U:H2'   | 26:iN:683:G:C8     | 2.50                     | 0.45              |
| 26:iN:716:U:H2'   | 26:iN:717:A:C8     | 2.51                     | 0.45              |
| 26:iN:1121:G:N2   | 26:iN:1124:A:OP2   | 2.47                     | 0.45              |
| 26:iN:1361:G:N2   | 26:iN:1363:A:H3'   | 2.31                     | 0.45              |
| 36:IX:8:PRO:O     | 36:IX:11:VAL:HG12  | 2.15                     | 0.45              |
| 5:Z2:9:G:O2'      | 5:Z2:10:U:OP1      | 2.30                     | 0.45              |
| 5:Z2:124:A:OP2    | 5:Z2:125:A:H2'     | 2.17                     | 0.45              |
| 5:Z2:659:G:O2'    | 12:E9:61:GLN:OE1   | 2.28                     | 0.45              |
| 5:Z2:1299:C:H2'   | 5:Z2:1300:A:H8     | 1.81                     | 0.45              |
| 5:Z2:1986:C:OP1   | 14:MB:5:LYS:NZ     | 2.45                     | 0.45              |
| 5:Z2:2347:C:H2'   | 5:Z2:2348:G:O4'    | 2.16                     | 0.45              |
| 5:Z2:2681:U:H2'   | 5:Z2:2682:C:C6     | 2.51                     | 0.45              |
| 10:F7:138:PHE:CE2 | 10:F7:152:MET:HE1  | 2.51                     | 0.45              |
| 23:HK:62:ASN:HD22 | 23:HK:62:ASN:C     | 2.23                     | 0.45              |
| 26:iN:751:U:H2'   | 26:iN:752:C:C6     | 2.52                     | 0.45              |
| 26:iN:1325:A:H5'  | 37:JY:43:PRO:HG2   | 1.99                     | 0.45              |
| 26:iN:1489:U:H2'  | 26:iN:1490:U:O4'   | 2.16                     | 0.45              |
| 29:BQ:55:GLU:H    | 29:BQ:55:GLU:CD    | 2.24                     | 0.45              |
| 30:GR:128:GLN:HG3 | 30:GR:129:THR:HG23 | 1.98                     | 0.45              |
| 37:JY:88:MET:SD   | 37:JY:88:MET:N     | 2.88                     | 0.45              |
| 41:Nc:98:TYR:CE2  | 41:Nc:103:LYS:HD2  | 2.52                     | 0.45              |
| 42:Kd:84:LEU:HD22 | 42:Kd:92:ILE:HD12  | 1.98                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:Af:181:ILE:HD11 | 44:Af:193:LYS:HB2 | 1.99                     | 0.45              |
| 51:Dm:178:LEU:HD23 | 51:Dm:189:PHE:HA  | 1.97                     | 0.45              |
| 54:ep:30:GLU:OE1   | 54:ep:32:ARG:HG2  | 2.16                     | 0.45              |
| 5:Z2:140:U:H2'     | 5:Z2:141:A:H8     | 1.81                     | 0.45              |
| 5:Z2:2005:A:H4'    | 27:PO:34:VAL:HG21 | 1.99                     | 0.45              |
| 5:Z2:2312:A:H2'    | 5:Z2:2313:G:C8    | 2.51                     | 0.45              |
| 5:Z2:2497:U:H2'    | 5:Z2:2498:C:C6    | 2.52                     | 0.45              |
| 6:R3:27:GLU:OE1    | 6:R3:27:GLU:N     | 2.47                     | 0.45              |
| 19:FG:25:TYR:OH    | 19:FG:81:ASN:ND2  | 2.50                     | 0.45              |
| 20:VH:19:LYS:HD3   | 20:VH:19:LYS:HA   | 1.75                     | 0.45              |
| 26:iN:266:A:H2'    | 26:iN:267:U:O4'   | 2.16                     | 0.45              |
| 26:iN:791:A:H2'    | 26:iN:792:U:C6    | 2.52                     | 0.45              |
| 26:iN:991:G:H2'    | 26:iN:992:C:C6    | 2.52                     | 0.45              |
| 26:iN:1084:G:H1'   | 26:iN:1085:A:OP1  | 2.17                     | 0.45              |
| 26:iN:1312:C:O2    | 26:iN:1372:C:H4'  | 2.17                     | 0.45              |
| 26:iN:1361:G:N2    | 26:iN:1364:A:OP2  | 2.44                     | 0.45              |
| 52:Sn:58:VAL:HG22  | 52:Sn:85:VAL:HG12 | 1.98                     | 0.45              |
| 5:Z2:665:G:H2'     | 5:Z2:666:A:C8     | 2.52                     | 0.45              |
| 5:Z2:1183:U:H1'    | 27:PO:4:VAL:HG22  | 1.99                     | 0.45              |
| 5:Z2:2426:U:OP1    | 12:E9:62:LYS:HD3  | 2.16                     | 0.45              |
| 5:Z2:2800:G:H2'    | 5:Z2:2845:A:H61   | 1.81                     | 0.45              |
| 6:R3:32:TYR:HB3    | 6:R3:55:LEU:HD21  | 1.97                     | 0.45              |
| 7:A4:170:ASP:OD2   | 7:A4:173:HIS:HB2  | 2.17                     | 0.45              |
| 26:iN:588:C:H5'    | 51:Dm:70:GLU:CB   | 2.46                     | 0.45              |
| 26:iN:1045:U:O4    | 26:iN:1046:A:N6   | 2.48                     | 0.45              |
| 32:CT:175:LEU:HD21 | 32:CT:201:TRP:CD1 | 2.51                     | 0.45              |
| 34:NV:6:VAL:HG23   | 34:NV:10:GLU:HG2  | 1.98                     | 0.45              |
| 37:JY:28:THR:HG21  | 37:JY:90:LEU:HD22 | 1.99                     | 0.45              |
| 50:Cl:33:LEU:HD21  | 50:Cl:102:ARG:HA  | 1.97                     | 0.45              |
| 5:Z2:1064:C:H2'    | 5:Z2:1065:U:H6    | 1.81                     | 0.45              |
| 5:Z2:1266:U:H2'    | 5:Z2:1267:G:O4'   | 2.16                     | 0.45              |
| 5:Z2:2224:A:H2'    | 5:Z2:2225:G:C8    | 2.51                     | 0.45              |
| 5:Z2:2812:G:H2'    | 5:Z2:2813:U:C6    | 2.51                     | 0.45              |
| 9:L6:82:ILE:HG23   | 9:L6:95:TYR:HB3   | 1.99                     | 0.45              |
| 22:fJ:3:LYS:O      | 22:fJ:5:ILE:HG23  | 2.16                     | 0.45              |
| 30:GR:86:ARG:HH11  | 30:GR:86:ARG:HG2  | 1.81                     | 0.45              |
| 38:QZ:63:ASP:N     | 38:QZ:63:ASP:OD2  | 2.49                     | 0.45              |
| 44:Af:149:THR:HA   | 44:Af:162:LYS:HE3 | 1.98                     | 0.45              |
| 53:To:29:ARG:O     | 53:To:33:LYS:HG2  | 2.15                     | 0.45              |
| 5:Z2:428:C:H2'     | 5:Z2:429:G:O4'    | 2.16                     | 0.45              |
| 5:Z2:562:G:H2'     | 5:Z2:563:G:C8     | 2.51                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2230:A:H2'   | 5:Z2:2231:C:H6     | 1.82                     | 0.45              |
| 5:Z2:2806:C:H2'   | 5:Z2:2807:A:H8     | 1.82                     | 0.45              |
| 5:Z2:2813:U:H2'   | 5:Z2:2814:G:O4'    | 2.17                     | 0.45              |
| 11:D8:112:A:H2'   | 11:D8:113:G:H8     | 1.82                     | 0.45              |
| 12:E9:116:ARG:NH1 | 42:Kd:3:LEU:O      | 2.43                     | 0.45              |
| 26:iN:1366:U:O3'  | 28:SP:78:ARG:NH2   | 2.49                     | 0.45              |
| 27:PO:48:ARG:NH2  | 27:PO:49:ASP:OD1   | 2.48                     | 0.45              |
| 30:GR:152:ARG:HB3 | 30:GR:162:ILE:HD12 | 1.98                     | 0.45              |
| 33:KU:87:LYS:HE2  | 33:KU:115:PRO:HD3  | 1.99                     | 0.45              |
| 1:B:47:ARG:HG3    | 1:B:47:ARG:NH1     | 2.31                     | 0.45              |
| 5:Z2:521:A:H2'    | 5:Z2:522:G:O4'     | 2.17                     | 0.45              |
| 5:Z2:732:U:O2     | 5:Z2:2000:A:H1'    | 2.17                     | 0.45              |
| 5:Z2:2081:A:H2'   | 5:Z2:2082:C:C6     | 2.52                     | 0.45              |
| 5:Z2:2531:U:H2'   | 5:Z2:2532:G:O4'    | 2.17                     | 0.45              |
| 5:Z2:2754:C:H2'   | 5:Z2:2755:C:C6     | 2.51                     | 0.45              |
| 7:A4:29:ASN:O     | 7:A4:32:MET:HB2    | 2.17                     | 0.45              |
| 7:A4:106:LEU:HD13 | 7:A4:186:ILE:HD11  | 1.99                     | 0.45              |
| 23:HK:76:LYS:HE2  | 37:JY:67:ILE:HD13  | 1.98                     | 0.45              |
| 32:CT:51:MET:HB2  | 32:CT:51:MET:HE2   | 1.82                     | 0.45              |
| 33:KU:24:HIS:HA   | 33:KU:87:LYS:HG2   | 1.99                     | 0.45              |
| 1:B:290:TYR:HA    | 1:B:338:ILE:HD12   | 1.98                     | 0.45              |
| 4:H:240:LYS:N     | 4:H:243:ASP:OD2    | 2.48                     | 0.45              |
| 5:Z2:315:U:H4'    | 21:TI:64:HIS:CD2   | 2.52                     | 0.45              |
| 5:Z2:800:C:OP2    | 40:Qb:85:LYS:HD2   | 2.16                     | 0.45              |
| 5:Z2:1384:A:H2'   | 5:Z2:1385:A:C8     | 2.52                     | 0.45              |
| 26:iN:133:C:H2'   | 26:iN:134:U:O4'    | 2.16                     | 0.45              |
| 26:iN:265:U:H2'   | 26:iN:266:A:C8     | 2.52                     | 0.45              |
| 26:iN:860:A:OP1   | 26:iN:1571:G:O2'   | 2.33                     | 0.45              |
| 32:CT:140:ASN:HA  | 32:CT:143:ARG:NH1  | 2.31                     | 0.45              |
| 50:Cl:109:LYS:HB3 | 50:Cl:126:PRO:HG2  | 1.99                     | 0.45              |
| 5:Z2:1776:C:H2'   | 5:Z2:1777:A:C5     | 2.52                     | 0.45              |
| 7:A4:30:PRO:HG2   | 26:iN:872:A:N3     | 2.31                     | 0.45              |
| 18:RF:29:ILE:HD11 | 18:RF:55:ILE:HG23  | 1.99                     | 0.45              |
| 26:iN:207:A:C5    | 26:iN:208:C:H1'    | 2.51                     | 0.45              |
| 26:iN:450:U:H2'   | 26:iN:451:G:H8     | 1.82                     | 0.45              |
| 43:Je:100:GLY:O   | 43:Je:119:PRO:HD2  | 2.17                     | 0.45              |
| 2:D:75:VAL:O      | 2:D:79:THR:HG22    | 2.17                     | 0.44              |
| 4:H:312:TYR:HE2   | 4:H:314:LEU:HD23   | 1.80                     | 0.44              |
| 5:Z2:584:A:H2'    | 5:Z2:585:G:C8      | 2.52                     | 0.44              |
| 5:Z2:817:U:H2'    | 5:Z2:818:A:C8      | 2.52                     | 0.44              |
| 19:FG:49:TYR:OH   | 19:FG:86:ARG:NH1   | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:HK:76:LYS:NZ   | 37:JY:47:GLU:OE1  | 2.29                     | 0.44              |
| 26:iN:298:G:H2'   | 26:iN:299:U:C6    | 2.53                     | 0.44              |
| 26:iN:1324:A:H4'  | 26:iN:1326:U:C5   | 2.53                     | 0.44              |
| 43:Je:8:LEU:HD22  | 43:Je:84:ALA:HB2  | 2.00                     | 0.44              |
| 52:Sn:88:LYS:HE3  | 52:Sn:88:LYS:HB3  | 1.67                     | 0.44              |
| 3:F:55:SER:O      | 3:F:55:SER:OG     | 2.32                     | 0.44              |
| 5:Z2:511:A:H5'    | 36:IX:113:PRO:HG3 | 2.00                     | 0.44              |
| 5:Z2:1063:C:H2'   | 5:Z2:1064:C:C6    | 2.51                     | 0.44              |
| 5:Z2:1394:U:H2'   | 5:Z2:1395:A:H8    | 1.83                     | 0.44              |
| 5:Z2:1866:U:H2'   | 5:Z2:1867:C:C6    | 2.53                     | 0.44              |
| 5:Z2:2197:C:H2'   | 5:Z2:2198:A:O4'   | 2.17                     | 0.44              |
| 10:F7:152:MET:HE2 | 10:F7:152:MET:HB3 | 1.66                     | 0.44              |
| 10:F7:159:SER:O   | 10:F7:159:SER:OG  | 2.28                     | 0.44              |
| 12:E9:155:ASN:OD1 | 12:E9:155:ASN:C   | 2.60                     | 0.44              |
| 26:iN:210:C:H2'   | 26:iN:211:G:H8    | 1.83                     | 0.44              |
| 42:Kd:91:VAL:O    | 42:Kd:96:THR:HG21 | 2.18                     | 0.44              |
| 5:Z2:312:A:H2'    | 5:Z2:313:G:C8     | 2.53                     | 0.44              |
| 5:Z2:448:G:H2'    | 5:Z2:449:A:C8     | 2.53                     | 0.44              |
| 5:Z2:727:G:H2'    | 5:Z2:728:U:H6     | 1.81                     | 0.44              |
| 5:Z2:847:G:H2'    | 5:Z2:848:A:O4'    | 2.17                     | 0.44              |
| 5:Z2:1802:C:H3'   | 50:Cl:62:TYR:CE1  | 2.52                     | 0.44              |
| 5:Z2:2184:A:C2    | 55:C1:29:PHE:HB2  | 2.53                     | 0.44              |
| 11:D8:30:U:C2     | 11:D8:31:G:C8     | 3.06                     | 0.44              |
| 19:FG:50:PRO:HB3  | 19:FG:55:HIS:CE1  | 2.52                     | 0.44              |
| 24:OL:74:LEU:O    | 24:OL:78:THR:HG23 | 2.17                     | 0.44              |
| 26:iN:1360:U:H2'  | 26:iN:1361:G:C8   | 2.52                     | 0.44              |
| 26:iN:1480:G:H2'  | 26:iN:1481:U:C6   | 2.52                     | 0.44              |
| 40:Qb:61:VAL:HG21 | 40:Qb:96:LEU:HD13 | 1.99                     | 0.44              |
| 45:Lg:27:VAL:HG13 | 45:Lg:105:GLU:HG2 | 1.99                     | 0.44              |
| 52:Sn:56:LEU:HD21 | 52:Sn:88:LYS:HG2  | 1.99                     | 0.44              |
| 5:Z2:341:C:H2'    | 5:Z2:342:G:C8     | 2.52                     | 0.44              |
| 5:Z2:398:A:H2'    | 5:Z2:399:U:C6     | 2.53                     | 0.44              |
| 5:Z2:574:U:H2'    | 5:Z2:575:A:C8     | 2.52                     | 0.44              |
| 5:Z2:1425:G:H2'   | 5:Z2:1426:U:C6    | 2.52                     | 0.44              |
| 5:Z2:1551:U:H2'   | 5:Z2:1552:C:C6    | 2.51                     | 0.44              |
| 8:E5:43:VAL:HG11  | 8:E5:119:VAL:HA   | 1.99                     | 0.44              |
| 9:L6:79:VAL:O     | 9:L6:103:ASP:HB2  | 2.17                     | 0.44              |
| 10:F7:123:ASP:OD2 | 10:F7:127:ASN:HB2 | 2.18                     | 0.44              |
| 11:D8:95:G:H1     | 15:UC:20:LYS:HB2  | 1.82                     | 0.44              |
| 12:E9:4:LYS:HD3   | 12:E9:4:LYS:HA    | 1.62                     | 0.44              |
| 18:RF:20:VAL:HG11 | 18:RF:44:ALA:HA   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:iN:587:G:OP1   | 51:Dm:60:GLN:HG3   | 2.17                     | 0.44              |
| 26:iN:990:A:O2'   | 26:iN:1378:A:N3    | 2.42                     | 0.44              |
| 26:iN:1002:A:C5   | 28:SP:55:ARG:HG3   | 2.53                     | 0.44              |
| 26:iN:1085:A:C8   | 26:iN:1086:A:C5    | 3.06                     | 0.44              |
| 28:SP:31:ILE:H    | 28:SP:49:LEU:HA    | 1.81                     | 0.44              |
| 5:Z2:612:A:O2'    | 42:Kd:78:GLU:OE2   | 2.33                     | 0.44              |
| 5:Z2:1283:G:O2'   | 5:Z2:1628:A:N6     | 2.51                     | 0.44              |
| 5:Z2:1625:A:H5'   | 5:Z2:1746:C:O2'    | 2.17                     | 0.44              |
| 7:A4:124:LYS:HD2  | 7:A4:124:LYS:C     | 2.43                     | 0.44              |
| 12:E9:21:GLU:HG3  | 12:E9:22:PHE:H     | 1.81                     | 0.44              |
| 12:E9:82:ARG:HB2  | 12:E9:85:ALA:HB2   | 1.99                     | 0.44              |
| 19:FG:9:LEU:O     | 19:FG:85:ILE:N     | 2.48                     | 0.44              |
| 26:iN:1040:A:H2'  | 26:iN:1041:U:C6    | 2.52                     | 0.44              |
| 26:iN:1079:A:N3   | 26:iN:1079:A:H2'   | 2.32                     | 0.44              |
| 34:NV:39:GLU:HA   | 34:NV:39:GLU:OE2   | 2.18                     | 0.44              |
| 36:IX:18:VAL:HG11 | 36:IX:28:LEU:HD11  | 1.98                     | 0.44              |
| 42:Kd:81:LEU:HD22 | 42:Kd:118:VAL:HG13 | 1.98                     | 0.44              |
| 50:Cl:245:THR:OG1 | 50:Cl:250:GLN:N    | 2.51                     | 0.44              |
| 5:Z2:134:C:H2'    | 5:Z2:135:C:H6      | 1.83                     | 0.44              |
| 5:Z2:2620:U:H2'   | 5:Z2:2621:G:O4'    | 2.17                     | 0.44              |
| 26:iN:211:G:H2'   | 26:iN:212:A:C8     | 2.52                     | 0.44              |
| 43:Je:19:VAL:HG12 | 43:Je:43:VAL:HA    | 2.00                     | 0.44              |
| 1:B:9:ARG:HH11    | 1:B:9:ARG:HG3      | 1.83                     | 0.44              |
| 4:H:104:LEU:HD11  | 4:H:116:THR:HG23   | 1.99                     | 0.44              |
| 5:Z2:781:U:H2'    | 5:Z2:782:C:C6      | 2.53                     | 0.44              |
| 5:Z2:810:A:H2'    | 5:Z2:811:U:C6      | 2.53                     | 0.44              |
| 5:Z2:1593:C:H2'   | 5:Z2:1594:C:O4'    | 2.17                     | 0.44              |
| 5:Z2:1816:U:H2'   | 5:Z2:1817:G:H8     | 1.82                     | 0.44              |
| 5:Z2:1845:U:H2'   | 5:Z2:1846:G:C8     | 2.53                     | 0.44              |
| 5:Z2:2598:U:H2'   | 5:Z2:2599:C:C6     | 2.53                     | 0.44              |
| 30:GR:106:ASN:OD1 | 30:GR:106:ASN:N    | 2.51                     | 0.44              |
| 32:CT:117:ALA:HB1 | 32:CT:187:VAL:HG22 | 1.98                     | 0.44              |
| 44:Af:85:ALA:HB1  | 44:Af:89:ASP:HB2   | 2.00                     | 0.44              |
| 51:Dm:11:LEU:HD23 | 51:Dm:64:ARG:HG2   | 2.00                     | 0.44              |
| 5:Z2:158:U:H2'    | 5:Z2:159:U:H6      | 1.82                     | 0.44              |
| 5:Z2:434:U:OP1    | 12:E9:46:LYS:HD3   | 2.18                     | 0.44              |
| 5:Z2:482:U:H2'    | 5:Z2:483:G:O4'     | 2.18                     | 0.44              |
| 5:Z2:959:A:H1'    | 5:Z2:974:A:C2      | 2.52                     | 0.44              |
| 5:Z2:1333:C:C2    | 5:Z2:1334:C:C5     | 3.06                     | 0.44              |
| 5:Z2:1369:A:H62   | 5:Z2:1386:U:H3     | 1.66                     | 0.44              |
| 5:Z2:1401:C:H2'   | 5:Z2:1402:G:C8     | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Z2:1479:A:H2'   | 5:Z2:1480:A:C8    | 2.52                     | 0.44              |
| 5:Z2:2526:G:H2'   | 5:Z2:2527:G:C8    | 2.53                     | 0.44              |
| 8:E5:111:ILE:HD11 | 8:E5:129:LEU:HD22 | 2.00                     | 0.44              |
| 15:UC:36:ILE:HD11 | 15:UC:46:ILE:HD13 | 2.00                     | 0.44              |
| 18:RF:34:ASP:OD1  | 18:RF:34:ASP:N    | 2.51                     | 0.44              |
| 24:OL:3:THR:O     | 24:OL:7:ARG:HB2   | 2.18                     | 0.44              |
| 26:iN:171:A:OP1   | 26:iN:648:U:O2'   | 2.15                     | 0.44              |
| 26:iN:339:U:H2'   | 26:iN:340:G:C8    | 2.53                     | 0.44              |
| 26:iN:716:U:H2'   | 26:iN:717:A:H8    | 1.81                     | 0.44              |
| 48:Pj:21:VAL:HG12 | 48:Pj:33:ILE:HB   | 1.99                     | 0.44              |
| 53:To:44:TYR:CE2  | 53:To:88:ALA:HA   | 2.52                     | 0.44              |
| 1:B:369:TYR:HB3   | 5:Z2:1079:A:C8    | 2.53                     | 0.44              |
| 5:Z2:619:C:H2'    | 5:Z2:620:C:C6     | 2.53                     | 0.44              |
| 5:Z2:818:A:H2'    | 5:Z2:819:G:H8     | 1.80                     | 0.44              |
| 5:Z2:887:C:H2'    | 5:Z2:888:C:H6     | 1.83                     | 0.44              |
| 5:Z2:1236:G:N2    | 27:PO:33:ARG:HG2  | 2.32                     | 0.44              |
| 5:Z2:1668:U:H2'   | 5:Z2:1669:G:O4'   | 2.17                     | 0.44              |
| 5:Z2:2065:U:O2'   | 16:WD:23:ASN:OD1  | 2.32                     | 0.44              |
| 5:Z2:2693:C:H2'   | 5:Z2:2694:A:C8    | 2.52                     | 0.44              |
| 5:Z2:2725:C:H5''  | 54:ep:1:MET:HE3   | 1.99                     | 0.44              |
| 5:Z2:2842:U:H5''  | 47:Oi:6:LEU:HD22  | 1.99                     | 0.44              |
| 10:F7:140:GLU:HA  | 22:fJ:29:VAL:HB   | 2.00                     | 0.44              |
| 11:D8:73:G:O2'    | 15:UC:94:HIS:NE2  | 2.43                     | 0.44              |
| 22:fJ:73:PHE:CD2  | 28:SP:42:PRO:HD3  | 2.52                     | 0.44              |
| 26:iN:167:A:N6    | 26:iN:282:U:H3    | 2.06                     | 0.44              |
| 26:iN:1104:U:H2'  | 26:iN:1105:G:H8   | 1.83                     | 0.44              |
| 29:BQ:88:HIS:CE1  | 29:BQ:126:GLU:HB2 | 2.53                     | 0.44              |
| 34:NV:41:PRO:O    | 34:NV:45:ARG:HG3  | 2.18                     | 0.44              |
| 5:Z2:573:U:H2'    | 5:Z2:574:U:C6     | 2.53                     | 0.43              |
| 5:Z2:856:U:H2'    | 5:Z2:857:U:C6     | 2.53                     | 0.43              |
| 5:Z2:1905:A:N1    | 26:iN:1540:U:O2'  | 2.36                     | 0.43              |
| 5:Z2:1932:U:H2'   | 5:Z2:1933:C:C6    | 2.53                     | 0.43              |
| 5:Z2:2298:U:H2'   | 5:Z2:2299:U:H6    | 1.82                     | 0.43              |
| 18:RF:42:LYS:O    | 18:RF:45:VAL:HG22 | 2.18                     | 0.43              |
| 25:MM:23:PHE:CE2  | 25:MM:69:LEU:HD23 | 2.53                     | 0.43              |
| 25:MM:23:PHE:CE2  | 25:MM:70:ARG:HG3  | 2.53                     | 0.43              |
| 25:MM:103:LYS:HD3 | 26:iN:1271:C:N4   | 2.33                     | 0.43              |
| 26:iN:470:U:OP2   | 26:iN:471:G:O2'   | 2.25                     | 0.43              |
| 26:iN:537:G:O2'   | 26:iN:539:A:H1'   | 2.17                     | 0.43              |
| 26:iN:727:G:N2    | 33:KU:39:GLY:O    | 2.50                     | 0.43              |
| 26:iN:964:U:H2'   | 26:iN:965:U:C6    | 2.53                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:Cl:120:GLU:HG3 | 50:Cl:131:PRO:HG2  | 2.00                     | 0.43              |
| 5:Z2:1072:A:N3    | 5:Z2:1072:A:H2'    | 2.34                     | 0.43              |
| 5:Z2:1369:A:H4'   | 5:Z2:1370:U:OP1    | 2.18                     | 0.43              |
| 5:Z2:1392:U:H2'   | 5:Z2:1393:U:H6     | 1.83                     | 0.43              |
| 5:Z2:1645:U:H2'   | 5:Z2:1646:C:H6     | 1.83                     | 0.43              |
| 5:Z2:2559:G:O2'   | 5:Z2:2562:C:OP2    | 2.28                     | 0.43              |
| 11:D8:7:G:C2      | 11:D8:8:A:C8       | 3.05                     | 0.43              |
| 11:D8:34:C:H2'    | 11:D8:35:C:C6      | 2.53                     | 0.43              |
| 18:RF:85:ILE:HG23 | 18:RF:93:ALA:HB1   | 2.00                     | 0.43              |
| 26:iN:226:A:C6    | 26:iN:240:A:C8     | 3.06                     | 0.43              |
| 26:iN:1046:A:H2'  | 26:iN:1047:G:H8    | 1.81                     | 0.43              |
| 26:iN:1315:U:H2'  | 26:iN:1316:G:H8    | 1.83                     | 0.43              |
| 28:SP:32:LYS:HE2  | 28:SP:32:LYS:HB2   | 1.88                     | 0.43              |
| 36:IX:31:GLN:HB3  | 36:IX:142:ILE:HG13 | 2.00                     | 0.43              |
| 38:QZ:68:LYS:HG2  | 38:QZ:82:VAL:HG11  | 1.99                     | 0.43              |
| 43:Je:101:PRO:HB3 | 43:Je:120:GLU:HB3  | 1.99                     | 0.43              |
| 45:Lg:43:THR:HG23 | 45:Lg:45:ARG:H     | 1.83                     | 0.43              |
| 1:B:289:VAL:HG12  | 1:B:338:ILE:HG21   | 2.00                     | 0.43              |
| 5:Z2:721:C:H2'    | 5:Z2:722:C:C6      | 2.54                     | 0.43              |
| 5:Z2:2056:A:H2'   | 5:Z2:2057:A:C8     | 2.53                     | 0.43              |
| 5:Z2:2523:U:H2'   | 5:Z2:2524:A:O4'    | 2.18                     | 0.43              |
| 17:XE:16:GLN:C    | 17:XE:16:GLN:OE1   | 2.61                     | 0.43              |
| 19:FG:2:ARG:NH2   | 26:iN:783:C:OP2    | 2.51                     | 0.43              |
| 19:FG:63:ASN:HD22 | 19:FG:96:ILE:HB    | 1.82                     | 0.43              |
| 20:VH:46:HIS:CE1  | 20:VH:77:ARG:HD2   | 2.52                     | 0.43              |
| 25:MM:103:LYS:HG2 | 25:MM:104:ASN:ND2  | 2.33                     | 0.43              |
| 26:iN:223:C:C2    | 26:iN:224:A:C8     | 3.06                     | 0.43              |
| 26:iN:1371:U:H2'  | 26:iN:1372:C:C6    | 2.53                     | 0.43              |
| 26:iN:1509:C:H2'  | 26:iN:1510:A:H8    | 1.82                     | 0.43              |
| 37:JY:50:ASN:HB3  | 37:JY:62:ARG:HD3   | 1.99                     | 0.43              |
| 41:Nc:16:ARG:NE   | 41:Nc:92:ASP:OD2   | 2.47                     | 0.43              |
| 51:Dm:108:PHE:CD2 | 51:Dm:152:ILE:HD11 | 2.53                     | 0.43              |
| 3:F:50:LEU:HD11   | 3:F:61:LEU:HD11    | 1.99                     | 0.43              |
| 5:Z2:179:A:H2'    | 5:Z2:180:C:C6      | 2.53                     | 0.43              |
| 5:Z2:582:G:H2'    | 5:Z2:583:U:C6      | 2.54                     | 0.43              |
| 5:Z2:695:G:H2'    | 5:Z2:696:C:H6      | 1.81                     | 0.43              |
| 5:Z2:1426:U:H2'   | 5:Z2:1427:C:H6     | 1.83                     | 0.43              |
| 5:Z2:2058:C:H2'   | 5:Z2:2059:C:C6     | 2.53                     | 0.43              |
| 5:Z2:2339:C:H2'   | 5:Z2:2340:C:O4'    | 2.18                     | 0.43              |
| 5:Z2:2842:U:H4'   | 47:Oi:6:LEU:HD11   | 2.01                     | 0.43              |
| 5:Z2:2865:G:H2'   | 5:Z2:2866:A:C8     | 2.53                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:L6:66:TYR:OH    | 26:iN:565:C:OP2    | 2.28                     | 0.43              |
| 10:F7:4:LEU:HD13  | 10:F7:101:ASP:HB2  | 1.99                     | 0.43              |
| 11:D8:61:C:H2'    | 11:D8:62:G:H8      | 1.83                     | 0.43              |
| 26:iN:1436:U:H2'  | 26:iN:1437:G:C8    | 2.53                     | 0.43              |
| 31:GS:2:PRO:HB2   | 31:GS:3:ARG:H      | 1.64                     | 0.43              |
| 31:GS:53:LYS:HB2  | 31:GS:53:LYS:HE2   | 1.77                     | 0.43              |
| 44:Af:105:GLU:OE2 | 44:Af:108:GLN:HB2  | 2.18                     | 0.43              |
| 5:Z2:669:G:OP1    | 39:Ba:16:HIS:ND1   | 2.46                     | 0.43              |
| 5:Z2:1059:C:C2    | 5:Z2:1060:C:C5     | 3.07                     | 0.43              |
| 5:Z2:1065:U:H2'   | 5:Z2:1066:U:C6     | 2.53                     | 0.43              |
| 5:Z2:1215:U:H2'   | 5:Z2:1216:G:H8     | 1.84                     | 0.43              |
| 5:Z2:1396:U:C2    | 5:Z2:1397:A:C8     | 3.07                     | 0.43              |
| 5:Z2:1738:C:H2'   | 5:Z2:1739:G:C8     | 2.54                     | 0.43              |
| 5:Z2:1875:A:H2'   | 5:Z2:1876:A:H8     | 1.83                     | 0.43              |
| 5:Z2:2450:C:H2'   | 5:Z2:2451:A:O4'    | 2.19                     | 0.43              |
| 5:Z2:2617:A:N1    | 5:Z2:2767:U:H5     | 2.16                     | 0.43              |
| 12:E9:47:THR:HG22 | 12:E9:85:ALA:HB3   | 2.00                     | 0.43              |
| 18:RF:80:ILE:O    | 18:RF:100:THR:OG1  | 2.30                     | 0.43              |
| 23:HK:27:LEU:HD21 | 23:HK:48:LEU:HB2   | 2.00                     | 0.43              |
| 26:iN:442:G:H2'   | 26:iN:443:C:C6     | 2.54                     | 0.43              |
| 38:QZ:23:MET:HB2  | 38:QZ:26:SER:HB2   | 2.00                     | 0.43              |
| 44:Af:106:GLN:OE1 | 44:Af:106:GLN:N    | 2.51                     | 0.43              |
