



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:35 AM UTC

PDB ID : 1M1K / pdb\_00001m1k  
Title : Co-crystal structure of azithromycin bound to the 50S ribosomal subunit of *Haloarcula marismortui*  
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2002-06-19  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

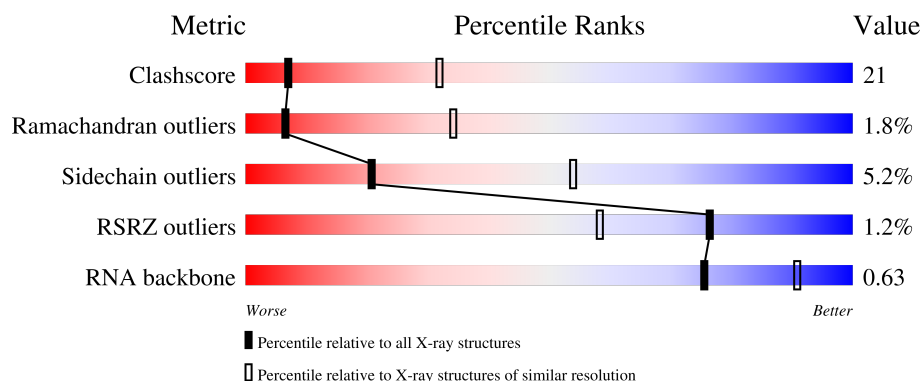
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |
| RNA backbone          | 3983                        | 1222 (3.50-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 2922   | <div> <div></div> <div>50%</div> <div>36%</div> <div>7%</div> <div>6%</div> </div>   |
| 2   | B     | 122    | <div> <div>3%</div> <div>43%</div> <div>41%</div> <div>9%</div> <div>7%</div> </div> |
| 3   | C     | 239    | <div> <div></div> <div>46%</div> <div>45%</div> <div>7%</div> <div></div> </div>     |
| 4   | D     | 337    | <div> <div></div> <div>48%</div> <div>44%</div> <div>8%</div> </div>                 |
| 5   | E     | 246    | <div> <div></div> <div>55%</div> <div>39%</div> <div>5%</div> </div>                 |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | F     | 176    |                  |
| 7   | G     | 177    |                  |
| 8   | H     | 119    |                  |
| 9   | I     | 348    |                  |
| 10  | J     | 167    |                  |
| 11  | K     | 145    |                  |
| 12  | L     | 132    |                  |
| 13  | M     | 164    |                  |
| 14  | N     | 194    |                  |
| 15  | O     | 186    |                  |
| 16  | P     | 115    |                  |
| 17  | Q     | 148    |                  |
| 18  | R     | 95     |                  |
| 19  | S     | 154    |                  |
| 20  | T     | 84     |                  |
| 21  | U     | 119    |                  |
| 22  | V     | 66     |                  |
| 23  | W     | 70     |                  |
| 24  | X     | 154    |                  |
| 25  | Y     | 91     |                  |
| 26  | Z     | 240    |                  |
| 27  | 1     | 73     |                  |
| 28  | 2     | 56     |                  |
| 29  | 3     | 48     |                  |
| 30  | 4     | 92     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 34  | NA   | A     | 8363 | -         | -        | -       | X                |
| 35  | CL   | A     | 8513 | -         | -        | X       | -                |
| 35  | CL   | K     | 8502 | -         | -        | X       | -                |
| 35  | CL   | N     | 8518 | -         | -        | X       | -                |
| 35  | CL   | O     | 8507 | -         | -        | X       | -                |

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98587 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S RRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | A     | 2754     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 59017 | 26346 | 10878 | 19048 | 2745 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 560     | C        | U      | conflict | GB 3377779 |

- Molecule 2 is a RNA chain called 5S RRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | B     | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2600  | 1160 | 472 | 847 | 121 |         |         |       |

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1754  | 1072 | 352 | 325 | 5 |         |         |       |

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 337      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2624  | 1616 | 493 | 510 | 5 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | ?       | -        | PRO    | deletion | UNP P20279 |
| D     | 310     | ARG      | PHE    | conflict | UNP P20279 |