| 1:B:69:LYS:NZ     | 1:B:70:GLU:HG3     | 2.33                     | 0.43              |
| 5:Z2:65:G:O2'     | 5:Z2:80:A:N1       | 2.41                     | 0.43              |
| 5:Z2:608:C:OP1    | 42:Kd:104:ARG:NH1  | 2.42                     | 0.43              |
| 5:Z2:834:A:H2'    | 5:Z2:835:C:H6      | 1.83                     | 0.43              |
| 5:Z2:866:G:H2'    | 5:Z2:866:G:N3      | 2.32                     | 0.43              |
| 5:Z2:895:A:H2'    | 5:Z2:896:A:C8      | 2.53                     | 0.43              |
| 5:Z2:1901:U:H2'   | 5:Z2:1902:A:O4'    | 2.18                     | 0.43              |
| 7:A4:188:VAL:HG13 | 7:A4:201:VAL:HA    | 1.99                     | 0.43              |
| 10:F7:24:ASN:ND2  | 11:D8:55:A:C8      | 2.87                     | 0.43              |
| 26:iN:159:U:H2'   | 26:iN:160:G:C8     | 2.53                     | 0.43              |
| 26:iN:277:C:H2'   | 26:iN:278:U:H6     | 1.83                     | 0.43              |
| 26:iN:513:C:H2'   | 26:iN:514:C:H6     | 1.84                     | 0.43              |
| 26:iN:1029:C:H2'  | 26:iN:1030:U:C6    | 2.53                     | 0.43              |
| 43:Je:120:GLU:HG2 | 43:Je:122:LEU:HD12 | 1.99                     | 0.43              |
| 53:To:24:GLN:O    | 53:To:28:VAL:HG23  | 2.19                     | 0.43              |
| 1:B:19:ILE:HB     | 1:B:82:ILE:HB      | 2.00                     | 0.43              |
| 4:H:71:ASP:HB3    | 4:H:76:HIS:ND1     | 2.34                     | 0.43              |
| 5:Z2:82:G:H2'     | 5:Z2:82:G:N3       | 2.34                     | 0.43              |
| 5:Z2:354:A:OP2    | 5:Z2:386:G:N2      | 2.50                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:822:C:N3     | 5:Z2:925:A:N6      | 2.67                     | 0.43              |
| 5:Z2:1708:A:N6    | 5:Z2:1724:G:O2'    | 2.47                     | 0.43              |
| 5:Z2:1787:A:H5'   | 5:Z2:2189:A:O2'    | 2.19                     | 0.43              |
| 5:Z2:1811:U:OP1   | 50:Cl:247:PRO:HD3  | 2.19                     | 0.43              |
| 32:CT:88:GLN:OE1  | 32:CT:101:VAL:HG12 | 2.18                     | 0.43              |
| 38:QZ:70:THR:OG1  | 38:QZ:71:ARG:N     | 2.52                     | 0.43              |
| 3:F:65:VAL:HG11   | 3:F:77:ILE:HD11    | 2.01                     | 0.43              |
| 5:Z2:793:G:OP2    | 42:Kd:38:LYS:HD3   | 2.18                     | 0.43              |
| 5:Z2:1051:A:H2'   | 5:Z2:1052:G:O4'    | 2.18                     | 0.43              |
| 5:Z2:1181:G:H2'   | 5:Z2:1182:U:H6     | 1.82                     | 0.43              |
| 6:R3:66:SER:HB2   | 19:FG:51:ILE:HD11  | 2.00                     | 0.43              |
| 7:A4:193:ASP:HB2  | 7:A4:209:ASP:OD2   | 2.18                     | 0.43              |
| 9:L6:67:ILE:HA    | 9:L6:97:THR:HG22   | 2.01                     | 0.43              |
| 10:F7:24:ASN:ND2  | 11:D8:55:A:H8      | 2.17                     | 0.43              |
| 10:F7:31:ILE:HA   | 10:F7:158:THR:HA   | 1.99                     | 0.43              |
| 19:FG:47:LEU:HD21 | 19:FG:57:ALA:HB3   | 2.00                     | 0.43              |
| 26:iN:136:C:C2    | 26:iN:137:U:C5     | 3.07                     | 0.43              |
| 26:iN:1541:C:H2'  | 26:iN:1542:G:O4'   | 2.18                     | 0.43              |
| 47:Oi:50:ILE:HG13 | 47:Oi:62:THR:HG23  | 2.00                     | 0.43              |
| 51:Dm:191:LYS:HE2 | 51:Dm:191:LYS:HB3  | 1.76                     | 0.43              |
| 52:Sn:25:SER:OG   | 52:Sn:26:LEU:HG    | 2.18                     | 0.43              |
| 5:Z2:1160:G:OP2   | 5:Z2:1160:G:N2     | 2.52                     | 0.43              |
| 5:Z2:1549:C:H2'   | 5:Z2:1550:U:C6     | 2.54                     | 0.43              |
| 5:Z2:1642:A:O2'   | 44:Af:121:PHE:O    | 2.32                     | 0.43              |
| 7:A4:76:GLY:O     | 7:A4:98:ASP:HA     | 2.18                     | 0.43              |
| 9:L6:4:THR:O      | 9:L6:8:ILE:HG12    | 2.19                     | 0.43              |
| 9:L6:9:ARG:HH21   | 26:iN:924:C:P      | 2.41                     | 0.43              |
| 24:OL:4:ASN:ND2   | 26:iN:704:G:OP1    | 2.48                     | 0.43              |
| 24:OL:73:ASP:HB3  | 24:OL:76:ARG:HB2   | 1.99                     | 0.43              |
| 26:iN:646:U:H2'   | 26:iN:647:G:C8     | 2.53                     | 0.43              |
| 26:iN:1221:A:H2'  | 26:iN:1222:G:C8    | 2.53                     | 0.43              |
| 26:iN:1469:U:H2'  | 26:iN:1470:U:C6    | 2.53                     | 0.43              |
| 26:iN:1557:U:H2'  | 26:iN:1558:A:C8    | 2.54                     | 0.43              |
| 41:Nc:34:LYS:HE3  | 41:Nc:34:LYS:HB3   | 1.91                     | 0.43              |
| 45:Lg:43:THR:HG22 | 45:Lg:46:GLN:CD    | 2.44                     | 0.43              |
| 5:Z2:179:A:H2'    | 5:Z2:180:C:H6      | 1.84                     | 0.43              |
| 5:Z2:572:C:H5'    | 12:E9:84:PHE:CE2   | 2.54                     | 0.43              |
| 5:Z2:802:C:O2'    | 5:Z2:824:U:H5''    | 2.19                     | 0.43              |
| 5:Z2:2295:U:H5'   | 10:F7:85:ILE:HD11  | 2.01                     | 0.43              |
| 5:Z2:2654:G:H2'   | 5:Z2:2655:U:C6     | 2.54                     | 0.43              |
| 17:XE:40:THR:HG23 | 17:XE:40:THR:O     | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:iN:450:U:O2'   | 51:Dm:114:GLU:HG3 | 2.19                     | 0.43              |
| 30:GR:177:LYS:HE2 | 30:GR:177:LYS:C   | 2.44                     | 0.43              |
| 37:JY:66:GLU:OE2  | 37:JY:68:ARG:NH1  | 2.52                     | 0.43              |
| 4:H:117:ARG:CZ    | 4:H:117:ARG:HB3   | 2.48                     | 0.42              |
| 5:Z2:140:U:H2'    | 5:Z2:141:A:C8     | 2.54                     | 0.42              |
| 5:Z2:441:G:C8     | 39:Ba:37:LYS:HG2  | 2.54                     | 0.42              |
| 5:Z2:1833:A:H1'   | 5:Z2:1834:A:N7    | 2.34                     | 0.42              |
| 5:Z2:2017:A:C6    | 5:Z2:2481:C:H1'   | 2.54                     | 0.42              |
| 5:Z2:2288:U:H5''  | 10:F7:131:GLY:HA3 | 2.01                     | 0.42              |
| 5:Z2:2810:G:H4'   | 47:Oi:2:SER:HB2   | 2.01                     | 0.42              |
| 9:L6:8:ILE:HD12   | 38:QZ:44:LEU:CD2  | 2.49                     | 0.42              |
| 26:iN:343:A:O2'   | 26:iN:607:C:H5    | 2.01                     | 0.42              |
| 26:iN:1084:G:O2'  | 26:iN:1085:A:C8   | 2.70                     | 0.42              |
| 29:BQ:10:MET:HE2  | 29:BQ:33:ARG:HA   | 2.00                     | 0.42              |
| 36:IX:120:LYS:O   | 36:IX:123:LYS:NZ  | 2.39                     | 0.42              |
| 51:Dm:51:GLU:OE1  | 51:Dm:51:GLU:HA   | 2.19                     | 0.42              |
| 1:B:157:MET:HG3   | 1:B:201:GLU:CD    | 2.44                     | 0.42              |
| 3:F:122:ARG:HB2   | 26:iN:1388:G:H4'  | 2.00                     | 0.42              |
| 4:H:38:ILE:HG22   | 4:H:39:THR:HG23   | 2.00                     | 0.42              |
| 4:H:133:VAL:HB    | 4:H:170:ILE:HG12  | 2.01                     | 0.42              |
| 5:Z2:71:G:H2'     | 5:Z2:72:C:H6      | 1.84                     | 0.42              |
| 5:Z2:728:U:O2'    | 5:Z2:1647:U:OP1   | 2.34                     | 0.42              |
| 5:Z2:773:A:H1'    | 39:Ba:4:THR:HG21  | 2.00                     | 0.42              |
| 5:Z2:886:A:O2'    | 5:Z2:887:C:OP1    | 2.32                     | 0.42              |
| 5:Z2:1775:A:OP1   | 50:Cl:221:ARG:HG3 | 2.19                     | 0.42              |
| 5:Z2:1869:U:H2'   | 5:Z2:1870:G:O4'   | 2.19                     | 0.42              |
| 10:F7:81:GLU:HB3  | 10:F7:82:GLU:OE1  | 2.19                     | 0.42              |
| 26:iN:298:G:H2'   | 26:iN:299:U:H6    | 1.84                     | 0.42              |
| 26:iN:447:G:O2'   | 26:iN:541:A:N1    | 2.47                     | 0.42              |
| 26:iN:997:U:H2'   | 26:iN:998:G:O4'   | 2.19                     | 0.42              |
| 26:iN:1349:G:H1'  | 26:iN:1379:G:N2   | 2.34                     | 0.42              |
| 26:iN:1361:G:N1   | 26:iN:1364:A:OP2  | 2.49                     | 0.42              |
| 27:PO:24:TYR:HB3  | 27:PO:28:ARG:HB2  | 2.01                     | 0.42              |
| 32:CT:32:TYR:O    | 32:CT:36:ASP:N    | 2.46                     | 0.42              |
| 50:Cl:225:MET:SD  | 50:Cl:230:HIS:HB2 | 2.59                     | 0.42              |
| 1:B:270:LEU:HD23  | 1:B:270:LEU:HA    | 1.91                     | 0.42              |
| 5:Z2:459:G:HO2'   | 5:Z2:485:A:H61    | 1.65                     | 0.42              |
| 5:Z2:614:G:H5''   | 5:Z2:635:C:O2'    | 2.20                     | 0.42              |
| 5:Z2:673:U:H2'    | 5:Z2:674:A:H8     | 1.84                     | 0.42              |
| 5:Z2:713:G:H4'    | 50:Cl:13:ARG:HD3  | 2.00                     | 0.42              |
| 5:Z2:792:U:OP2    | 42:Kd:38:LYS:HD2  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:2711:U:H2'   | 5:Z2:2712:U:C6     | 2.54                     | 0.42              |
| 9:L6:20:LYS:HD3   | 9:L6:20:LYS:HA     | 1.79                     | 0.42              |
| 10:F7:54:VAL:HG13 | 10:F7:65:PRO:HG2   | 2.01                     | 0.42              |
| 11:D8:29:C:C2     | 11:D8:30:U:C5      | 3.07                     | 0.42              |
| 14:MB:38:LEU:HB3  | 14:MB:39:PRO:HD3   | 2.01                     | 0.42              |
| 23:HK:58:VAL:HG13 | 26:iN:1405:A:N7    | 2.34                     | 0.42              |
| 26:iN:450:U:H2'   | 26:iN:451:G:C8     | 2.54                     | 0.42              |
| 26:iN:482:U:C2    | 26:iN:483:A:C8     | 3.07                     | 0.42              |
| 26:iN:844:G:H2'   | 26:iN:845:U:C6     | 2.54                     | 0.42              |
| 26:iN:905:G:O2'   | 26:iN:918:G:O2'    | 2.35                     | 0.42              |
| 26:iN:922:A:H5'   | 29:BQ:83:PRO:HG2   | 2.00                     | 0.42              |
| 26:iN:1261:A:H2'  | 26:iN:1262:C:C6    | 2.54                     | 0.42              |
| 26:iN:1364:A:C8   | 26:iN:1368:G:C5    | 3.07                     | 0.42              |
| 33:KU:85:LEU:HD23 | 33:KU:111:SER:HB3  | 2.01                     | 0.42              |
| 37:JY:18:ILE:HD12 | 37:JY:72:ARG:HG3   | 2.00                     | 0.42              |
| 53:To:47:ALA:HB1  | 53:To:83:ILE:HD13  | 2.01                     | 0.42              |
| 5:Z2:341:C:H2'    | 5:Z2:342:G:H8      | 1.85                     | 0.42              |
| 5:Z2:629:A:H2'    | 5:Z2:631:A:N7      | 2.35                     | 0.42              |
| 5:Z2:956:G:H3'    | 5:Z2:957:A:H2'     | 2.01                     | 0.42              |
| 5:Z2:1160:G:C4'   | 5:Z2:1161:U:H3'    | 2.50                     | 0.42              |
| 5:Z2:2754:C:H2'   | 5:Z2:2755:C:H6     | 1.85                     | 0.42              |
| 12:E9:170:ASP:O   | 12:E9:174:VAL:HG23 | 2.20                     | 0.42              |
| 24:OL:25:GLU:OE1  | 24:OL:76:ARG:NE    | 2.51                     | 0.42              |
| 30:GR:52:LEU:HD23 | 30:GR:52:LEU:H     | 1.84                     | 0.42              |
| 38:QZ:16:GLY:HA3  | 38:QZ:31:ILE:HD13  | 2.01                     | 0.42              |
| 43:Je:17:ARG:NE   | 43:Je:17:ARG:HA    | 2.34                     | 0.42              |
| 3:F:118:LYS:NZ    | 26:iN:1396:U:O4    | 2.47                     | 0.42              |
| 5:Z2:295:G:H2'    | 5:Z2:296:G:C8      | 2.54                     | 0.42              |
| 5:Z2:375:U:H2'    | 5:Z2:376:C:H6      | 1.83                     | 0.42              |
| 5:Z2:726:U:H2'    | 5:Z2:727:G:C8      | 2.54                     | 0.42              |
| 5:Z2:1155:A:H2'   | 5:Z2:1156:A:C8     | 2.54                     | 0.42              |
| 5:Z2:1372:G:H2'   | 5:Z2:1373:G:C8     | 2.54                     | 0.42              |
| 5:Z2:2864:U:H2'   | 5:Z2:2865:G:C8     | 2.55                     | 0.42              |
| 8:E5:94:HIS:CE1   | 8:E5:143:ARG:HD2   | 2.54                     | 0.42              |
| 26:iN:109:U:H2'   | 26:iN:110:C:C6     | 2.55                     | 0.42              |
| 27:PO:112:LYS:HE2 | 27:PO:112:LYS:HB2  | 1.83                     | 0.42              |
| 41:Nc:52:ALA:HB3  | 41:Nc:77:ILE:HB    | 2.01                     | 0.42              |
| 53:To:84:LYS:O    | 53:To:88:ALA:HB2   | 2.19                     | 0.42              |
| 4:H:89:VAL:HA     | 4:H:122:LEU:HD21   | 2.01                     | 0.42              |
| 5:Z2:275:U:H2'    | 5:Z2:276:A:C8      | 2.54                     | 0.42              |
| 5:Z2:400:C:H2'    | 5:Z2:401:C:H6      | 1.85                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:462:A:N3     | 5:Z2:464:G:H5''    | 2.34                     | 0.42              |
| 5:Z2:741:A:H2'    | 5:Z2:742:G:O4'     | 2.20                     | 0.42              |
| 5:Z2:1655:G:O2'   | 5:Z2:1977:U:O4     | 2.23                     | 0.42              |
| 5:Z2:2496:A:H2'   | 5:Z2:2497:U:C6     | 2.54                     | 0.42              |
| 23:HK:53:ARG:HH22 | 26:iN:1265:G:P     | 2.42                     | 0.42              |
| 26:iN:811:A:H2'   | 26:iN:812:A:O4'    | 2.19                     | 0.42              |
| 26:iN:1307:C:H2'  | 26:iN:1308:A:H8    | 1.85                     | 0.42              |
| 26:iN:1431:G:H2'  | 26:iN:1432:G:H8    | 1.83                     | 0.42              |
| 33:KU:35:THR:OG1  | 33:KU:36:ASP:N     | 2.52                     | 0.42              |
| 43:Je:24:VAL:HG13 | 43:Je:33:ALA:HB2   | 2.02                     | 0.42              |
| 47:Oi:89:LYS:HE3  | 47:Oi:89:LYS:HB3   | 1.77                     | 0.42              |
| 1:B:285:ASP:O     | 1:B:289:VAL:HG23   | 2.19                     | 0.42              |
| 4:H:135:MET:SD    | 4:H:172:LYS:HG2    | 2.60                     | 0.42              |
| 4:H:384:ARG:HG3   | 5:Z2:2643:A:H1'    | 2.01                     | 0.42              |
| 5:Z2:247:G:H2'    | 5:Z2:248:A:C8      | 2.54                     | 0.42              |
| 5:Z2:288:C:OP2    | 21:TI:80:ARG:NH2   | 2.49                     | 0.42              |
| 5:Z2:311:U:H5     | 5:Z2:1189:A:OP2    | 2.02                     | 0.42              |
| 5:Z2:1706:U:H2'   | 5:Z2:1707:G:O4'    | 2.20                     | 0.42              |
| 5:Z2:1729:U:H2'   | 5:Z2:1730:U:C6     | 2.54                     | 0.42              |
| 5:Z2:2283:A:H2'   | 5:Z2:2284:A:C8     | 2.55                     | 0.42              |
| 9:L6:54:ARG:HE    | 9:L6:54:ARG:HB2    | 1.75                     | 0.42              |
| 26:iN:1316:G:H2'  | 26:iN:1317:U:C6    | 2.54                     | 0.42              |
| 36:IX:17:VAL:HG23 | 36:IX:137:PRO:HB2  | 2.01                     | 0.42              |
| 40:Qb:64:ILE:HB   | 40:Qb:95:LEU:HB3   | 2.01                     | 0.42              |
| 44:Af:106:GLN:HG3 | 44:Af:182:SER:HA   | 2.02                     | 0.42              |
| 49:bk:39:ILE:HG13 | 49:bk:41:GLN:HB2   | 2.01                     | 0.42              |
| 1:B:17:VAL:HG11   | 1:B:44:VAL:HG21    | 2.02                     | 0.42              |
| 3:F:53:LEU:HD23   | 3:F:96:LEU:HD11    | 2.01                     | 0.42              |
| 5:Z2:749:A:H5''   | 50:Cl:209:GLY:HA2  | 2.02                     | 0.42              |
| 5:Z2:919:U:H2'    | 5:Z2:920:C:C6      | 2.55                     | 0.42              |
| 5:Z2:1273:C:H2'   | 5:Z2:1274:U:C6     | 2.54                     | 0.42              |
| 5:Z2:2515:G:N2    | 5:Z2:2646:G:O2'    | 2.53                     | 0.42              |
| 26:iN:1283:A:C8   | 26:iN:1348:C:H1'   | 2.55                     | 0.42              |
| 26:iN:1491:A:O2'  | 26:iN:1492:A:H5'   | 2.20                     | 0.42              |
| 26:iN:1492:A:OP1  | 26:iN:1493:C:N4    | 2.42                     | 0.42              |
| 42:Kd:63:LEU:HD13 | 46:dh:24:ARG:HD3   | 2.02                     | 0.42              |
| 44:Af:6:VAL:HG22  | 44:Af:205:ILE:HG13 | 2.01                     | 0.42              |
| 44:Af:128:HIS:HB3 | 44:Af:163:LYS:HD3  | 2.01                     | 0.42              |
| 51:Dm:182:HIS:N   | 51:Dm:182:HIS:ND1  | 2.68                     | 0.42              |
| 53:To:35:VAL:HG11 | 53:To:79:LEU:HD13  | 2.02                     | 0.42              |
| 4:H:74:SER:OG     | 4:H:75:ARG:N       | 2.52                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:565:U:H2'    | 5:Z2:566:C:H6      | 1.85                     | 0.42              |
| 5:Z2:817:U:H2'    | 5:Z2:818:A:H8      | 1.85                     | 0.42              |
| 5:Z2:912:A:O2'    | 35:YW:38:GLU:OE2   | 2.30                     | 0.42              |
| 5:Z2:1127:A:O2'   | 5:Z2:1128:A:H3'    | 2.20                     | 0.42              |
| 5:Z2:1580:A:HO2'  | 5:Z2:1581:A:P      | 2.39                     | 0.42              |
| 5:Z2:2819:U:H2'   | 5:Z2:2820:G:H8     | 1.84                     | 0.42              |
| 8:E5:70:GLU:OE2   | 8:E5:70:GLU:HA     | 2.20                     | 0.42              |
| 9:L6:8:ILE:HG22   | 38:QZ:37:HIS:CD2   | 2.55                     | 0.42              |
| 10:F7:134:GLU:HB3 | 10:F7:136:ILE:HG12 | 2.02                     | 0.42              |
| 26:iN:211:G:H2'   | 26:iN:212:A:H8     | 1.85                     | 0.42              |
| 26:iN:587:G:H5''  | 51:Dm:56:LEU:HD21  | 2.02                     | 0.42              |
| 26:iN:865:G:H2'   | 26:iN:866:U:C6     | 2.54                     | 0.42              |
| 26:iN:1076:G:C5   | 26:iN:1077:G:H1'   | 2.54                     | 0.42              |
| 26:iN:1361:G:H22  | 26:iN:1364:A:H5'   | 1.85                     | 0.42              |
| 41:Nc:55:LEU:HA   | 41:Nc:60:ARG:HD3   | 2.02                     | 0.42              |
| 47:Oi:108:LYS:O   | 47:Oi:111:ARG:NE   | 2.38                     | 0.42              |
| 1:B:220:SER:OG    | 5:Z2:2541:C:H5'    | 2.19                     | 0.42              |
| 5:Z2:248:A:OP1    | 42:Kd:60:TYR:OH    | 2.32                     | 0.42              |
| 5:Z2:694:U:H2'    | 5:Z2:695:G:C8      | 2.55                     | 0.42              |
| 5:Z2:779:A:H2'    | 5:Z2:780:C:C6      | 2.55                     | 0.42              |
| 5:Z2:1394:U:H2'   | 5:Z2:1395:A:C8     | 2.55                     | 0.42              |
| 5:Z2:1888:C:H4'   | 50:Cl:242:ARG:O    | 2.19                     | 0.42              |
| 5:Z2:2296:C:H2'   | 5:Z2:2297:G:H8     | 1.85                     | 0.42              |
| 5:Z2:2438:G:H2'   | 5:Z2:2439:C:H6     | 1.82                     | 0.42              |
| 8:E5:89:PRO:HA    | 8:E5:102:GLN:HA    | 2.02                     | 0.42              |
| 26:iN:337:U:H2'   | 26:iN:338:C:C6     | 2.55                     | 0.42              |
| 26:iN:364:A:H2'   | 26:iN:365:C:C6     | 2.55                     | 0.42              |
| 26:iN:425:A:H2'   | 26:iN:426:A:C8     | 2.54                     | 0.42              |
| 26:iN:1054:G:H2'  | 26:iN:1055:C:C6    | 2.55                     | 0.42              |
| 44:Af:86:ASN:ND2  | 44:Af:89:ASP:OD2   | 2.53                     | 0.42              |
| 50:Cl:251:LYS:HB2 | 50:Cl:255:LEU:HB2  | 2.02                     | 0.42              |
| 3:F:5:TYR:CE2     | 26:iN:1192:C:H4'   | 2.55                     | 0.41              |
| 3:F:61:LEU:HB3    | 3:F:63:ILE:HD11    | 2.02                     | 0.41              |
| 5:Z2:1044:U:C2    | 5:Z2:1046:G:H5'    | 2.55                     | 0.41              |
| 5:Z2:1174:G:H2'   | 5:Z2:1175:G:C8     | 2.55                     | 0.41              |
| 5:Z2:1592:C:H2'   | 5:Z2:1593:C:C6     | 2.55                     | 0.41              |
| 26:iN:309:G:H1'   | 26:iN:311:C:OP2    | 2.20                     | 0.41              |
| 26:iN:377:C:H2'   | 26:iN:378:C:C6     | 2.56                     | 0.41              |
| 26:iN:797:A:H4'   | 26:iN:798:C:O5'    | 2.20                     | 0.41              |
| 28:SP:52:HIS:CD2  | 28:SP:54:GLY:H     | 2.38                     | 0.41              |
| 32:CT:173:VAL:HA  | 32:CT:203:PHE:HB2  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:KU:25:ALA:HA   | 33:KU:30:THR:HA    | 2.02                     | 0.41              |
| 33:KU:89:PRO:HB3  | 34:NV:32:VAL:HG21  | 2.02                     | 0.41              |
| 36:IX:55:VAL:HA   | 36:IX:123:LYS:O    | 2.20                     | 0.41              |
| 41:Nc:35:HIS:ND1  | 41:Nc:54:THR:OG1   | 2.45                     | 0.41              |
| 43:Je:17:ARG:HD2  | 43:Je:47:ILE:HD13  | 2.02                     | 0.41              |
| 43:Je:38:ILE:HD13 | 43:Je:91:LYS:HG2   | 2.02                     | 0.41              |
| 44:Af:78:ARG:NH2  | 44:Af:203:ASP:OD1  | 2.46                     | 0.41              |
| 48:Pj:4:ILE:O     | 48:Pj:71:VAL:HG11  | 2.19                     | 0.41              |
| 1:B:355:GLU:HG2   | 1:B:356:MET:HE2    | 2.01                     | 0.41              |
| 5:Z2:221:U:O4     | 5:Z2:402:U:O2'     | 2.36                     | 0.41              |
| 5:Z2:476:G:H2'    | 5:Z2:477:G:O4'     | 2.20                     | 0.41              |
| 5:Z2:494:U:H4'    | 5:Z2:1219:G:H4'    | 2.03                     | 0.41              |
| 5:Z2:843:G:N3     | 5:Z2:2251:A:H2'    | 2.35                     | 0.41              |
| 5:Z2:1558:A:H5'   | 50:Cl:36:SER:HB2   | 2.03                     | 0.41              |
| 5:Z2:1671:U:H2'   | 5:Z2:1672:A:C8     | 2.56                     | 0.41              |
| 5:Z2:2355:U:O2'   | 5:Z2:2356:A:OP1    | 2.33                     | 0.41              |
| 21:TI:92:GLN:HG3  | 21:TI:101:VAL:HG13 | 2.02                     | 0.41              |
| 26:iN:718:G:N2    | 33:KU:118:HIS:HB2  | 2.35                     | 0.41              |
| 26:iN:1303:G:H2'  | 26:iN:1304:C:C6    | 2.55                     | 0.41              |
| 30:GR:47:ASP:OD1  | 30:GR:47:ASP:N     | 2.51                     | 0.41              |
| 31:GS:27:ILE:HD13 | 31:GS:40:GLU:HG2   | 2.02                     | 0.41              |
| 32:CT:68:ILE:H    | 32:CT:68:ILE:HD12  | 1.85                     | 0.41              |
| 39:Ba:15:THR:HG23 | 39:Ba:16:HIS:CD2   | 2.55                     | 0.41              |
| 53:To:52:LYS:NZ   | 53:To:52:LYS:HB2   | 2.34                     | 0.41              |
| 5:Z2:299:A:C2     | 5:Z2:300:G:C8      | 3.08                     | 0.41              |
| 5:Z2:1602:A:N1    | 18:RF:93:ALA:HB2   | 2.34                     | 0.41              |
| 5:Z2:1672:A:H2'   | 5:Z2:1673:C:H6     | 1.85                     | 0.41              |
| 5:Z2:1914:A:H2'   | 5:Z2:1915:G:O4'    | 2.20                     | 0.41              |
| 5:Z2:2369:U:H2'   | 5:Z2:2370:U:C6     | 2.54                     | 0.41              |
| 5:Z2:2714:G:H2'   | 5:Z2:2715:G:C8     | 2.55                     | 0.41              |
| 5:Z2:2791:U:H3'   | 5:Z2:2792:A:H8     | 1.85                     | 0.41              |
| 14:MB:1:MET:HE3   | 14:MB:1:MET:HB2    | 1.87                     | 0.41              |
| 26:iN:539:A:H2'   | 26:iN:540:U:H5     | 1.82                     | 0.41              |
| 26:iN:748:A:C4    | 26:iN:749:G:C8     | 3.07                     | 0.41              |
| 26:iN:909:A:H2'   | 26:iN:910:C:C6     | 2.55                     | 0.41              |
| 26:iN:1045:U:O2   | 26:iN:1084:G:C2    | 2.73                     | 0.41              |
| 50:Cl:29:PRO:HG2  | 50:Cl:34:LEU:HD11  | 2.02                     | 0.41              |
| 51:Dm:195:ARG:HA  | 51:Dm:195:ARG:HD2  | 1.74                     | 0.41              |
| 4:H:233:ARG:HA    | 4:H:276:ASN:HA     | 2.02                     | 0.41              |
| 5:Z2:85:U:H2'     | 5:Z2:86:C:C6       | 2.56                     | 0.41              |
| 5:Z2:87:G:O2'     | 5:Z2:281:A:N1      | 2.45                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:174:A:H3'    | 5:Z2:175:G:C8      | 2.55                     | 0.41              |
| 5:Z2:1158:U:O2'   | 5:Z2:1159:U:O5'    | 2.35                     | 0.41              |
| 5:Z2:1700:U:H2'   | 5:Z2:1701:G:H8     | 1.84                     | 0.41              |
| 9:L6:110:ARG:HD2  | 9:L6:110:ARG:HA    | 1.92                     | 0.41              |
| 19:FG:26:ILE:HD13 | 19:FG:26:ILE:HA    | 1.86                     | 0.41              |
| 22:fJ:75:LYS:C    | 22:fJ:76:ARG:HD3   | 2.45                     | 0.41              |
| 26:iN:186:A:H2'   | 26:iN:187:G:O4'    | 2.21                     | 0.41              |
| 26:iN:367:G:OP1   | 53:To:17:ARG:NH1   | 2.53                     | 0.41              |
| 26:iN:539:A:H5'   | 26:iN:540:U:OP2    | 2.19                     | 0.41              |
| 26:iN:642:C:H2'   | 26:iN:643:A:C8     | 2.56                     | 0.41              |
| 26:iN:781:U:H2'   | 26:iN:782:U:H6     | 1.85                     | 0.41              |
| 26:iN:801:U:OP1   | 26:iN:866:U:O2'    | 2.35                     | 0.41              |
| 26:iN:966:G:N3    | 26:iN:1443:A:H2    | 2.18                     | 0.41              |
| 26:iN:1140:C:H2'  | 26:iN:1141:C:C6    | 2.56                     | 0.41              |
| 36:IX:73:LYS:HE3  | 36:IX:88:ASN:ND2   | 2.34                     | 0.41              |
| 37:JY:37:CYS:SG   | 37:JY:75:ASP:HB2   | 2.61                     | 0.41              |
| 46:dh:10:GLY:O    | 46:dh:14:ARG:NH1   | 2.53                     | 0.41              |
| 47:Oi:62:THR:HA   | 47:Oi:75:ALA:HA    | 2.02                     | 0.41              |
| 5:Z2:694:U:H2'    | 5:Z2:695:G:H8      | 1.84                     | 0.41              |
| 5:Z2:1299:C:H2'   | 5:Z2:1300:A:C8     | 2.55                     | 0.41              |
| 5:Z2:1485:G:H5''  | 50:Cl:95:LYS:HZ2   | 1.85                     | 0.41              |
| 5:Z2:1806:U:H5    | 50:Cl:177:ARG:HH12 | 1.68                     | 0.41              |
| 16:WD:39:TRP:CD1  | 55:C1:32:PRO:HA    | 2.55                     | 0.41              |
| 26:iN:279:A:H2'   | 26:iN:280:A:H8     | 1.85                     | 0.41              |
| 26:iN:401:U:H2'   | 26:iN:402:G:H8     | 1.83                     | 0.41              |
| 26:iN:805:G:H2'   | 26:iN:806:C:C6     | 2.55                     | 0.41              |
| 26:iN:807:U:H2'   | 26:iN:808:C:C6     | 2.54                     | 0.41              |
| 26:iN:1048:A:H5'' | 26:iN:1069:U:O2    | 2.21                     | 0.41              |
| 26:iN:1229:G:C2   | 26:iN:1230:G:C8    | 3.08                     | 0.41              |
| 31:GS:15:ASP:OD2  | 31:GS:18:PHE:HB2   | 2.20                     | 0.41              |
| 33:KU:112:ASP:HB3 | 34:NV:2:PRO:HB2    | 2.02                     | 0.41              |
| 46:dh:26:GLN:NE2  | 46:dh:48:LYS:HD3   | 2.36                     | 0.41              |
| 1:B:53:ASP:OD2    | 1:B:55:ARG:HB3     | 2.21                     | 0.41              |
| 1:B:74:LYS:HE2    | 1:B:74:LYS:HB2     | 1.68                     | 0.41              |
| 5:Z2:205:C:H2'    | 5:Z2:206:C:C6      | 2.56                     | 0.41              |
| 5:Z2:857:U:H2'    | 5:Z2:858:C:C6      | 2.56                     | 0.41              |
| 5:Z2:2435:C:H2'   | 5:Z2:2436:A:C8     | 2.56                     | 0.41              |
| 5:Z2:2815:G:C6    | 5:Z2:2833:U:C2     | 3.09                     | 0.41              |
| 5:Z2:2853:C:H2'   | 5:Z2:2854:U:H6     | 1.85                     | 0.41              |
| 6:R3:61:GLN:HE22  | 19:FG:90:MET:HE1   | 1.86                     | 0.41              |
| 23:HK:6:MET:HE3   | 23:HK:6:MET:HB3    | 1.76                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:HK:63:ARG:HG2  | 23:HK:68:GLY:HA2   | 2.02                     | 0.41              |
| 26:iN:680:U:H2'   | 26:iN:681:C:C6     | 2.56                     | 0.41              |
| 26:iN:979:A:O2'   | 26:iN:1428:C:N3    | 2.52                     | 0.41              |
| 26:iN:1202:A:H4'  | 26:iN:1203:C:O4'   | 2.19                     | 0.41              |
| 45:Lg:32:PHE:CZ   | 45:Lg:115:ARG:HG3  | 2.55                     | 0.41              |
| 47:Oi:94:VAL:HG11 | 47:Oi:99:LEU:HD11  | 2.03                     | 0.41              |
| 50:Cl:8:PRO:HB3   | 50:Cl:14:ARG:HG3   | 2.03                     | 0.41              |
| 5:Z2:592:U:C5     | 5:Z2:605:G:C5      | 3.08                     | 0.41              |
| 5:Z2:1428:A:C4    | 5:Z2:1429:G:C8     | 3.09                     | 0.41              |
| 5:Z2:1480:A:H2'   | 5:Z2:1482:C:C5     | 2.56                     | 0.41              |
| 5:Z2:1721:C:H2'   | 5:Z2:1722:U:C6     | 2.55                     | 0.41              |
| 5:Z2:2374:G:O6    | 5:Z2:2408:A:H8     | 2.03                     | 0.41              |
| 5:Z2:2428:G:P     | 12:E9:68:ARG:HH12  | 2.41                     | 0.41              |
| 7:A4:69:LYS:NZ    | 7:A4:69:LYS:HB3    | 2.35                     | 0.41              |
| 26:iN:367:G:N2    | 26:iN:369:G:H3'    | 2.36                     | 0.41              |
| 26:iN:662:U:H1'   | 51:Dm:137:VAL:HG12 | 2.02                     | 0.41              |
| 26:iN:908:A:H2'   | 26:iN:909:A:C8     | 2.55                     | 0.41              |
| 26:iN:948:U:H2'   | 26:iN:949:U:C6     | 2.56                     | 0.41              |
| 26:iN:1317:U:C2   | 26:iN:1318:G:C8    | 3.09                     | 0.41              |
| 26:iN:1387:C:H2'  | 26:iN:1388:G:H8    | 1.85                     | 0.41              |
| 32:CT:150:LYS:HB2 | 32:CT:169:ARG:HG3  | 2.03                     | 0.41              |
| 38:QZ:21:ASP:OD2  | 38:QZ:60:GLN:HA    | 2.21                     | 0.41              |
| 51:Dm:177:TRP:CZ3 | 51:Dm:197:ASP:HB3  | 2.55                     | 0.41              |
| 5:Z2:515:A:H4'    | 5:Z2:516:G:C8      | 2.56                     | 0.41              |
| 5:Z2:578:U:H2'    | 5:Z2:579:U:H6      | 1.85                     | 0.41              |
| 5:Z2:2441:G:O2'   | 5:Z2:2443:U:O4     | 2.31                     | 0.41              |
| 5:Z2:2723:A:H2'   | 5:Z2:2724:A:C8     | 2.56                     | 0.41              |
| 12:E9:97:ARG:HG2  | 12:E9:101:ARG:HE   | 1.85                     | 0.41              |
| 19:FG:4:TYR:CZ    | 19:FG:71:LEU:HD22  | 2.55                     | 0.41              |
| 25:MM:28:THR:HG21 | 26:iN:1373:C:OP1   | 2.20                     | 0.41              |
| 26:iN:173:G:O2'   | 26:iN:174:A:H5'    | 2.20                     | 0.41              |
| 26:iN:451:G:H2'   | 26:iN:452:U:O4'    | 2.21                     | 0.41              |
| 26:iN:759:A:H2'   | 26:iN:760:A:H8     | 1.83                     | 0.41              |
| 27:PO:6:ARG:H     | 27:PO:6:ARG:HG2    | 1.71                     | 0.41              |
| 29:BQ:5:ASP:CG    | 29:BQ:79:ARG:HE    | 2.29                     | 0.41              |
| 33:KU:19:GLY:C    | 33:KU:82:ILE:HG13  | 2.45                     | 0.41              |
| 33:KU:31:ILE:HG12 | 33:KU:46:THR:HG22  | 2.03                     | 0.41              |
| 54:ep:3:VAL:HA    | 54:ep:36:ARG:O     | 2.21                     | 0.41              |
| 4:H:98:GLN:OE1    | 4:H:376:ARG:NH2    | 2.48                     | 0.41              |
| 5:Z2:157:C:H2'    | 5:Z2:158:U:C6      | 2.55                     | 0.41              |
| 5:Z2:309:A:OP1    | 12:E9:161:ARG:NE   | 2.43                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:497:A:N3     | 5:Z2:566:C:O2'     | 2.50                     | 0.41              |
| 5:Z2:711:G:HO2'   | 5:Z2:712:A:P       | 2.43                     | 0.41              |
| 5:Z2:1559:A:H2'   | 5:Z2:1560:A:C8     | 2.56                     | 0.41              |
| 5:Z2:1979:U:H4'   | 44:Af:136:THR:OG1  | 2.21                     | 0.41              |
| 9:L6:43:LYS:HG3   | 9:L6:91:PRO:HD3    | 2.03                     | 0.41              |
| 9:L6:114:ARG:HG2  | 9:L6:119:ALA:HB3   | 2.02                     | 0.41              |
| 23:HK:45:MET:HE2  | 23:HK:45:MET:HB3   | 1.79                     | 0.41              |
| 26:iN:82:G:H2'    | 26:iN:83:C:C6      | 2.55                     | 0.41              |
| 26:iN:646:U:H2'   | 26:iN:647:G:H8     | 1.85                     | 0.41              |
| 26:iN:806:C:H2'   | 26:iN:807:U:C6     | 2.55                     | 0.41              |
| 26:iN:1027:A:H5'  | 26:iN:1028:C:OP2   | 2.21                     | 0.41              |
| 26:iN:1224:A:H2'  | 26:iN:1225:A:O4'   | 2.21                     | 0.41              |
| 26:iN:1481:U:C2   | 26:iN:1482:G:C8    | 3.08                     | 0.41              |
| 31:GS:5:ARG:HG3   | 31:GS:6:VAL:H      | 1.85                     | 0.41              |
| 31:GS:58:ASP:OD1  | 31:GS:60:VAL:HG22  | 2.20                     | 0.41              |
| 33:KU:86:VAL:HG11 | 33:KU:93:ARG:HB2   | 2.03                     | 0.41              |
| 36:IX:105:VAL:O   | 36:IX:109:LEU:HD13 | 2.21                     | 0.41              |
| 37:JY:7:ARG:O     | 37:JY:7:ARG:HG3    | 2.21                     | 0.41              |
| 42:Kd:93:SER:H    | 42:Kd:96:THR:HB    | 1.85                     | 0.41              |
| 1:B:17:VAL:HG22   | 1:B:104:ILE:HG12   | 2.02                     | 0.41              |
| 5:Z2:302:U:H2'    | 5:Z2:303:G:O4'     | 2.21                     | 0.41              |
| 5:Z2:728:U:OP1    | 44:Af:138:GLY:HA2  | 2.20                     | 0.41              |
| 5:Z2:824:U:H2'    | 5:Z2:825:C:C6      | 2.56                     | 0.41              |
| 5:Z2:1644:C:H2'   | 5:Z2:1645:U:H6     | 1.86                     | 0.41              |
| 5:Z2:2660:G:H2'   | 5:Z2:2661:A:C8     | 2.56                     | 0.41              |
| 5:Z2:2819:U:H2'   | 5:Z2:2820:G:C8     | 2.56                     | 0.41              |
| 12:E9:5:THR:OG1   | 12:E9:6:VAL:N      | 2.54                     | 0.41              |
| 14:MB:56:LYS:HD3  | 14:MB:87:TYR:O     | 2.21                     | 0.41              |
| 18:RF:82:LEU:HB2  | 18:RF:98:LYS:HB2   | 2.03                     | 0.41              |
| 22:fJ:10:HIS:C    | 22:fJ:26:ARG:HG3   | 2.46                     | 0.41              |
| 23:HK:37:SER:HB3  | 23:HK:40:VAL:HG23  | 2.02                     | 0.41              |
| 26:iN:751:U:H2'   | 26:iN:752:C:H6     | 1.86                     | 0.41              |
| 26:iN:944:A:H2'   | 26:iN:945:A:C8     | 2.56                     | 0.41              |
| 40:Qb:24:LEU:HA   | 40:Qb:94:THR:HG23  | 2.02                     | 0.41              |
| 52:Sn:64:LYS:HD3  | 52:Sn:64:LYS:N     | 2.35                     | 0.41              |
| 1:B:218:ASN:ND2   | 5:Z2:1929:U:OP2    | 2.54                     | 0.40              |
| 1:B:282:LEU:HD11  | 1:B:364:ALA:HB1    | 2.03                     | 0.40              |
| 5:Z2:194:A:N6     | 5:Z2:2413:A:O2'    | 2.54                     | 0.40              |
| 5:Z2:374:A:H1'    | 5:Z2:394:G:O4'     | 2.20                     | 0.40              |
| 5:Z2:582:G:O2'    | 42:Kd:13:GLY:O     | 2.39                     | 0.40              |
| 5:Z2:625:C:H2'    | 5:Z2:626:U:H6      | 1.86                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:Z2:1198:A:H61   | 5:Z2:1219:G:H1'    | 1.85                     | 0.40              |
| 5:Z2:1306:A:C5    | 5:Z2:1307:C:C5     | 3.09                     | 0.40              |
| 5:Z2:1760:C:O2    | 5:Z2:1760:C:H2'    | 2.20                     | 0.40              |
| 5:Z2:2025:U:H2'   | 5:Z2:2026:G:C8     | 2.56                     | 0.40              |
| 5:Z2:2052:C:O2'   | 5:Z2:2053:G:H5'    | 2.21                     | 0.40              |
| 5:Z2:2755:C:H2'   | 5:Z2:2756:U:C6     | 2.56                     | 0.40              |
| 9:L6:9:ARG:NH2    | 26:iN:924:C:OP1    | 2.40                     | 0.40              |
| 11:D8:46:U:H4'    | 41:Nc:99:HIS:HD2   | 1.85                     | 0.40              |
| 23:HK:22:ASP:OD1  | 23:HK:23:LYS:N     | 2.54                     | 0.40              |
| 26:iN:176:U:H2'   | 26:iN:177:C:C6     | 2.56                     | 0.40              |
| 26:iN:469:U:H2'   | 26:iN:470:U:C6     | 2.56                     | 0.40              |
| 26:iN:543:G:H2'   | 26:iN:544:C:C6     | 2.55                     | 0.40              |
| 26:iN:980:C:C2    | 26:iN:981:A:C8     | 3.08                     | 0.40              |
| 31:GS:76:VAL:HG12 | 31:GS:87:GLN:HG3   | 2.02                     | 0.40              |
| 40:Qb:68:ARG:HB3  | 40:Qb:90:ARG:HB3   | 2.03                     | 0.40              |
| 45:Lg:71:ASP:N    | 45:Lg:71:ASP:OD1   | 2.54                     | 0.40              |
| 51:Dm:37:ARG:NH2  | 51:Dm:42:HIS:O     | 2.40                     | 0.40              |
| 5:Z2:189:G:O6     | 5:Z2:200:C:O2'     | 2.25                     | 0.40              |
| 5:Z2:616:A:OP2    | 46:dh:47:LEU:HD11  | 2.21                     | 0.40              |
| 5:Z2:957:A:H5'    | 5:Z2:1172:U:H1'    | 2.03                     | 0.40              |
| 7:A4:136:LYS:HB2  | 7:A4:136:LYS:HE2   | 1.91                     | 0.40              |
| 23:HK:13:ARG:NH1  | 26:iN:1024:C:O2'   | 2.54                     | 0.40              |
| 26:iN:1336:C:OP1  | 31:GS:41:ARG:NH2   | 2.54                     | 0.40              |
| 26:iN:1401:G:H2'  | 26:iN:1402:A:H8    | 1.83                     | 0.40              |
| 26:iN:1469:U:H2'  | 26:iN:1470:U:H6    | 1.86                     | 0.40              |
| 36:IX:89:PHE:CE2  | 36:IX:100:VAL:HG11 | 2.57                     | 0.40              |
| 38:QZ:68:LYS:HG2  | 38:QZ:82:VAL:CG1   | 2.51                     | 0.40              |
| 51:Dm:151:ALA:HB2 | 51:Dm:186:GLN:HG3  | 2.02                     | 0.40              |
| 52:Sn:22:LEU:HB3  | 52:Sn:28:VAL:CG2   | 2.51                     | 0.40              |
| 1:B:64:ILE:HG12   | 1:B:65:HIS:N       | 2.37                     | 0.40              |
| 1:B:269:ALA:HB1   | 1:B:302:TYR:CE1    | 2.57                     | 0.40              |
| 4:H:30:ALA:O      | 4:H:34:THR:HG23    | 2.21                     | 0.40              |
| 4:H:90:LYS:O      | 4:H:94:THR:HG23    | 2.22                     | 0.40              |
| 5:Z2:40:U:O4      | 5:Z2:429:G:O2'     | 2.33                     | 0.40              |
| 5:Z2:816:G:H2'    | 5:Z2:817:U:O4'     | 2.21                     | 0.40              |
| 5:Z2:1090:A:C4    | 5:Z2:1091:G:C8     | 3.09                     | 0.40              |
| 5:Z2:1485:G:OP1   | 50:Cl:101:ARG:NH2  | 2.50                     | 0.40              |
| 5:Z2:2633:U:H2'   | 5:Z2:2634:C:H6     | 1.86                     | 0.40              |
| 5:Z2:2675:G:H1'   | 5:Z2:2813:U:H1'    | 2.03                     | 0.40              |
| 7:A4:166:ILE:HG22 | 7:A4:168:VAL:HG13  | 2.02                     | 0.40              |
| 8:E5:34:ARG:C     | 8:E5:35:ILE:HD13   | 2.46                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:D8:30:U:H2'    | 11:D8:31:G:C8      | 2.56                     | 0.40              |
| 17:XE:30:MET:O    | 17:XE:34:THR:HG22  | 2.22                     | 0.40              |
| 23:HK:67:THR:HG22 | 26:iN:1248:C:H4'   | 2.02                     | 0.40              |
| 26:iN:210:C:H2'   | 26:iN:211:G:C8     | 2.56                     | 0.40              |
| 26:iN:1195:U:O4   | 26:iN:1196:A:N6    | 2.55                     | 0.40              |
| 26:iN:1236:A:H2'  | 26:iN:1237:C:C6    | 2.57                     | 0.40              |
| 29:BQ:104:ALA:O   | 29:BQ:106:VAL:HG23 | 2.21                     | 0.40              |
| 29:BQ:115:ASP:OD1 | 29:BQ:116:ARG:N    | 2.54                     | 0.40              |
| 36:IX:15:TRP:CE2  | 36:IX:135:GLN:HG2  | 2.56                     | 0.40              |
| 40:Qb:28:GLU:OE1  | 40:Qb:28:GLU:N     | 2.53                     | 0.40              |
| 50:Cl:171:TYR:HB3 | 50:Cl:183:ARG:HB2  | 2.02                     | 0.40              |
| 50:Cl:227:PRO:HD3 | 50:Cl:234:GLY:CA   | 2.52                     | 0.40              |
| 53:To:32:LEU:HD21 | 53:To:58:LEU:HD12  | 2.03                     | 0.40              |
| 4:H:150:VAL:O     | 4:H:154:VAL:HG22   | 2.21                     | 0.40              |
| 5:Z2:824:U:H1'    | 5:Z2:1175:G:H1'    | 2.03                     | 0.40              |
| 5:Z2:891:U:O2'    | 45:Lg:67:ARG:NH2   | 2.54                     | 0.40              |
| 5:Z2:1116:U:OP2   | 5:Z2:1117:A:H2'    | 2.21                     | 0.40              |
| 5:Z2:1338:A:H2'   | 5:Z2:1339:G:O4'    | 2.20                     | 0.40              |
| 5:Z2:1844:A:N6    | 5:Z2:1870:G:H1'    | 2.37                     | 0.40              |
| 5:Z2:1985:G:H5''  | 5:Z2:2706:C:O2'    | 2.21                     | 0.40              |
| 8:E5:98:LYS:HB2   | 8:E5:133:TYR:HB2   | 2.03                     | 0.40              |
| 20:VH:81:MET:HE2  | 20:VH:81:MET:HB2   | 1.96                     | 0.40              |
| 22:fJ:15:HIS:HB3  | 22:fJ:44:TYR:CE1   | 2.52                     | 0.40              |
| 26:iN:480:U:H5''  | 51:Dm:159:GLN:OE1  | 2.22                     | 0.40              |
| 26:iN:1317:U:H2'  | 26:iN:1318:G:H8    | 1.85                     | 0.40              |
| 32:CT:190:GLU:OE1 | 32:CT:195:THR:OG1  | 2.35                     | 0.40              |
| 50:Cl:210:ALA:HA  | 50:Cl:213:TRP:CE3  | 2.56                     | 0.40              |
| 51:Dm:106:MET:CE  | 51:Dm:187:GLY:HA3  | 2.51                     | 0.40              |
| 52:Sn:77:ARG:HH11 | 52:Sn:77:ARG:HG3   | 1.87                     | 0.40              |
| 4:H:34:THR:HG22   | 4:H:44:ALA:HA      | 2.04                     | 0.40              |
| 4:H:321:ARG:HB2   | 4:H:386:VAL:HG12   | 2.04                     | 0.40              |
| 5:Z2:205:C:H2'    | 5:Z2:206:C:H6      | 1.87                     | 0.40              |
| 5:Z2:396:C:H2'    | 5:Z2:397:C:C6      | 2.56                     | 0.40              |
| 5:Z2:1098:C:H2'   | 5:Z2:1099:G:C8     | 2.56                     | 0.40              |
| 5:Z2:1137:C:H2'   | 5:Z2:1138:C:H6     | 1.87                     | 0.40              |
| 5:Z2:1276:G:H2'   | 5:Z2:1277:C:H6     | 1.87                     | 0.40              |
| 5:Z2:1707:G:C6    | 5:Z2:1724:G:C6     | 3.09                     | 0.40              |
| 5:Z2:1781:C:H2'   | 5:Z2:1782:U:C6     | 2.57                     | 0.40              |
| 5:Z2:1909:U:H2'   | 5:Z2:1910:C:H6     | 1.86                     | 0.40              |
| 8:E5:35:ILE:HD13  | 8:E5:35:ILE:N      | 2.37                     | 0.40              |
| 15:UC:77:GLN:HB3  | 15:UC:100:ILE:HG22 | 2.04                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:HK:4:LYS:HA    | 23:HK:7:ILE:HD12   | 2.04                     | 0.40              |
| 25:MM:40:ALA:HB3  | 25:MM:43:THR:HG23  | 2.03                     | 0.40              |
| 26:iN:247:G:HO2'  | 26:iN:511:A:H8     | 1.66                     | 0.40              |
| 26:iN:313:A:H2'   | 26:iN:314:C:C6     | 2.57                     | 0.40              |
| 26:iN:643:A:H2'   | 26:iN:644:G:C8     | 2.56                     | 0.40              |
| 34:NV:57:LYS:HE3  | 34:NV:57:LYS:HB3   | 1.83                     | 0.40              |
| 35:YW:5:LYS:HB2   | 35:YW:57:GLU:HB2   | 2.03                     | 0.40              |
| 36:IX:45:THR:HG23 | 36:IX:48:VAL:HB    | 2.02                     | 0.40              |
| 50:Cl:122:SER:HB2 | 50:Cl:130:LEU:HD21 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | B     | 366/369 (99%) | 345 (94%) | 21 (6%) | 0        | 100         | 100 |
| 2   | D     | 23/123 (19%)  | 23 (100%) | 0       | 0        | 100         | 100 |
| 3   | F     | 122/128 (95%) | 111 (91%) | 11 (9%) | 0        | 100         | 100 |
| 4   | H     | 384/396 (97%) | 371 (97%) | 13 (3%) | 0        | 100         | 100 |
| 6   | R3    | 54/76 (71%)   | 54 (100%) | 0       | 0        | 100         | 100 |
| 7   | A4    | 231/269 (86%) | 217 (94%) | 14 (6%) | 0        | 100         | 100 |
| 8   | E5    | 154/171 (90%) | 148 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 9   | L6    | 120/124 (97%) | 113 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 10  | F7    | 175/178 (98%) | 167 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 12  | E9    | 197/200 (98%) | 191 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 13  | aA    | 51/60 (85%)   | 50 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 14  | MB    | 117/119 (98%) | 112 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 15  | UC    | 95/219 (43%)  | 91 (96%)  | 4 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 16  | WD    | 74/78 (95%)   | 72 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 17  | XE    | 60/65 (92%)   | 59 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 18  | RF    | 107/109 (98%) | 104 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 19  | FG    | 100/134 (75%) | 98 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 20  | VH    | 82/85 (96%)   | 77 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 21  | TI    | 100/105 (95%) | 95 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 22  | fJ    | 57/93 (61%)   | 54 (95%)   | 3 (5%)  | 0        | 100         | 100 |
| 23  | HK    | 98/101 (97%)  | 96 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 24  | OL    | 84/88 (96%)   | 80 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 25  | MM    | 114/118 (97%) | 113 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 27  | PO    | 114/118 (97%) | 114 (100%) | 0       | 0        | 100         | 100 |
| 28  | SP    | 76/91 (84%)   | 76 (100%)  | 0       | 0        | 100         | 100 |
| 29  | BQ    | 129/132 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 30  | GR    | 173/177 (98%) | 164 (95%)  | 9 (5%)  | 0        | 100         | 100 |
| 31  | GS    | 151/157 (96%) | 148 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 32  | CT    | 203/241 (84%) | 190 (94%)  | 13 (6%) | 0        | 100         | 100 |
| 33  | KU    | 113/129 (88%) | 108 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 34  | NV    | 55/71 (78%)   | 55 (100%)  | 0       | 0        | 100         | 100 |
| 35  | YW    | 54/59 (92%)   | 53 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 36  | IX    | 140/142 (99%) | 137 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 37  | JY    | 98/103 (95%)  | 93 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 38  | QZ    | 77/91 (85%)   | 75 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 39  | Ba    | 42/44 (96%)   | 39 (93%)   | 3 (7%)  | 0        | 100         | 100 |
| 40  | Qb    | 101/103 (98%) | 98 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 41  | Nc    | 111/116 (96%) | 106 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 42  | Kd    | 143/146 (98%) | 133 (93%)  | 10 (7%) | 0        | 100         | 100 |
| 43  | Je    | 120/122 (98%) | 117 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 44  | Af    | 209/212 (99%) | 198 (95%)  | 10 (5%) | 1 (0%)   | 24          | 40  |
| 45  | Lg    | 135/137 (98%) | 132 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 46  | dh    | 62/65 (95%)   | 61 (98%)   | 0       | 1 (2%)   | 7           | 13  |
| 47  | Oi    | 113/130 (87%) | 105 (93%)  | 8 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 48  | Pj    | 79/89 (89%)     | 79 (100%)  | 0        | 0        | 100         | 100 |
| 49  | bk    | 47/51 (92%)     | 46 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 50  | Cl    | 270/274 (98%)   | 260 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 51  | Dm    | 210/213 (99%)   | 201 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 52  | Sn    | 86/116 (74%)    | 85 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 53  | To    | 85/88 (97%)     | 84 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 54  | ep    | 36/38 (95%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 55  | C1    | 47/166 (28%)    | 45 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| All | All   | 6244/7029 (89%) | 6007 (96%) | 235 (4%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | dh    | 32  | ILE  |
| 44  | Af    | 141 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | B     | 306/310 (99%)  | 270 (88%)  | 36 (12%) | 5           | 9   |
| 2   | D     | 2/87 (2%)      | 2 (100%)   | 0        | 100         | 100 |
| 3   | F     | 101/105 (96%)  | 99 (98%)   | 2 (2%)   | 48          | 67  |
| 4   | H     | 314/327 (96%)  | 312 (99%)  | 2 (1%)   | 78          | 87  |
| 6   | R3    | 51/67 (76%)    | 50 (98%)   | 1 (2%)   | 48          | 67  |
| 7   | A4    | 188/211 (89%)  | 187 (100%) | 1 (0%)   | 81          | 88  |
| 8   | E5    | 118/131 (90%)  | 116 (98%)  | 2 (2%)   | 53          | 71  |
| 9   | L6    | 102/103 (99%)  | 93 (91%)   | 9 (9%)   | 9           | 17  |
| 10  | F7    | 139/146 (95%)  | 138 (99%)  | 1 (1%)   | 76          | 85  |
| 12  | E9    | 159/159 (100%) | 158 (99%)  | 1 (1%)   | 78          | 87  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 13  | aA    | 46/53 (87%)    | 45 (98%)   | 1 (2%)   | 45          | 65  |
| 14  | MB    | 101/102 (99%)  | 99 (98%)   | 2 (2%)   | 48          | 67  |
| 15  | UC    | 79/184 (43%)   | 78 (99%)   | 1 (1%)   | 61          | 75  |
| 16  | WD    | 67/71 (94%)    | 65 (97%)   | 2 (3%)   | 36          | 58  |
| 17  | XE    | 54/57 (95%)    | 53 (98%)   | 1 (2%)   | 50          | 68  |
| 18  | RF    | 88/88 (100%)   | 87 (99%)   | 1 (1%)   | 65          | 79  |
| 19  | FG    | 92/121 (76%)   | 92 (100%)  | 0        | 100         | 100 |
| 20  | VH    | 60/62 (97%)    | 59 (98%)   | 1 (2%)   | 53          | 71  |
| 21  | TI    | 83/85 (98%)    | 83 (100%)  | 0        | 100         | 100 |
| 22  | fJ    | 52/81 (64%)    | 52 (100%)  | 0        | 100         | 100 |
| 23  | HK    | 87/88 (99%)    | 86 (99%)   | 1 (1%)   | 65          | 79  |
| 24  | OL    | 75/77 (97%)    | 73 (97%)   | 2 (3%)   | 39          | 61  |
| 25  | MM    | 97/99 (98%)    | 97 (100%)  | 0        | 100         | 100 |
| 27  | PO    | 88/90 (98%)    | 87 (99%)   | 1 (1%)   | 65          | 79  |
| 28  | SP    | 69/79 (87%)    | 69 (100%)  | 0        | 100         | 100 |
| 29  | BQ    | 103/104 (99%)  | 103 (100%) | 0        | 100         | 100 |
| 30  | GR    | 149/151 (99%)  | 147 (99%)  | 2 (1%)   | 61          | 75  |
| 31  | GS    | 124/128 (97%)  | 123 (99%)  | 1 (1%)   | 73          | 83  |
| 32  | CT    | 168/198 (85%)  | 165 (98%)  | 3 (2%)   | 51          | 69  |
| 33  | KU    | 85/98 (87%)    | 83 (98%)   | 2 (2%)   | 43          | 63  |
| 34  | NV    | 49/63 (78%)    | 47 (96%)   | 2 (4%)   | 27          | 48  |
| 35  | YW    | 50/52 (96%)    | 50 (100%)  | 0        | 100         | 100 |
| 36  | IX    | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 37  | JY    | 88/90 (98%)    | 88 (100%)  | 0        | 100         | 100 |
| 38  | QZ    | 73/84 (87%)    | 71 (97%)   | 2 (3%)   | 39          | 61  |
| 39  | Ba    | 37/37 (100%)   | 37 (100%)  | 0        | 100         | 100 |
| 40  | Qb    | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 79  |
| 41  | Nc    | 81/85 (95%)    | 81 (100%)  | 0        | 100         | 100 |
| 42  | Kd    | 108/110 (98%)  | 106 (98%)  | 2 (2%)   | 50          | 68  |
| 43  | Je    | 102/102 (100%) | 100 (98%)  | 2 (2%)   | 48          | 67  |
| 44  | Af    | 161/162 (99%)  | 159 (99%)  | 2 (1%)   | 63          | 77  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 45  | Lg    | 114/114 (100%)  | 112 (98%)  | 2 (2%)   | 51          | 69  |
| 46  | dh    | 55/56 (98%)     | 54 (98%)   | 1 (2%)   | 51          | 69  |
| 47  | Oi    | 97/108 (90%)    | 94 (97%)   | 3 (3%)   | 35          | 57  |
| 48  | Pj    | 63/68 (93%)     | 62 (98%)   | 1 (2%)   | 55          | 72  |
| 49  | bk    | 42/46 (91%)     | 42 (100%)  | 0        | 100         | 100 |
| 50  | Cl    | 219/221 (99%)   | 218 (100%) | 1 (0%)   | 81          | 88  |
| 51  | Dm    | 177/181 (98%)   | 158 (89%)  | 19 (11%) | 6           | 12  |
| 52  | Sn    | 76/97 (78%)     | 75 (99%)   | 1 (1%)   | 61          | 75  |
| 53  | To    | 67/69 (97%)     | 65 (97%)   | 2 (3%)   | 36          | 58  |
| 54  | ep    | 33/33 (100%)    | 33 (100%)  | 0        | 100         | 100 |
| 55  | C1    | 39/135 (29%)    | 33 (85%)   | 6 (15%)  | 2           | 3   |
| All | All   | 5183/5781 (90%) | 5060 (98%) | 123 (2%) | 43          | 63  |