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 246      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1858  | 1131 | 344 | 382 | 1 |         |         |       |

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1094  | 685 | 195 | 210 | 4 |         |         |       |

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1357  | 840 | 224 | 289 | 4 |         |         |       |

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 552 | 141 | 191 | 1 |         |         |       |

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | I     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 240   | 149 | 39 | 51 | 1 |         |         |       |

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1215  | 766 | 233 | 212 | 4 |         |         |       |

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 696 | 199 | 221 | 3 |         |         |       |

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 993   | 609 | 189 | 191 | 4 |         |         |       |

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 13  | M     | 145      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1114  | 668 | 222 | 224 |  |         |         |       |

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | N     | 194      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 988 | 346 | 266 | 5 |         |         |       |

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | O     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1444  | 895 | 262 | 285 | 2 |         |         |       |

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 16  | P     | 115      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 864   | 529 | 161 | 174 |  |         |         |       |

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17  | Q     | 143      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1133  | 680 | 230 | 223 |  |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Q     | 71      | LYS      | TYR    | conflict | UNP P14119 |

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18  | R     | 95       | Total | C   | N   | O   |         |         |       |
|     |       |          | 734   | 450 | 141 | 143 | 0       | 0       | 0     |

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19  | S     | 150      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 1149  | 713 | 209 | 223 | 4       | 0       | 0     |

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 20  | T     | 81       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 641   | 389 | 111 | 138 | 3       | 0       | 0     |

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 21  | U     | 119      | Total | C   | N   | O   |         |         |       |
|     |       |          | 949   | 568 | 180 | 201 |         | 0       | 0     |

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 22  | V     | 53       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 410   | 244 | 75 | 86 | 5       | 0       | 0     |

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms |     |    |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|---------|-------|
| 23  | W     | 65       | Total | C   | N  | O   | S       |         |       |
|     |       |          | 499   | 304 | 94 | 100 | 1       | 0       | 0     |

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 24  | X     | 154      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 1195  | 737 | 209 | 243 | 6       | 0       | 0     |

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | Y     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 654   | 402 | 129 | 122 | 1 |         |         |       |

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 26  | Z     | 142      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1130  | 686 | 228 | 216 |  |         |         |       |

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 27  | 1     | 73       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 563   | 359 | 111 | 86 | 7 |         |         |       |

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | 2     | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 258 | 86 | 82 | 4 |         |         |       |

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29  | 3     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 393   | 238 | 86 | 68 | 1 |         |         |       |

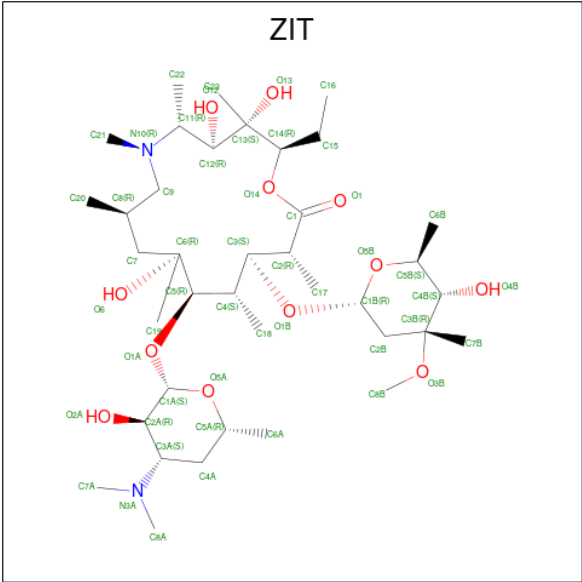
There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 3     | ?       | -        | ARG    | deletion | UNP P22452 |

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | 4     | 92       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 458 | 153 | 137 | 7 |         |         |       |

- Molecule 31 is AZITHROMYCIN (CCD ID: ZIT) (formula: C<sub>38</sub>H<sub>72</sub>N<sub>2</sub>O<sub>12</sub>).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 31  | A     | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 52    | 38 | 2 | 12 |         |         |