All (123) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 4   | THR  |
| 1   | B     | 12  | LYS  |
| 1   | B     | 25  | ARG  |
| 1   | B     | 31  | ASP  |
| 1   | B     | 49  | THR  |
| 1   | B     | 54  | LYS  |
| 1   | B     | 56  | THR  |
| 1   | B     | 62  | ASP  |
| 1   | B     | 64  | ILE  |
| 1   | B     | 69  | LYS  |
| 1   | B     | 71  | TYR  |
| 1   | B     | 74  | LYS  |
| 1   | B     | 79  | THR  |
| 1   | B     | 98  | THR  |
| 1   | B     | 106 | ASN  |
| 1   | B     | 114 | VAL  |
| 1   | B     | 115 | ARG  |
| 1   | B     | 137 | GLU  |
| 1   | B     | 143 | VAL  |
| 1   | B     | 148 | ASP  |
| 1   | B     | 149 | THR  |
| 1   | B     | 172 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 188 | LEU  |
| 1   | B     | 210 | LEU  |
| 1   | B     | 216 | VAL  |
| 1   | B     | 219 | ILE  |
| 1   | B     | 225 | VAL  |
| 1   | B     | 239 | LEU  |
| 1   | B     | 265 | LEU  |
| 1   | B     | 300 | THR  |
| 1   | B     | 303 | VAL  |
| 1   | B     | 316 | ASP  |
| 1   | B     | 331 | THR  |
| 1   | B     | 332 | ASP  |
| 1   | B     | 337 | LEU  |
| 1   | B     | 342 | VAL  |
| 3   | F     | 19  | LEU  |
| 3   | F     | 53  | LEU  |
| 4   | H     | 140 | MET  |
| 4   | H     | 332 | GLN  |
| 6   | R3    | 73  | ASN  |
| 7   | A4    | 189 | ILE  |
| 8   | E5    | 37  | SER  |
| 8   | E5    | 127 | ASP  |
| 9   | L6    | 10  | LYS  |
| 9   | L6    | 13  | LYS  |
| 9   | L6    | 20  | LYS  |
| 9   | L6    | 33  | VAL  |
| 9   | L6    | 47  | SER  |
| 9   | L6    | 54  | ARG  |
| 9   | L6    | 55  | VAL  |
| 9   | L6    | 78  | SER  |
| 9   | L6    | 86  | ARG  |
| 10  | F7    | 159 | SER  |
| 12  | E9    | 114 | GLN  |
| 13  | aA    | 23  | THR  |
| 14  | MB    | 89  | ASN  |
| 14  | MB    | 95  | LEU  |
| 15  | UC    | 8   | LEU  |
| 16  | WD    | 25  | THR  |
| 16  | WD    | 65  | ASP  |
| 17  | XE    | 57  | ILE  |
| 18  | RF    | 94  | ASP  |
| 20  | VH    | 14  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | HK    | 62  | ASN  |
| 24  | OL    | 46  | LYS  |
| 24  | OL    | 58  | MET  |
| 27  | PO    | 74  | LEU  |
| 30  | GR    | 175 | LYS  |
| 30  | GR    | 177 | LYS  |
| 31  | GS    | 48  | GLU  |
| 32  | CT    | 16  | LYS  |
| 32  | CT    | 19  | ASN  |
| 32  | CT    | 141 | SER  |
| 33  | KU    | 65  | VAL  |
| 33  | KU    | 86  | VAL  |
| 34  | NV    | 7   | LYS  |
| 34  | NV    | 10  | GLU  |
| 38  | QZ    | 29  | VAL  |
| 38  | QZ    | 35  | VAL  |
| 40  | Qb    | 7   | THR  |
| 42  | Kd    | 57  | THR  |
| 42  | Kd    | 96  | THR  |
| 43  | Je    | 43  | VAL  |
| 43  | Je    | 47  | ILE  |
| 44  | Af    | 40  | ASN  |
| 44  | Af    | 165 | PRO  |
| 45  | Lg    | 76  | ASN  |
| 45  | Lg    | 136 | ILE  |
| 46  | dh    | 17  | ARG  |
| 47  | Oi    | 3   | ASN  |
| 47  | Oi    | 5   | HIS  |
| 47  | Oi    | 112 | ILE  |
| 48  | Pj    | 42  | LEU  |
| 50  | Cl    | 153 | GLN  |
| 51  | Dm    | 25  | VAL  |
| 51  | Dm    | 29  | ASP  |
| 51  | Dm    | 32  | THR  |
| 51  | Dm    | 51  | GLU  |
| 51  | Dm    | 61  | LYS  |
| 51  | Dm    | 103 | VAL  |
| 51  | Dm    | 111 | THR  |
| 51  | Dm    | 117 | GLN  |
| 51  | Dm    | 131 | ARG  |
| 51  | Dm    | 133 | GLU  |
| 51  | Dm    | 153 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | Dm    | 163 | LYS  |
| 51  | Dm    | 170 | THR  |
| 51  | Dm    | 179 | ASP  |
| 51  | Dm    | 182 | HIS  |
| 51  | Dm    | 191 | LYS  |
| 51  | Dm    | 194 | ASP  |
| 51  | Dm    | 195 | ARG  |
| 51  | Dm    | 207 | ILE  |
| 52  | Sn    | 35  | SER  |
| 53  | To    | 58  | LEU  |
| 53  | To    | 77  | SER  |
| 55  | C1    | 9   | ILE  |
| 55  | C1    | 11  | ASN  |
| 55  | C1    | 14  | LYS  |
| 55  | C1    | 18  | THR  |
| 55  | C1    | 31  | ILE  |
| 55  | C1    | 40  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 151 | ASN  |
| 1   | B     | 156 | ASN  |
| 1   | B     | 318 | GLN  |
| 1   | B     | 341 | HIS  |
| 4   | H     | 67  | HIS  |
| 4   | H     | 358 | ASN  |
| 6   | R3    | 61  | GLN  |
| 7   | A4    | 41  | ASN  |
| 7   | A4    | 173 | HIS  |
| 7   | A4    | 234 | GLN  |
| 9   | L6    | 5   | ASN  |
| 13  | aA    | 52  | GLN  |
| 14  | MB    | 31  | HIS  |
| 15  | UC    | 5   | HIS  |
| 15  | UC    | 9   | ASN  |
| 15  | UC    | 98  | GLN  |
| 16  | WD    | 22  | ASN  |
| 19  | FG    | 30  | GLN  |
| 20  | VH    | 3   | HIS  |
| 20  | VH    | 12  | ASN  |
| 20  | VH    | 46  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | fJ    | 74  | ASN  |
| 23  | HK    | 82  | ASN  |
| 28  | SP    | 43  | GLN  |
| 31  | GS    | 154 | HIS  |
| 33  | KU    | 40  | ASN  |
| 34  | NV    | 43  | GLN  |
| 36  | IX    | 47  | HIS  |
| 36  | IX    | 136 | GLN  |
| 38  | QZ    | 43  | GLN  |
| 40  | Qb    | 89  | HIS  |
| 42  | Kd    | 56  | GLN  |
| 43  | Je    | 13  | ASN  |
| 43  | Je    | 20  | GLN  |
| 43  | Je    | 29  | HIS  |
| 43  | Je    | 110 | GLN  |
| 44  | Af    | 40  | ASN  |
| 44  | Af    | 65  | GLN  |
| 44  | Af    | 129 | ASN  |
| 44  | Af    | 176 | GLN  |
| 47  | Oi    | 9   | GLN  |
| 50  | Cl    | 90  | HIS  |
| 50  | Cl    | 200 | ASN  |
| 50  | Cl    | 239 | ASN  |
| 51  | Dm    | 72  | GLN  |
| 52  | Sn    | 20  | GLN  |
| 53  | To    | 3   | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | D8    | 114/115 (99%)   | 16 (14%)          | 0               |
| 26  | iN    | 1499/1590 (94%) | 272 (18%)         | 0               |
| 5   | Z2    | 2723/2882 (94%) | 425 (15%)         | 19 (0%)         |
| All | All   | 4336/4587 (94%) | 713 (16%)         | 19 (0%)         |

All (713) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Z2    | 10  | U    |
| 5   | Z2    | 16  | A    |
| 5   | Z2    | 19  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Z2    | 22  | G    |
| 5   | Z2    | 30  | G    |
| 5   | Z2    | 34  | G    |
| 5   | Z2    | 41  | U    |
| 5   | Z2    | 49  | A    |
| 5   | Z2    | 53  | G    |
| 5   | Z2    | 58  | G    |
| 5   | Z2    | 61  | A    |
| 5   | Z2    | 70  | A    |
| 5   | Z2    | 78  | A    |
| 5   | Z2    | 81  | A    |
| 5   | Z2    | 82  | G    |
| 5   | Z2    | 99  | A    |
| 5   | Z2    | 124 | A    |
| 5   | Z2    | 125 | A    |
| 5   | Z2    | 126 | U    |
| 5   | Z2    | 131 | A    |
| 5   | Z2    | 137 | A    |
| 5   | Z2    | 146 | A    |
| 5   | Z2    | 148 | G    |
| 5   | Z2    | 155 | A    |
| 5   | Z2    | 161 | U    |
| 5   | Z2    | 169 | C    |
| 5   | Z2    | 170 | A    |
| 5   | Z2    | 193 | A    |
| 5   | Z2    | 196 | A    |
| 5   | Z2    | 202 | G    |
| 5   | Z2    | 213 | A    |
| 5   | Z2    | 219 | C    |
| 5   | Z2    | 220 | A    |
| 5   | Z2    | 222 | C    |
| 5   | Z2    | 226 | U    |
| 5   | Z2    | 227 | G    |
| 5   | Z2    | 245 | G    |
| 5   | Z2    | 262 | A    |
| 5   | Z2    | 267 | A    |
| 5   | Z2    | 278 | U    |
| 5   | Z2    | 298 | A    |
| 5   | Z2    | 311 | U    |
| 5   | Z2    | 314 | G    |
| 5   | Z2    | 317 | A    |
| 5   | Z2    | 325 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Z2    | 333 | A    |
| 5   | Z2    | 346 | A    |
| 5   | Z2    | 354 | A    |
| 5   | Z2    | 355 | G    |
| 5   | Z2    | 366 | C    |
| 5   | Z2    | 369 | G    |
| 5   | Z2    | 379 | G    |
| 5   | Z2    | 387 | A    |
| 5   | Z2    | 394 | G    |
| 5   | Z2    | 409 | C    |
| 5   | Z2    | 418 | C    |
| 5   | Z2    | 419 | C    |
| 5   | Z2    | 430 | A    |
| 5   | Z2    | 431 | U    |
| 5   | Z2    | 434 | U    |
| 5   | Z2    | 439 | C    |
| 5   | Z2    | 440 | A    |
| 5   | Z2    | 456 | G    |
| 5   | Z2    | 461 | A    |
| 5   | Z2    | 462 | A    |
| 5   | Z2    | 464 | G    |
| 5   | Z2    | 475 | A    |
| 5   | Z2    | 487 | U    |
| 5   | Z2    | 488 | A    |
| 5   | Z2    | 491 | A    |
| 5   | Z2    | 501 | G    |
| 5   | Z2    | 512 | A    |
| 5   | Z2    | 515 | A    |
| 5   | Z2    | 519 | G    |
| 5   | Z2    | 530 | U    |
| 5   | Z2    | 531 | U    |
| 5   | Z2    | 532 | A    |
| 5   | Z2    | 533 | U    |
| 5   | Z2    | 548 | A    |
| 5   | Z2    | 558 | U    |
| 5   | Z2    | 559 | A    |
| 5   | Z2    | 560 | A    |
| 5   | Z2    | 573 | U    |
| 5   | Z2    | 588 | A    |
| 5   | Z2    | 589 | G    |
| 5   | Z2    | 592 | U    |
| 5   | Z2    | 598 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Z2    | 599 | U    |
| 5   | Z2    | 612 | A    |
| 5   | Z2    | 622 | A    |
| 5   | Z2    | 630 | U    |
| 5   | Z2    | 638 | C    |
| 5   | Z2    | 639 | U    |
| 5   | Z2    | 640 | A    |
| 5   | Z2    | 654 | G    |
| 5   | Z2    | 655 | A    |
| 5   | Z2    | 656 | C    |
| 5   | Z2    | 670 | A    |
| 5   | Z2    | 671 | U    |
| 5   | Z2    | 689 | G    |
| 5   | Z2    | 691 | A    |
| 5   | Z2    | 715 | A    |
| 5   | Z2    | 732 | U    |
| 5   | Z2    | 749 | A    |
| 5   | Z2    | 750 | C    |
| 5   | Z2    | 760 | G    |
| 5   | Z2    | 761 | G    |
| 5   | Z2    | 767 | A    |
| 5   | Z2    | 769 | G    |
| 5   | Z2    | 770 | G    |
| 5   | Z2    | 774 | A    |
| 5   | Z2    | 776 | C    |
| 5   | Z2    | 790 | G    |
| 5   | Z2    | 797 | C    |
| 5   | Z2    | 812 | U    |
| 5   | Z2    | 813 | U    |
| 5   | Z2    | 815 | G    |
| 5   | Z2    | 844 | G    |
| 5   | Z2    | 849 | G    |
| 5   | Z2    | 854 | G    |
| 5   | Z2    | 864 | G    |
| 5   | Z2    | 872 | U    |
| 5   | Z2    | 873 | A    |
| 5   | Z2    | 874 | C    |
| 5   | Z2    | 875 | C    |
| 5   | Z2    | 876 | G    |
| 5   | Z2    | 878 | C    |
| 5   | Z2    | 879 | U    |
| 5   | Z2    | 887 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 892  | G    |
| 5   | Z2    | 895  | A    |
| 5   | Z2    | 912  | A    |
| 5   | Z2    | 917  | U    |
| 5   | Z2    | 929  | A    |
| 5   | Z2    | 930  | C    |
| 5   | Z2    | 945  | C    |
| 5   | Z2    | 958  | G    |
| 5   | Z2    | 966  | C    |
| 5   | Z2    | 967  | A    |
| 5   | Z2    | 969  | C    |
| 5   | Z2    | 980  | A    |
| 5   | Z2    | 983  | U    |
| 5   | Z2    | 987  | G    |
| 5   | Z2    | 995  | U    |
| 5   | Z2    | 996  | U    |
| 5   | Z2    | 997  | C    |
| 5   | Z2    | 1001 | G    |
| 5   | Z2    | 1010 | G    |
| 5   | Z2    | 1018 | G    |
| 5   | Z2    | 1023 | A    |
| 5   | Z2    | 1024 | A    |
| 5   | Z2    | 1025 | G    |
| 5   | Z2    | 1030 | A    |
| 5   | Z2    | 1031 | G    |
| 5   | Z2    | 1044 | U    |
| 5   | Z2    | 1053 | A    |
| 5   | Z2    | 1054 | A    |
| 5   | Z2    | 1055 | G    |
| 5   | Z2    | 1063 | C    |
| 5   | Z2    | 1066 | U    |
| 5   | Z2    | 1072 | A    |
| 5   | Z2    | 1074 | A    |
| 5   | Z2    | 1081 | U    |
| 5   | Z2    | 1085 | U    |
| 5   | Z2    | 1095 | A    |
| 5   | Z2    | 1096 | G    |
| 5   | Z2    | 1113 | A    |
| 5   | Z2    | 1114 | U    |
| 5   | Z2    | 1116 | U    |
| 5   | Z2    | 1117 | A    |
| 5   | Z2    | 1119 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 1120 | G    |
| 5   | Z2    | 1123 | G    |
| 5   | Z2    | 1133 | G    |
| 5   | Z2    | 1155 | A    |
| 5   | Z2    | 1156 | A    |
| 5   | Z2    | 1157 | C    |
| 5   | Z2    | 1158 | U    |
| 5   | Z2    | 1159 | U    |
| 5   | Z2    | 1160 | G    |
| 5   | Z2    | 1161 | U    |
| 5   | Z2    | 1162 | U    |
| 5   | Z2    | 1168 | G    |
| 5   | Z2    | 1179 | G    |
| 5   | Z2    | 1190 | G    |
| 5   | Z2    | 1196 | G    |
| 5   | Z2    | 1211 | G    |
| 5   | Z2    | 1232 | G    |
| 5   | Z2    | 1234 | G    |
| 5   | Z2    | 1237 | A    |
| 5   | Z2    | 1240 | G    |
| 5   | Z2    | 1255 | G    |
| 5   | Z2    | 1256 | A    |
| 5   | Z2    | 1257 | U    |
| 5   | Z2    | 1259 | A    |
| 5   | Z2    | 1260 | U    |
| 5   | Z2    | 1284 | G    |
| 5   | Z2    | 1285 | A    |
| 5   | Z2    | 1298 | C    |
| 5   | Z2    | 1305 | A    |
| 5   | Z2    | 1309 | U    |
| 5   | Z2    | 1313 | U    |
| 5   | Z2    | 1336 | U    |
| 5   | Z2    | 1343 | A    |
| 5   | Z2    | 1349 | A    |
| 5   | Z2    | 1362 | A    |
| 5   | Z2    | 1363 | U    |
| 5   | Z2    | 1364 | G    |
| 5   | Z2    | 1367 | A    |
| 5   | Z2    | 1369 | A    |
| 5   | Z2    | 1370 | U    |
| 5   | Z2    | 1371 | U    |
| 5   | Z2    | 1379 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 1400 | G    |
| 5   | Z2    | 1404 | U    |
| 5   | Z2    | 1405 | G    |
| 5   | Z2    | 1411 | A    |
| 5   | Z2    | 1412 | C    |
| 5   | Z2    | 1419 | G    |
| 5   | Z2    | 1435 | C    |
| 5   | Z2    | 1436 | G    |
| 5   | Z2    | 1443 | G    |
| 5   | Z2    | 1444 | U    |
| 5   | Z2    | 1466 | U    |
| 5   | Z2    | 1474 | A    |
| 5   | Z2    | 1475 | G    |
| 5   | Z2    | 1477 | C    |
| 5   | Z2    | 1478 | A    |
| 5   | Z2    | 1489 | G    |
| 5   | Z2    | 1497 | G    |
| 5   | Z2    | 1501 | A    |
| 5   | Z2    | 1515 | G    |
| 5   | Z2    | 1532 | A    |
| 5   | Z2    | 1536 | G    |
| 5   | Z2    | 1542 | U    |
| 5   | Z2    | 1543 | A    |
| 5   | Z2    | 1548 | G    |
| 5   | Z2    | 1554 | A    |
| 5   | Z2    | 1557 | A    |
| 5   | Z2    | 1564 | U    |
| 5   | Z2    | 1566 | U    |
| 5   | Z2    | 1580 | A    |
| 5   | Z2    | 1581 | A    |
| 5   | Z2    | 1596 | A    |
| 5   | Z2    | 1598 | A    |
| 5   | Z2    | 1603 | C    |
| 5   | Z2    | 1606 | A    |
| 5   | Z2    | 1635 | U    |
| 5   | Z2    | 1636 | U    |
| 5   | Z2    | 1649 | C    |
| 5   | Z2    | 1662 | G    |
| 5   | Z2    | 1663 | C    |
| 5   | Z2    | 1681 | U    |
| 5   | Z2    | 1684 | G    |
| 5   | Z2    | 1707 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 1718 | C    |
| 5   | Z2    | 1719 | U    |
| 5   | Z2    | 1724 | G    |
| 5   | Z2    | 1732 | G    |
| 5   | Z2    | 1750 | G    |
| 5   | Z2    | 1759 | A    |
| 5   | Z2    | 1762 | G    |
| 5   | Z2    | 1768 | U    |
| 5   | Z2    | 1770 | A    |
| 5   | Z2    | 1777 | A    |
| 5   | Z2    | 1785 | G    |
| 5   | Z2    | 1786 | C    |
| 5   | Z2    | 1787 | A    |
| 5   | Z2    | 1796 | A    |
| 5   | Z2    | 1802 | C    |
| 5   | Z2    | 1815 | A    |
| 5   | Z2    | 1819 | C    |
| 5   | Z2    | 1824 | C    |
| 5   | Z2    | 1843 | G    |
| 5   | Z2    | 1848 | G    |
| 5   | Z2    | 1851 | U    |
| 5   | Z2    | 1852 | A    |
| 5   | Z2    | 1855 | G    |
| 5   | Z2    | 1856 | U    |
| 5   | Z2    | 1857 | A    |
| 5   | Z2    | 1881 | C    |
| 5   | Z2    | 1892 | G    |
| 5   | Z2    | 1893 | G    |
| 5   | Z2    | 1899 | A    |
| 5   | Z2    | 1915 | G    |
| 5   | Z2    | 1916 | G    |
| 5   | Z2    | 1918 | A    |
| 5   | Z2    | 1923 | A    |
| 5   | Z2    | 1924 | A    |
| 5   | Z2    | 1925 | U    |
| 5   | Z2    | 1928 | C    |
| 5   | Z2    | 1931 | G    |
| 5   | Z2    | 1941 | U    |
| 5   | Z2    | 1948 | C    |
| 5   | Z2    | 1949 | U    |
| 5   | Z2    | 1950 | G    |
| 5   | Z2    | 1953 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 1956 | A    |
| 5   | Z2    | 1957 | U    |
| 5   | Z2    | 1958 | G    |
| 5   | Z2    | 1968 | U    |
| 5   | Z2    | 1977 | U    |
| 5   | Z2    | 1979 | U    |
| 5   | Z2    | 1983 | C    |
| 5   | Z2    | 2007 | A    |
| 5   | Z2    | 2009 | C    |
| 5   | Z2    | 2017 | A    |
| 5   | Z2    | 2019 | A    |
| 5   | Z2    | 2041 | C    |
| 5   | Z2    | 2042 | G    |
| 5   | Z2    | 2046 | A    |
| 5   | Z2    | 2047 | G    |
| 5   | Z2    | 2048 | A    |
| 5   | Z2    | 2054 | U    |
| 5   | Z2    | 2055 | G    |
| 5   | Z2    | 2079 | G    |
| 5   | Z2    | 2178 | G    |
| 5   | Z2    | 2184 | A    |
| 5   | Z2    | 2189 | A    |
| 5   | Z2    | 2190 | G    |
| 5   | Z2    | 2195 | A    |
| 5   | Z2    | 2197 | C    |
| 5   | Z2    | 2206 | G    |
| 5   | Z2    | 2208 | A    |
| 5   | Z2    | 2221 | G    |
| 5   | Z2    | 2222 | G    |
| 5   | Z2    | 2224 | A    |
| 5   | Z2    | 2252 | G    |
| 5   | Z2    | 2262 | G    |
| 5   | Z2    | 2266 | U    |
| 5   | Z2    | 2270 | A    |
| 5   | Z2    | 2271 | A    |
| 5   | Z2    | 2288 | U    |
| 5   | Z2    | 2302 | U    |
| 5   | Z2    | 2303 | A    |
| 5   | Z2    | 2305 | A    |
| 5   | Z2    | 2306 | G    |
| 5   | Z2    | 2308 | A    |
| 5   | Z2    | 2309 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 2310 | A    |
| 5   | Z2    | 2314 | G    |
| 5   | Z2    | 2317 | A    |
| 5   | Z2    | 2328 | A    |
| 5   | Z2    | 2330 | C    |
| 5   | Z2    | 2333 | C    |
| 5   | Z2    | 2337 | A    |
| 5   | Z2    | 2356 | A    |
| 5   | Z2    | 2360 | A    |
| 5   | Z2    | 2365 | G    |
| 5   | Z2    | 2366 | G    |
| 5   | Z2    | 2368 | C    |
| 5   | Z2    | 2374 | G    |
| 5   | Z2    | 2385 | U    |
| 5   | Z2    | 2386 | C    |
| 5   | Z2    | 2389 | U    |
| 5   | Z2    | 2405 | C    |
| 5   | Z2    | 2408 | A    |
| 5   | Z2    | 2412 | G    |
| 5   | Z2    | 2419 | G    |
| 5   | Z2    | 2422 | A    |
| 5   | Z2    | 2424 | U    |
| 5   | Z2    | 2431 | A    |
| 5   | Z2    | 2453 | G    |
| 5   | Z2    | 2457 | U    |
| 5   | Z2    | 2458 | C    |
| 5   | Z2    | 2459 | A    |
| 5   | Z2    | 2474 | U    |
| 5   | Z2    | 2481 | C    |
| 5   | Z2    | 2485 | G    |
| 5   | Z2    | 2486 | A    |
| 5   | Z2    | 2488 | G    |
| 5   | Z2    | 2501 | A    |
| 5   | Z2    | 2503 | C    |
| 5   | Z2    | 2512 | G    |
| 5   | Z2    | 2530 | A    |
| 5   | Z2    | 2537 | U    |
| 5   | Z2    | 2539 | C    |
| 5   | Z2    | 2545 | U    |
| 5   | Z2    | 2549 | A    |
| 5   | Z2    | 2550 | G    |
| 5   | Z2    | 2556 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 2561 | G    |
| 5   | Z2    | 2565 | G    |
| 5   | Z2    | 2568 | U    |
| 5   | Z2    | 2585 | A    |
| 5   | Z2    | 2592 | U    |
| 5   | Z2    | 2596 | U    |
| 5   | Z2    | 2598 | U    |
| 5   | Z2    | 2604 | G    |
| 5   | Z2    | 2612 | U    |
| 5   | Z2    | 2619 | U    |
| 5   | Z2    | 2623 | G    |
| 5   | Z2    | 2646 | G    |
| 5   | Z2    | 2654 | G    |
| 5   | Z2    | 2656 | G    |
| 5   | Z2    | 2657 | G    |
| 5   | Z2    | 2658 | A    |
| 5   | Z2    | 2665 | U    |
| 5   | Z2    | 2668 | G    |
| 5   | Z2    | 2672 | U    |
| 5   | Z2    | 2673 | U    |
| 5   | Z2    | 2697 | G    |
| 5   | Z2    | 2701 | G    |
| 5   | Z2    | 2709 | C    |
| 5   | Z2    | 2715 | G    |
| 5   | Z2    | 2716 | A    |
| 5   | Z2    | 2731 | A    |
| 5   | Z2    | 2740 | A    |
| 5   | Z2    | 2748 | A    |
| 5   | Z2    | 2749 | G    |
| 5   | Z2    | 2761 | A    |
| 5   | Z2    | 2762 | U    |
| 5   | Z2    | 2763 | U    |
| 5   | Z2    | 2773 | U    |
| 5   | Z2    | 2774 | A    |
| 5   | Z2    | 2775 | A    |
| 5   | Z2    | 2784 | U    |
| 5   | Z2    | 2786 | A    |
| 5   | Z2    | 2787 | A    |
| 5   | Z2    | 2801 | A    |
| 5   | Z2    | 2802 | U    |
| 5   | Z2    | 2815 | G    |
| 5   | Z2    | 2827 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 2839 | A    |
| 5   | Z2    | 2850 | U    |
| 11  | D8    | 6    | C    |
| 11  | D8    | 22   | G    |
| 11  | D8    | 24   | A    |
| 11  | D8    | 28   | C    |
| 11  | D8    | 35   | C    |
| 11  | D8    | 38   | U    |
| 11  | D8    | 39   | C    |
| 11  | D8    | 49   | G    |
| 11  | D8    | 50   | A    |
| 11  | D8    | 51   | A    |
| 11  | D8    | 54   | G    |
| 11  | D8    | 88   | A    |
| 11  | D8    | 96   | A    |
| 11  | D8    | 105  | C    |
| 11  | D8    | 106  | A    |
| 11  | D8    | 108  | C    |
| 26  | iN    | 51   | C    |
| 26  | iN    | 52   | U    |
| 26  | iN    | 54   | A    |
| 26  | iN    | 56   | G    |
| 26  | iN    | 69   | G    |
| 26  | iN    | 79   | A    |
| 26  | iN    | 80   | A    |
| 26  | iN    | 86   | G    |
| 26  | iN    | 94   | C    |
| 26  | iN    | 95   | U    |
| 26  | iN    | 97   | A    |
| 26  | iN    | 98   | A    |
| 26  | iN    | 116  | G    |
| 26  | iN    | 118  | A    |
| 26  | iN    | 122  | G    |
| 26  | iN    | 125  | G    |
| 26  | iN    | 127  | A    |
| 26  | iN    | 128  | G    |
| 26  | iN    | 130  | U    |
| 26  | iN    | 131  | U    |
| 26  | iN    | 132  | G    |
| 26  | iN    | 135  | U    |
| 26  | iN    | 136  | C    |
| 26  | iN    | 137  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | iN    | 139 | G    |
| 26  | iN    | 141 | U    |
| 26  | iN    | 143 | A    |
| 26  | iN    | 164 | A    |
| 26  | iN    | 166 | U    |
| 26  | iN    | 167 | A    |
| 26  | iN    | 172 | G    |
| 26  | iN    | 174 | A    |
| 26  | iN    | 175 | A    |
| 26  | iN    | 176 | U    |
| 26  | iN    | 187 | G    |
| 26  | iN    | 189 | G    |
| 26  | iN    | 197 | G    |
| 26  | iN    | 200 | C    |
| 26  | iN    | 202 | G    |
| 26  | iN    | 206 | A    |
| 26  | iN    | 208 | C    |
| 26  | iN    | 210 | C    |
| 26  | iN    | 218 | U    |
| 26  | iN    | 225 | U    |
| 26  | iN    | 233 | A    |
| 26  | iN    | 234 | C    |
| 26  | iN    | 238 | A    |
| 26  | iN    | 240 | A    |
| 26  | iN    | 242 | A    |
| 26  | iN    | 247 | G    |
| 26  | iN    | 259 | U    |
| 26  | iN    | 263 | G    |
| 26  | iN    | 275 | G    |
| 26  | iN    | 286 | A    |
| 26  | iN    | 288 | U    |
| 26  | iN    | 290 | G    |
| 26  | iN    | 294 | G    |
| 26  | iN    | 309 | G    |
| 26  | iN    | 310 | C    |
| 26  | iN    | 317 | U    |
| 26  | iN    | 332 | G    |
| 26  | iN    | 364 | A    |
| 26  | iN    | 371 | C    |
| 26  | iN    | 372 | A    |
| 26  | iN    | 373 | C    |
| 26  | iN    | 375 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | iN    | 395 | C    |
| 26  | iN    | 397 | G    |
| 26  | iN    | 398 | C    |
| 26  | iN    | 406 | A    |
| 26  | iN    | 410 | U    |
| 26  | iN    | 415 | C    |
| 26  | iN    | 425 | A    |
| 26  | iN    | 435 | C    |
| 26  | iN    | 449 | G    |
| 26  | iN    | 450 | U    |
| 26  | iN    | 451 | G    |
| 26  | iN    | 452 | U    |
| 26  | iN    | 454 | A    |
| 26  | iN    | 456 | G    |
| 26  | iN    | 457 | A    |
| 26  | iN    | 464 | U    |
| 26  | iN    | 465 | U    |
| 26  | iN    | 466 | U    |
| 26  | iN    | 467 | G    |
| 26  | iN    | 472 | U    |
| 26  | iN    | 482 | U    |
| 26  | iN    | 488 | G    |
| 26  | iN    | 496 | G    |
| 26  | iN    | 497 | A    |
| 26  | iN    | 502 | G    |
| 26  | iN    | 508 | A    |
| 26  | iN    | 510 | U    |
| 26  | iN    | 511 | A    |
| 26  | iN    | 514 | C    |
| 26  | iN    | 521 | G    |
| 26  | iN    | 522 | A    |
| 26  | iN    | 524 | G    |
| 26  | iN    | 527 | A    |
| 26  | iN    | 529 | U    |
| 26  | iN    | 538 | A    |
| 26  | iN    | 552 | A    |
| 26  | iN    | 554 | C    |
| 26  | iN    | 561 | C    |
| 26  | iN    | 567 | G    |
| 26  | iN    | 574 | U    |
| 26  | iN    | 575 | A    |
| 26  | iN    | 578 | A    |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | iN    | 582 | A    |
| 26  | iN    | 590 | A    |
| 26  | iN    | 592 | C    |
| 26  | iN    | 607 | C    |
| 26  | iN    | 609 | G    |
| 26  | iN    | 614 | U    |
| 26  | iN    | 615 | A    |
| 26  | iN    | 616 | A    |
| 26  | iN    | 617 | A    |
| 26  | iN    | 619 | G    |
| 26  | iN    | 620 | G    |
| 26  | iN    | 631 | G    |
| 26  | iN    | 639 | A    |
| 26  | iN    | 658 | G    |
| 26  | iN    | 660 | G    |
| 26  | iN    | 662 | U    |
| 26  | iN    | 675 | U    |
| 26  | iN    | 677 | G    |
| 26  | iN    | 686 | A    |
| 26  | iN    | 697 | A    |
| 26  | iN    | 709 | A    |
| 26  | iN    | 730 | U    |
| 26  | iN    | 731 | A    |
| 26  | iN    | 732 | G    |
| 26  | iN    | 739 | A    |
| 26  | iN    | 747 | G    |
| 26  | iN    | 761 | U    |
| 26  | iN    | 765 | G    |
| 26  | iN    | 767 | U    |
| 26  | iN    | 768 | G    |
| 26  | iN    | 773 | A    |
| 26  | iN    | 789 | U    |
| 26  | iN    | 798 | C    |
| 26  | iN    | 799 | A    |
| 26  | iN    | 803 | A    |
| 26  | iN    | 821 | A    |
| 26  | iN    | 825 | A    |
| 26  | iN    | 837 | U    |
| 26  | iN    | 838 | A    |
| 26  | iN    | 843 | G    |
| 26  | iN    | 859 | A    |
| 26  | iN    | 861 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | iN    | 872  | A    |
| 26  | iN    | 880  | G    |
| 26  | iN    | 891  | G    |
| 26  | iN    | 897  | G    |
| 26  | iN    | 911  | G    |
| 26  | iN    | 916  | A    |
| 26  | iN    | 956  | C    |
| 26  | iN    | 958  | A    |
| 26  | iN    | 970  | G    |
| 26  | iN    | 971  | G    |
| 26  | iN    | 978  | C    |
| 26  | iN    | 979  | A    |
| 26  | iN    | 1002 | A    |
| 26  | iN    | 1004 | U    |
| 26  | iN    | 1011 | C    |
| 26  | iN    | 1013 | A    |
| 26  | iN    | 1019 | A    |
| 26  | iN    | 1020 | G    |
| 26  | iN    | 1021 | A    |
| 26  | iN    | 1023 | C    |
| 26  | iN    | 1033 | U    |
| 26  | iN    | 1043 | U    |
| 26  | iN    | 1048 | A    |
| 26  | iN    | 1050 | U    |
| 26  | iN    | 1053 | U    |
| 26  | iN    | 1056 | A    |
| 26  | iN    | 1070 | G    |
| 26  | iN    | 1072 | C    |
| 26  | iN    | 1074 | U    |
| 26  | iN    | 1075 | C    |
| 26  | iN    | 1076 | G    |
| 26  | iN    | 1077 | G    |
| 26  | iN    | 1078 | G    |
| 26  | iN    | 1080 | A    |
| 26  | iN    | 1081 | U    |
| 26  | iN    | 1085 | A    |
| 26  | iN    | 1089 | C    |
| 26  | iN    | 1109 | U    |
| 26  | iN    | 1110 | C    |
| 26  | iN    | 1114 | U    |
| 26  | iN    | 1129 | U    |
| 26  | iN    | 1133 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | iN    | 1138 | G    |
| 26  | iN    | 1139 | U    |
| 26  | iN    | 1145 | A    |
| 26  | iN    | 1168 | G    |
| 26  | iN    | 1197 | A    |
| 26  | iN    | 1202 | A    |
| 26  | iN    | 1204 | U    |
| 26  | iN    | 1209 | G    |
| 26  | iN    | 1210 | U    |
| 26  | iN    | 1213 | C    |
| 26  | iN    | 1214 | A    |
| 26  | iN    | 1216 | A    |
| 26  | iN    | 1219 | G    |
| 26  | iN    | 1241 | A    |
| 26  | iN    | 1242 | A    |
| 26  | iN    | 1247 | U    |
| 26  | iN    | 1257 | U    |
| 26  | iN    | 1258 | A    |
| 26  | iN    | 1271 | C    |
| 26  | iN    | 1272 | A    |
| 26  | iN    | 1273 | C    |
| 26  | iN    | 1278 | G    |
| 26  | iN    | 1281 | A    |
| 26  | iN    | 1283 | A    |
| 26  | iN    | 1284 | A    |
| 26  | iN    | 1286 | G    |
| 26  | iN    | 1291 | G    |
| 26  | iN    | 1302 | A    |
| 26  | iN    | 1303 | G    |
| 26  | iN    | 1305 | U    |
| 26  | iN    | 1323 | G    |
| 26  | iN    | 1331 | A    |
| 26  | iN    | 1332 | A    |
| 26  | iN    | 1333 | A    |
| 26  | iN    | 1345 | G    |
| 26  | iN    | 1347 | C    |
| 26  | iN    | 1348 | C    |
| 26  | iN    | 1350 | G    |
| 26  | iN    | 1360 | U    |
| 26  | iN    | 1362 | C    |
| 26  | iN    | 1363 | A    |
| 26  | iN    | 1365 | C    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | iN    | 1367 | C    |
| 26  | iN    | 1377 | A    |
| 26  | iN    | 1383 | G    |
| 26  | iN    | 1391 | A    |
| 26  | iN    | 1398 | G    |
| 26  | iN    | 1408 | A    |
| 26  | iN    | 1415 | G    |
| 26  | iN    | 1424 | G    |
| 26  | iN    | 1426 | U    |
| 26  | iN    | 1427 | C    |
| 26  | iN    | 1428 | C    |
| 26  | iN    | 1439 | A    |
| 26  | iN    | 1443 | A    |
| 26  | iN    | 1464 | G    |
| 26  | iN    | 1472 | C    |
| 26  | iN    | 1473 | A    |
| 26  | iN    | 1477 | G    |
| 26  | iN    | 1486 | A    |
| 26  | iN    | 1490 | U    |
| 26  | iN    | 1491 | A    |
| 26  | iN    | 1496 | U    |
| 26  | iN    | 1497 | C    |
| 26  | iN    | 1513 | A    |
| 26  | iN    | 1520 | G    |
| 26  | iN    | 1527 | G    |
| 26  | iN    | 1532 | G    |
| 26  | iN    | 1538 | A    |
| 26  | iN    | 1539 | G    |
| 26  | iN    | 1542 | G    |
| 26  | iN    | 1548 | A    |
| 26  | iN    | 1549 | G    |
| 26  | iN    | 1551 | U    |
| 26  | iN    | 1562 | G    |
| 26  | iN    | 1564 | A    |
| 26  | iN    | 1574 | G    |
| 26  | iN    | 1575 | G    |
| 26  | iN    | 1577 | U    |
| 26  | iN    | 1578 | C    |