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32  | A     | 109      | Total | Mg  | 0       | 0       |
|     |       |          | 109   | 109 |         |         |
| 32  | B     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | C     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | D     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | L     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | U     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | Z     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | 1     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | 4     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 33  | A     | 2        | Total K<br>2 2 | 0       | 0       |

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms             | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 34  | A     | 71       | Total Na<br>71 71 | 0       | 0       |
| 34  | B     | 2        | Total Na<br>2 2   | 0       | 0       |
| 34  | C     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | E     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | J     | 2        | Total Na<br>2 2   | 0       | 0       |
| 34  | K     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | M     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | N     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | R     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | S     | 3        | Total Na<br>3 3   | 0       | 0       |
| 34  | T     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | U     | 1        | Total Na<br>1 1   | 0       | 0       |

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 35  | A     | 9        | Total Cl<br>9 9 | 0       | 0       |
| 35  | C     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 35  | D     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 35  | K     | 4        | Total Cl<br>4 4 | 0       | 0       |
| 35  | L     | 1        | Total Cl<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35  | N     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |
| 35  | O     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |
| 35  | P     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |
| 35  | R     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |
| 35  | S     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |
| 35  | 4     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 36  | P     | 1        | Total<br>1 | Cd<br>1 | 0       | 0       |
| 36  | V     | 1        | Total<br>1 | Cd<br>1 | 0       | 0       |
| 36  | 1     | 1        | Total<br>1 | Cd<br>1 | 0       | 0       |
| 36  | 2     | 1        | Total<br>1 | Cd<br>1 | 0       | 0       |
| 36  | 4     | 1        | Total<br>1 | Cd<br>1 | 0       | 0       |

- Molecule 37 is water.

| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 37  | A     | 5898     | Total<br>5898 | O<br>5898 | 0       | 0       |
| 37  | B     | 140      | Total<br>140  | O<br>140  | 0       | 0       |
| 37  | C     | 129      | Total<br>129  | O<br>129  | 0       | 0       |
| 37  | D     | 152      | Total<br>152  | O<br>152  | 0       | 0       |
| 37  | E     | 169      | Total<br>169  | O<br>169  | 0       | 0       |
| 37  | F     | 52       | Total<br>52   | O<br>52   | 0       | 0       |

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*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 37  | G     | 42       | Total<br>42  | O<br>42  | 0       | 0       |
| 37  | H     | 28       | Total<br>28  | O<br>28  | 0       | 0       |
| 37  | I     | 21       | Total<br>21  | O<br>21  | 0       | 0       |
| 37  | J     | 81       | Total<br>81  | O<br>81  | 0       | 0       |
| 37  | K     | 56       | Total<br>56  | O<br>56  | 0       | 0       |
| 37  | L     | 61       | Total<br>61  | O<br>61  | 0       | 0       |
| 37  | M     | 81       | Total<br>81  | O<br>81  | 0       | 0       |
| 37  | N     | 129      | Total<br>129 | O<br>129 | 0       | 0       |
| 37  | O     | 68       | Total<br>68  | O<br>68  | 0       | 0       |
| 37  | P     | 45       | Total<br>45  | O<br>45  | 0       | 0       |
| 37  | Q     | 69       | Total<br>69  | O<br>69  | 0       | 0       |
| 37  | R     | 56       | Total<br>56  | O<br>56  | 0       | 0       |
| 37  | S     | 89       | Total<br>89  | O<br>89  | 0       | 0       |
| 37  | T     | 36       | Total<br>36  | O<br>36  | 0       | 0       |
| 37  | U     | 39       | Total<br>39  | O<br>39  | 0       | 0       |
| 37  | V     | 27       | Total<br>27  | O<br>27  | 0       | 0       |
| 37  | W     | 15       | Total<br>15  | O<br>15  | 0       | 0       |
| 37  | X     | 73       | Total<br>73  | O<br>73  | 0       | 0       |
| 37  | Y     | 30       | Total<br>30  | O<br>30  | 0       | 0       |
| 37  | Z     | 93       | Total<br>93  | O<br>93  | 0       | 0       |
| 37  | 1     | 38       | Total<br>38  | O<br>38  | 0       | 0       |