All (19) RNA pucker outliers are listed below:

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
|-----|-------|-----|------|

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Z2    | 9    | G    |
| 5   | Z2    | 169  | C    |
| 5   | Z2    | 532  | A    |
| 5   | Z2    | 637  | U    |
| 5   | Z2    | 769  | G    |
| 5   | Z2    | 812  | U    |
| 5   | Z2    | 875  | C    |
| 5   | Z2    | 886  | A    |
| 5   | Z2    | 916  | A    |
| 5   | Z2    | 1580 | A    |
| 5   | Z2    | 1717 | U    |
| 5   | Z2    | 1856 | U    |
| 5   | Z2    | 1927 | C    |
| 5   | Z2    | 2196 | A    |
| 5   | Z2    | 2223 | U    |
| 5   | Z2    | 2309 | U    |
| 5   | Z2    | 2355 | U    |
| 5   | Z2    | 2457 | U    |
| 5   | Z2    | 2739 | U    |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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 |
| 56  | GDP  | H     | 401 | 57   | 29,30,30     | 1.18 | 3 (10%)  | 45,47,47    | 1.75 | 7 (15%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 56  | GDP  | H     | 401 | 57   | -       | 3/16/32/32 | 0/3/3/3 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 56  | H     | 401 | GDP  | C5-C4 | 3.27  | 1.47        | 1.38     |
| 56  | H     | 401 | GDP  | C6-N1 | -2.52 | 1.34        | 1.38     |
| 56  | H     | 401 | GDP  | C5-N7 | -2.11 | 1.34        | 1.39     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | H     | 401 | GDP  | C5-C4-N3    | -6.24 | 118.46      | 128.39   |
| 56  | H     | 401 | GDP  | N9-C4-N3    | 4.78  | 135.51      | 125.95   |
| 56  | H     | 401 | GDP  | C2-N3-C4    | 4.77  | 120.52      | 112.30   |
| 56  | H     | 401 | GDP  | C6-C5-N7    | 2.81  | 135.41      | 130.29   |
| 56  | H     | 401 | GDP  | C4-C5-N7    | -2.46 | 106.78      | 110.67   |
| 56  | H     | 401 | GDP  | C3'-C2'-C1' | 2.28  | 105.78      | 101.46   |
| 56  | H     | 401 | GDP  | O6-C6-C5    | -2.08 | 121.05      | 126.53   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

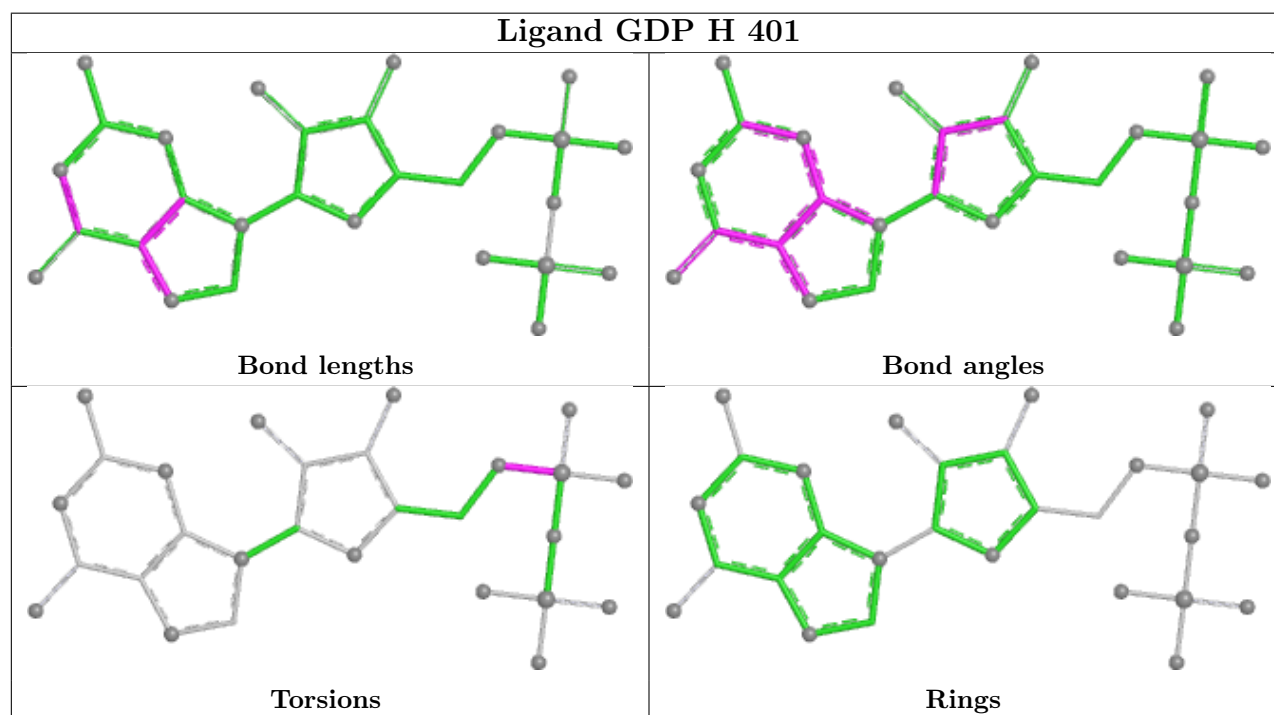
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 56  | H     | 401 | GDP  | C5'-O5'-PA-O1A |
| 56  | H     | 401 | GDP  | C5'-O5'-PA-O3A |
| 56  | H     | 401 | GDP  | C5'-O5'-PA-O2A |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56  | H     | 401 | GDP  | 1       | 0            |

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



## 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.

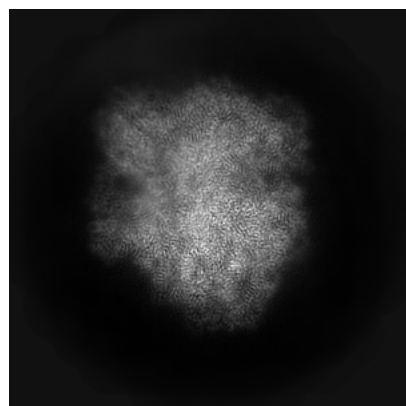
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19077. These allow visual inspection of the internal detail of the map and identification of artifacts.

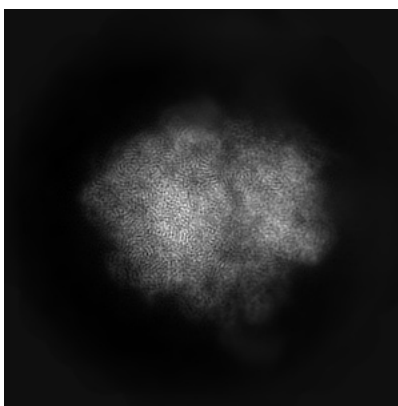
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

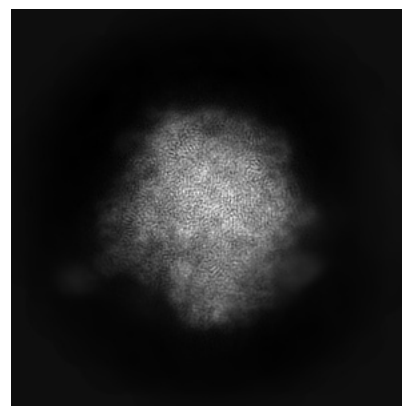
#### 6.1.1 Primary map



X

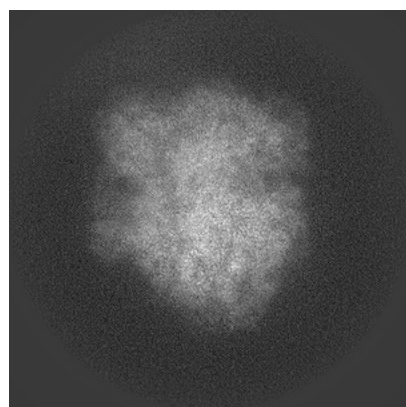


Y

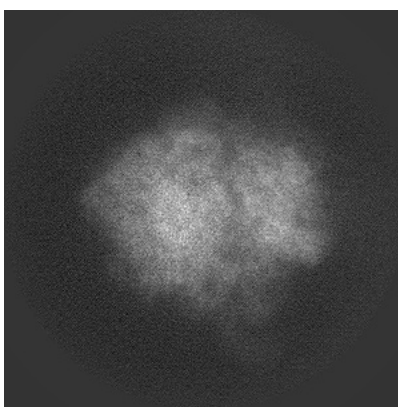


Z

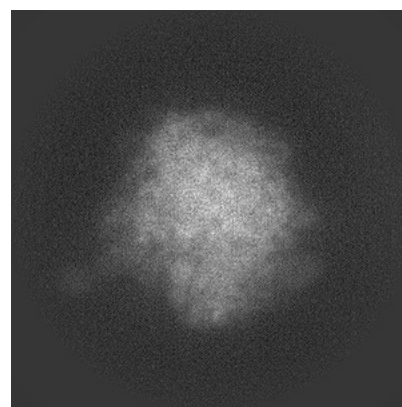
#### 6.1.2 Raw map



X



Y

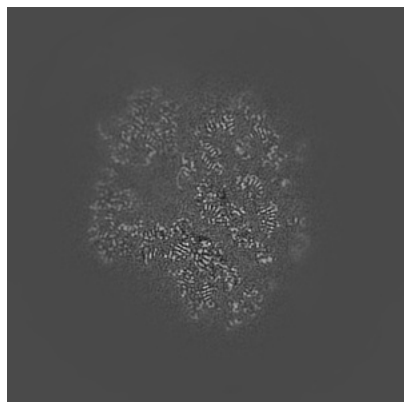


Z

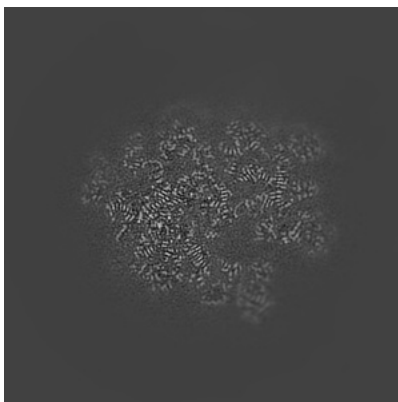
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

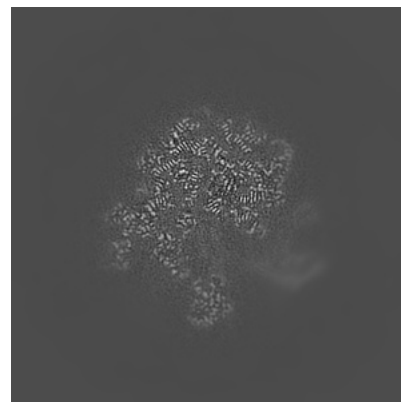
### 6.2.1 Primary map



X Index: 270

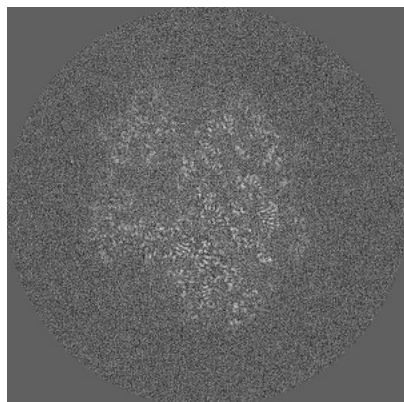


Y Index: 270

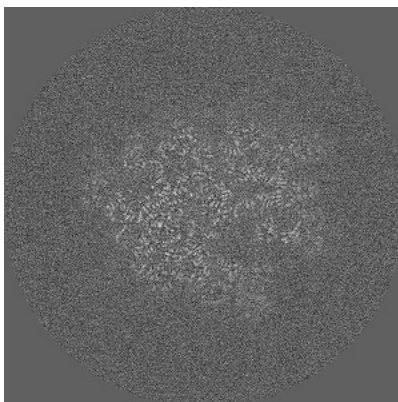


Z Index: 270

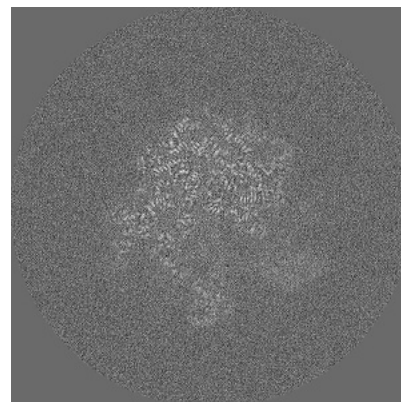
### 6.2.2 Raw map



X Index: 270



Y Index: 270

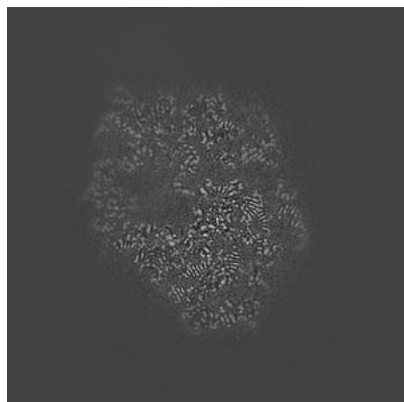


Z Index: 270

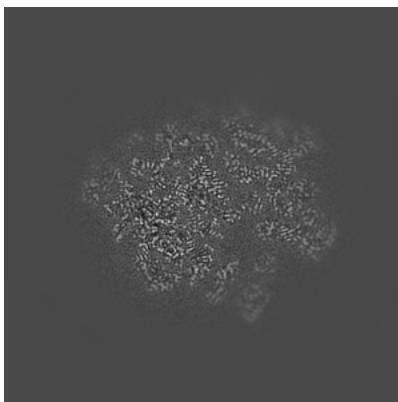
The images above show central slices of the map in three orthogonal directions.

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

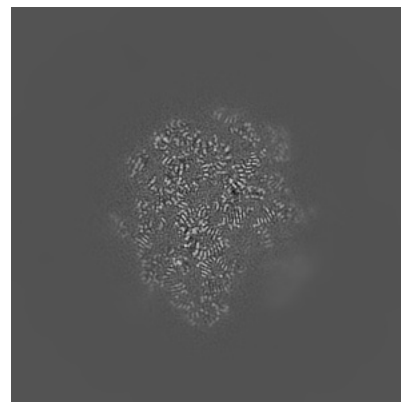
### 6.3.1 Primary map



X Index: 286

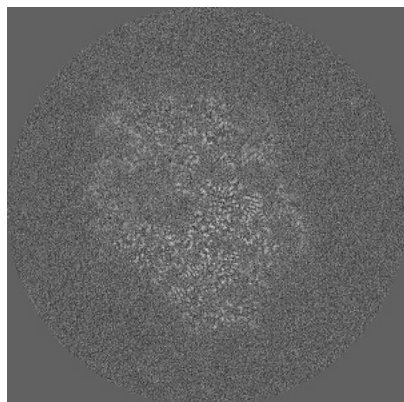


Y Index: 277

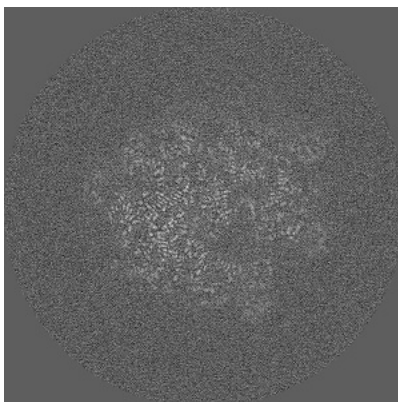


Z Index: 237

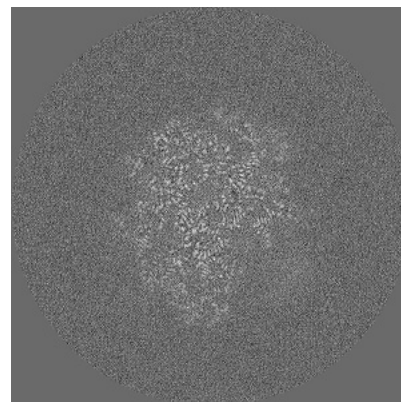
### 6.3.2 Raw map



X Index: 286



Y Index: 268

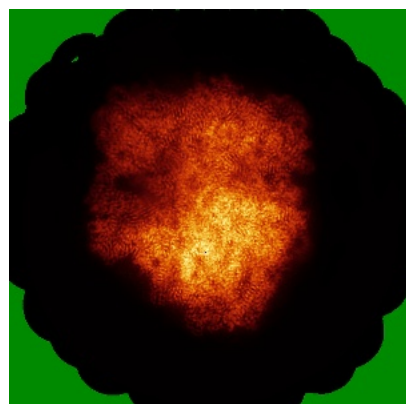


Z Index: 237

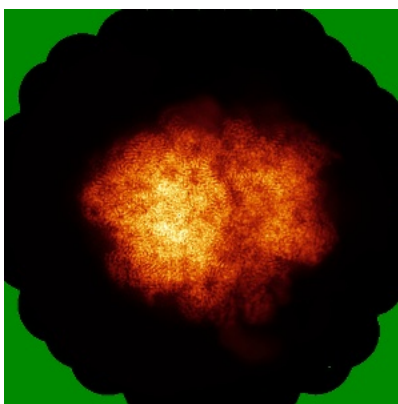
The images above show the largest variance slices of the map in three orthogonal directions.

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

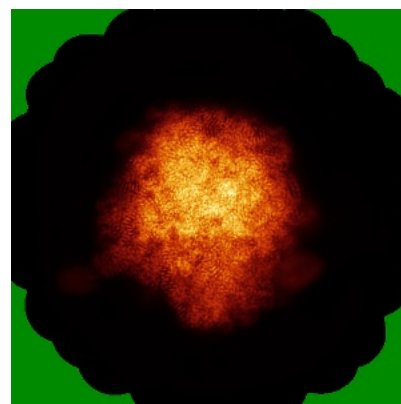
### 6.4.1 Primary map



X

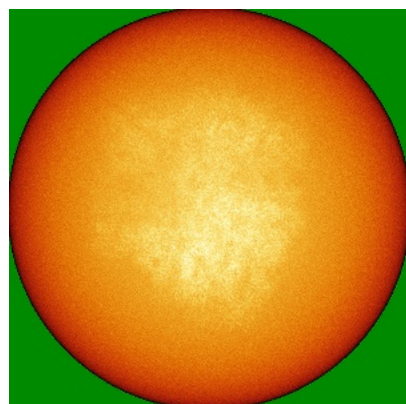


Y

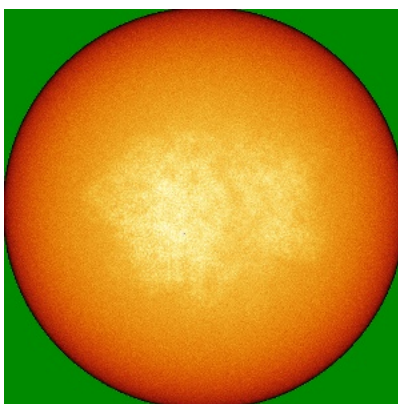


Z

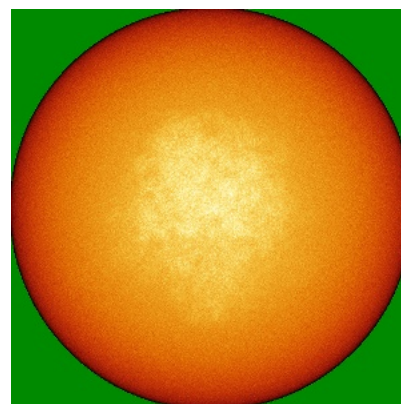
### 6.4.2 Raw map



X



Y

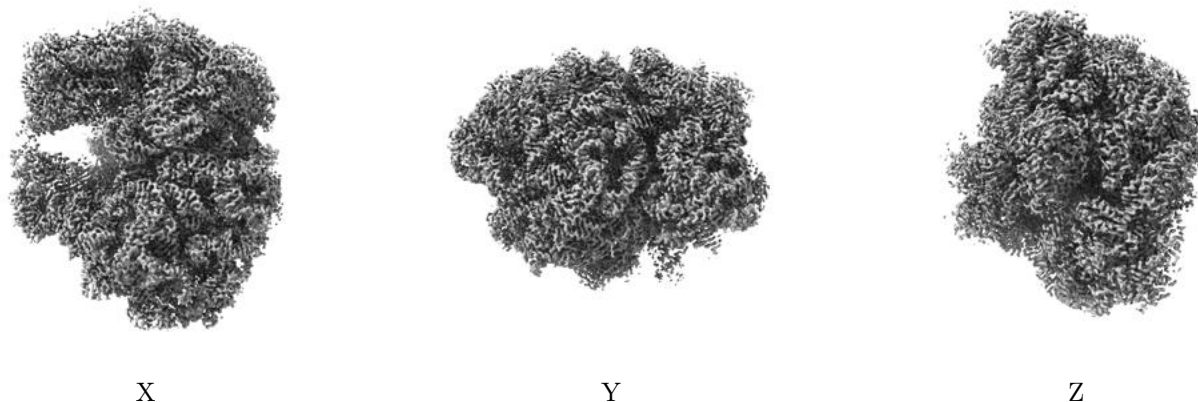


Z

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

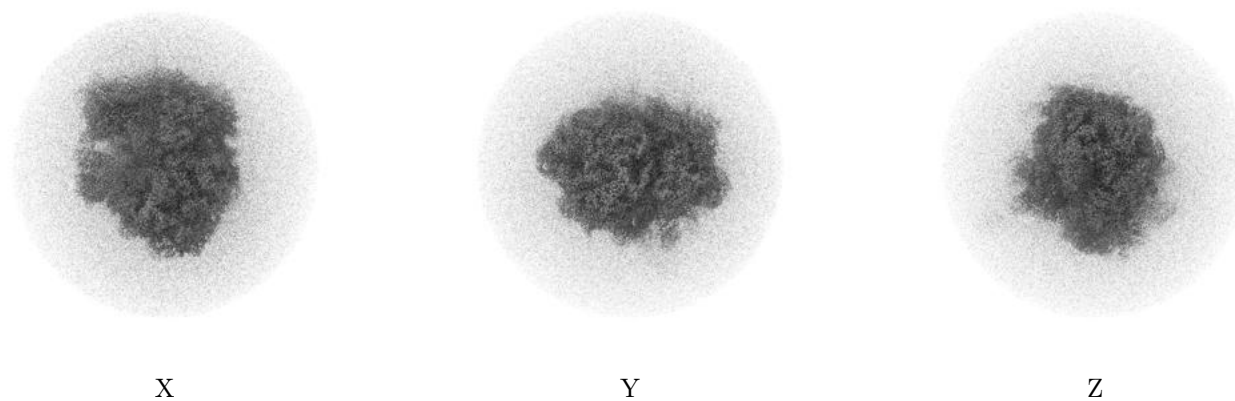
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0189. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

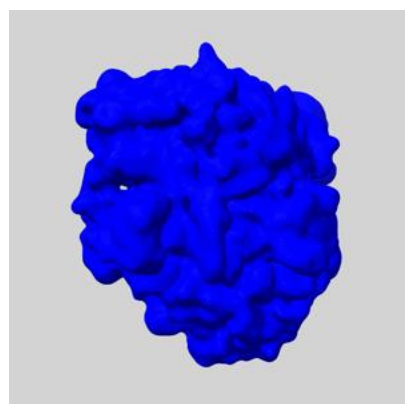
## 6.6 Mask visualisation [i](#)

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

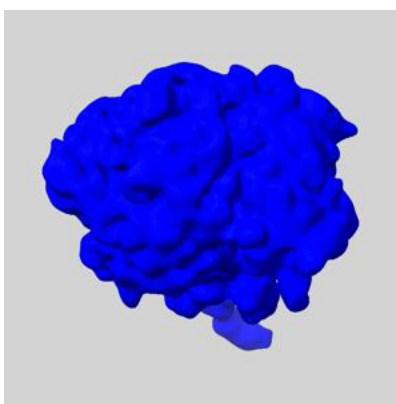
A mask typically either:

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

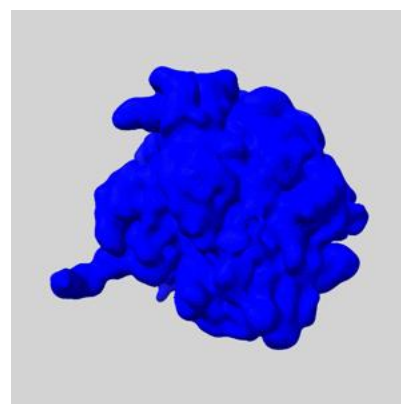
### 6.6.1 emd\_19077\_msk\_1.map [i](#)



X



Y

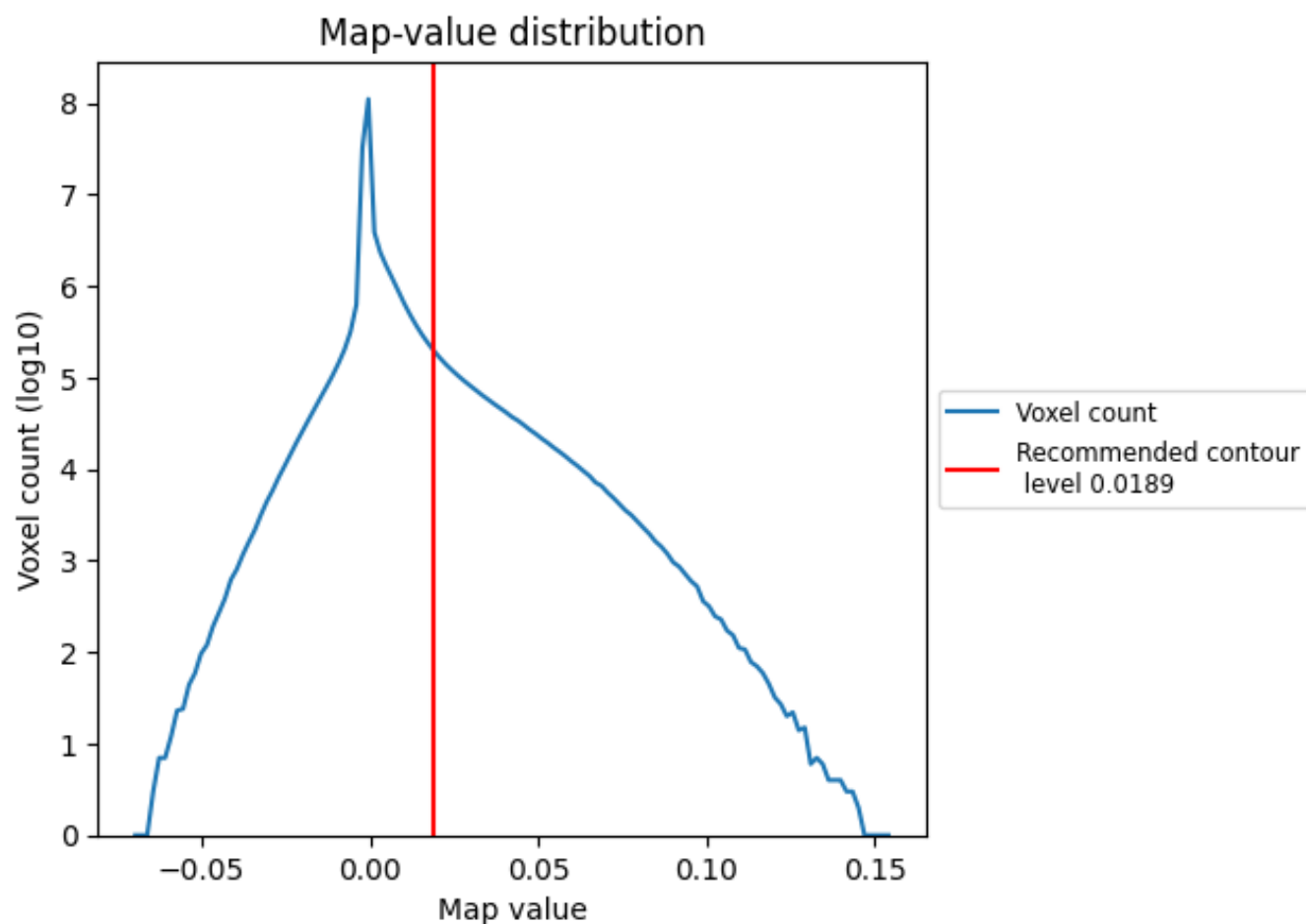


Z

## 7 Map analysis [i](#)

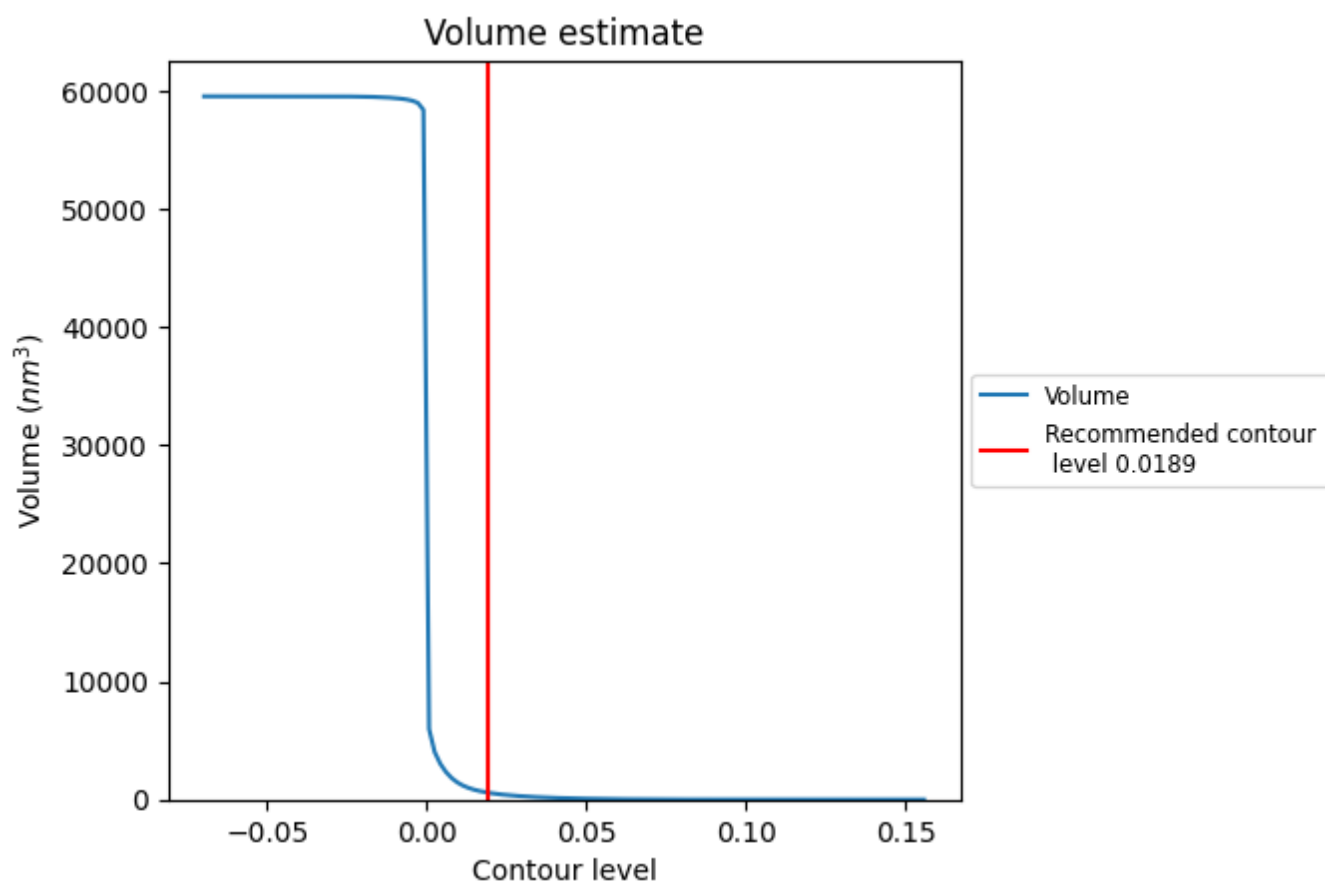
This section contains the results of statistical analysis of the map.

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



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

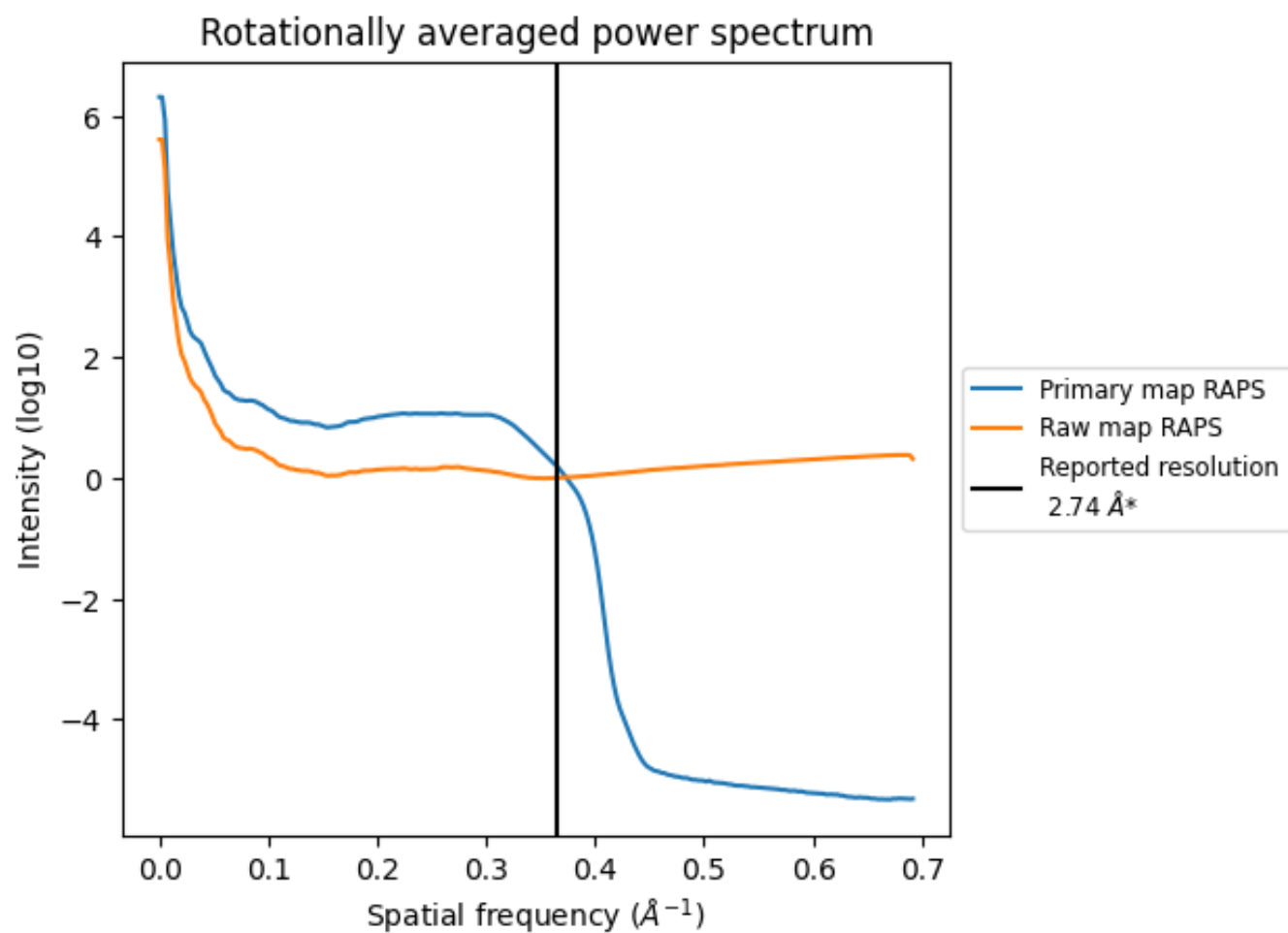
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 597  $\text{nm}^3$ ; this corresponds to an approximate mass of 539 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 [i](#)

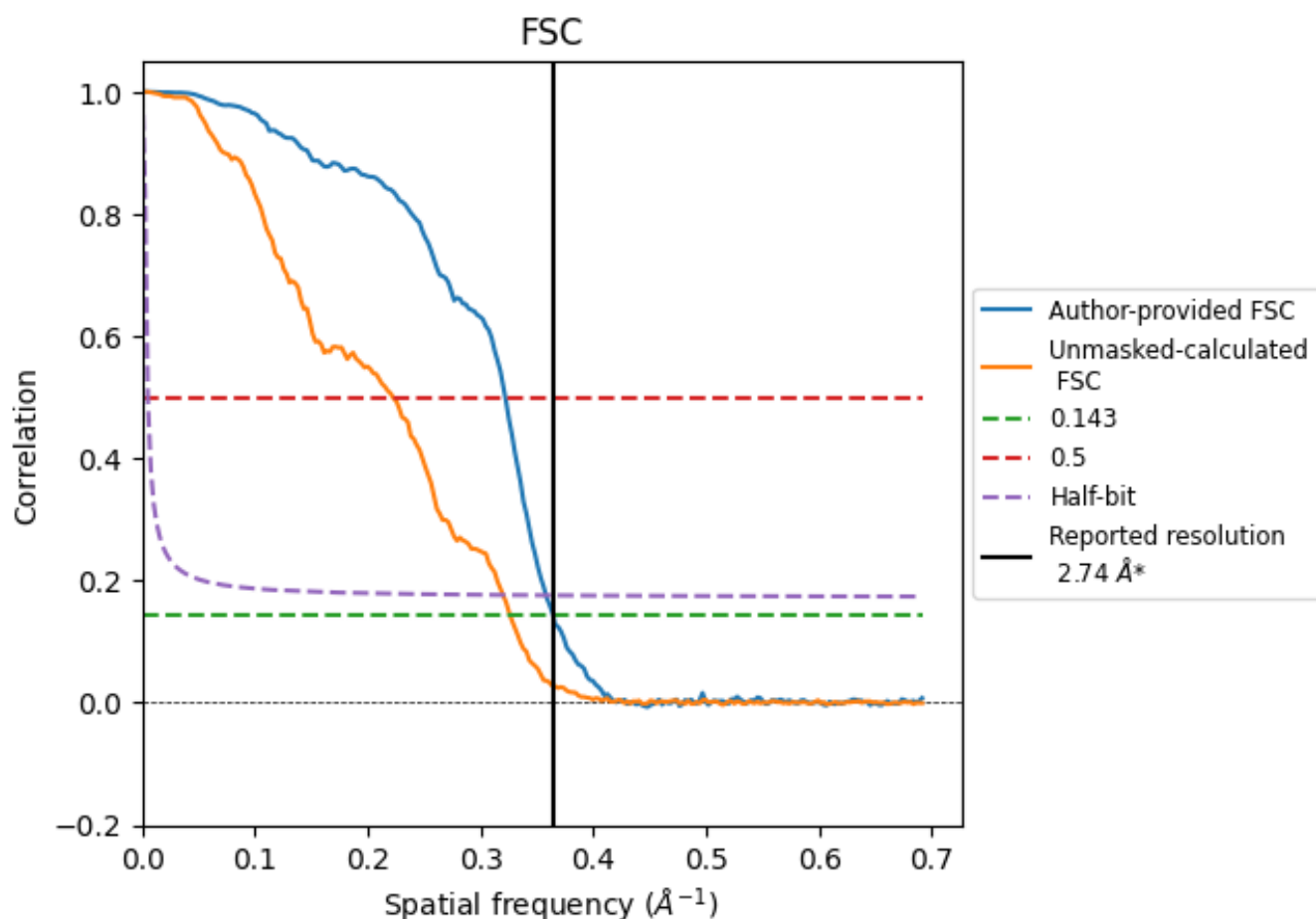


\*Reported resolution corresponds to spatial frequency of 0.365  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.365  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

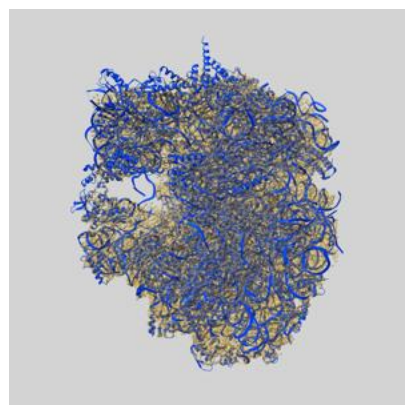
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.74                               | -    | -        |
| Author-provided FSC curve | 2.74                               | 3.11 | 2.79     |
| Unmasked-calculated*      | 3.07                               | 4.50 | 3.12     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.74 by more than 10 %

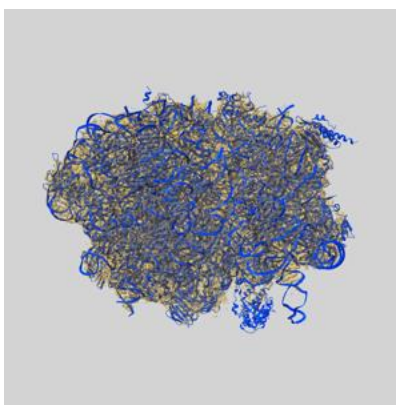
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19077 and PDB model 8RDW. Per-residue inclusion information can be found in section [3](#) on page [15](#).

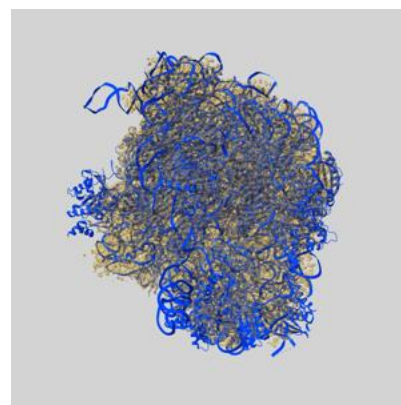
### 9.1 Map-model overlay [i](#)



X



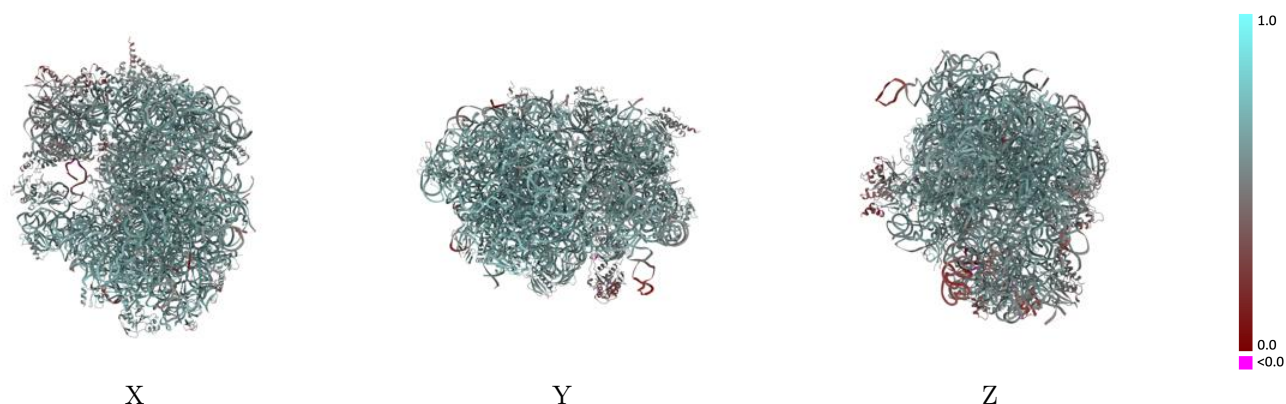
Y



Z

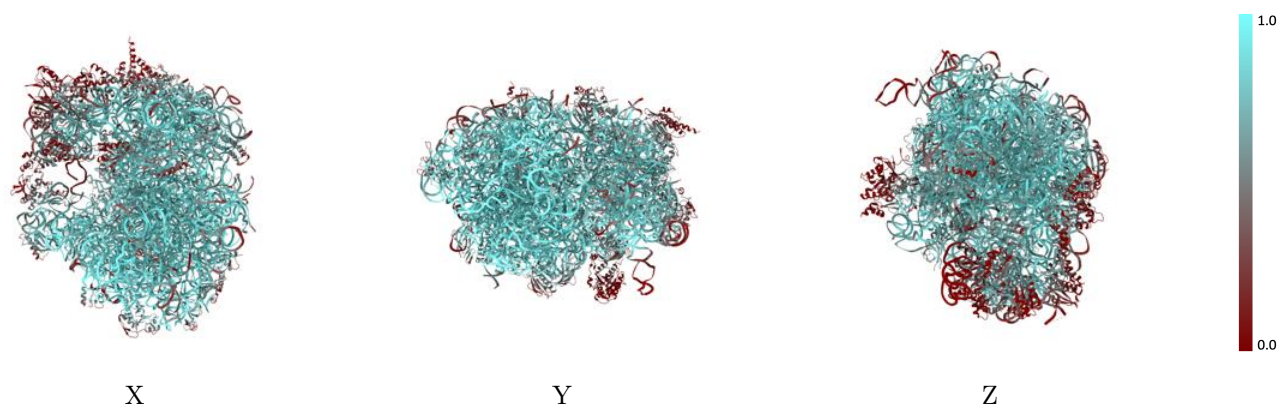
The images above show the 3D surface view of the map at the recommended contour level 0.0189 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



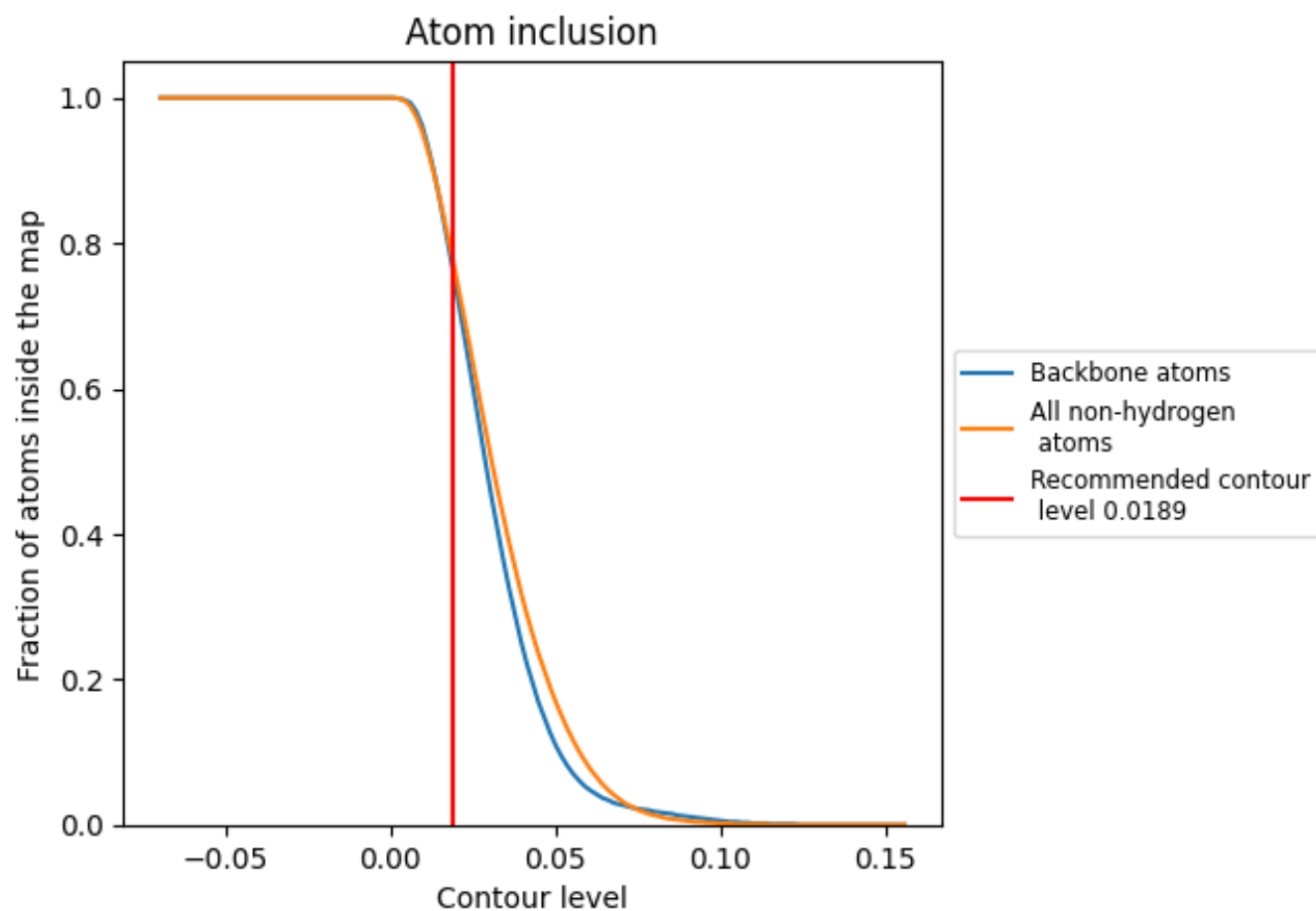
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0189).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 78% 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 (0.0189) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7760   |  0.6040   |
| A4    |  0.2830   |  0.4890   |
| Af    |  0.8530   |  0.6440   |
| B     |  0.7490   |  0.6110   |
| BQ    |  0.7080   |  0.6110   |
| Ba    |  0.9710   |  0.6650   |
| C1    |  0.3960   |  0.5530   |
| CT    |  0.3990   |  0.5150   |
| Cl    |  0.8880   |  0.6460   |
| D     |  0.0000   |  0.2270   |
| D8    |  0.8080   |  0.6110   |
| Dm    |  0.4900   |  0.5720   |
| E5    |  0.7180   |  0.6030   |
| E9    |  0.7330   |  0.6190   |
| F     |  0.3380  |  0.5080  |
| F7    |  0.4150 |  0.5300 |
| FG    |  0.4120 |  0.5320 |
| GR    |  0.5370 |  0.5720 |
| GS    |  0.2850 |  0.4850 |
| H     |  0.2960 |  0.4770 |
| HK    |  0.4000 |  0.5100 |
| IX    |  0.8760 |  0.6450 |
| JY    |  0.2760 |  0.4470 |
| Je    |  0.8530 |  0.6380 |
| KU    |  0.5010 |  0.5470 |
| Kd    |  0.7870 |  0.6230 |
| L6    |  0.8680 |  0.6290 |
| Lg    |  0.8420 |  0.6270 |
| MB    |  0.9170 |  0.6520 |
| MM    |  0.2040 |  0.4770 |
| NV    |  0.3550 |  0.5370 |
| Nc    |  0.6620 |  0.5960 |
| OL    |  0.6830 |  0.5870 |
| Oi    |  0.8200 |  0.6290 |
| PO    |  0.8940 |  0.6550 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Pj    |  0.6810   |  0.5980   |
| QZ    |  0.6480   |  0.5710   |
| Qb    |  0.6910   |  0.6110   |
| R3    |  0.6300   |  0.5580   |
| RF    |  0.8600   |  0.6440   |
| SP    |  0.1560   |  0.4680   |
| Sn    |  0.7180   |  0.6030   |
| TI    |  0.5490   |  0.5430   |
| To    |  0.6740   |  0.5890   |
| UC    |  0.6960   |  0.6080   |
| VH    |  0.8710   |  0.6360   |
| WD    |  0.7850   |  0.6210   |
| XE    |  0.4510   |  0.5510   |
| YW    |  0.8570   |  0.6500   |
| Z2    |  0.9100   |  0.6350   |
| aA    |  0.8740   |  0.6530   |
| bk    |  0.8010   |  0.6280   |
| dh    |  0.9620  |  0.6560  |
| ep    |  0.9170 |  0.6340 |
| fJ    |  0.1690 |  0.4860 |
| iN    |  0.7760 |  0.5870 |