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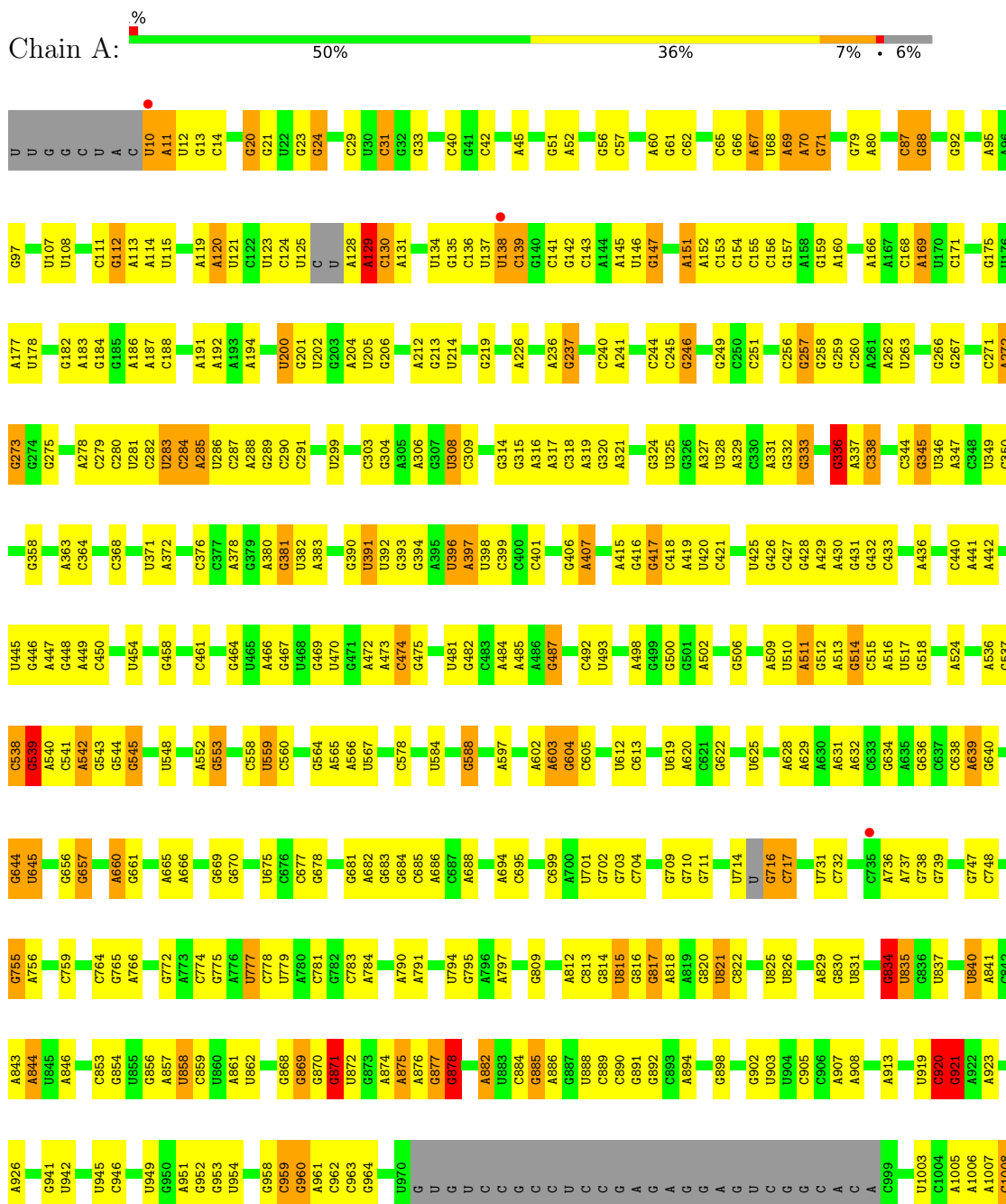
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 37  | 2     | 57       | Total<br>57 | O<br>57 | 0       | 0       |
| 37  | 3     | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 37  | 4     | 72       | Total<br>72 | O<br>72 | 0       | 0       |

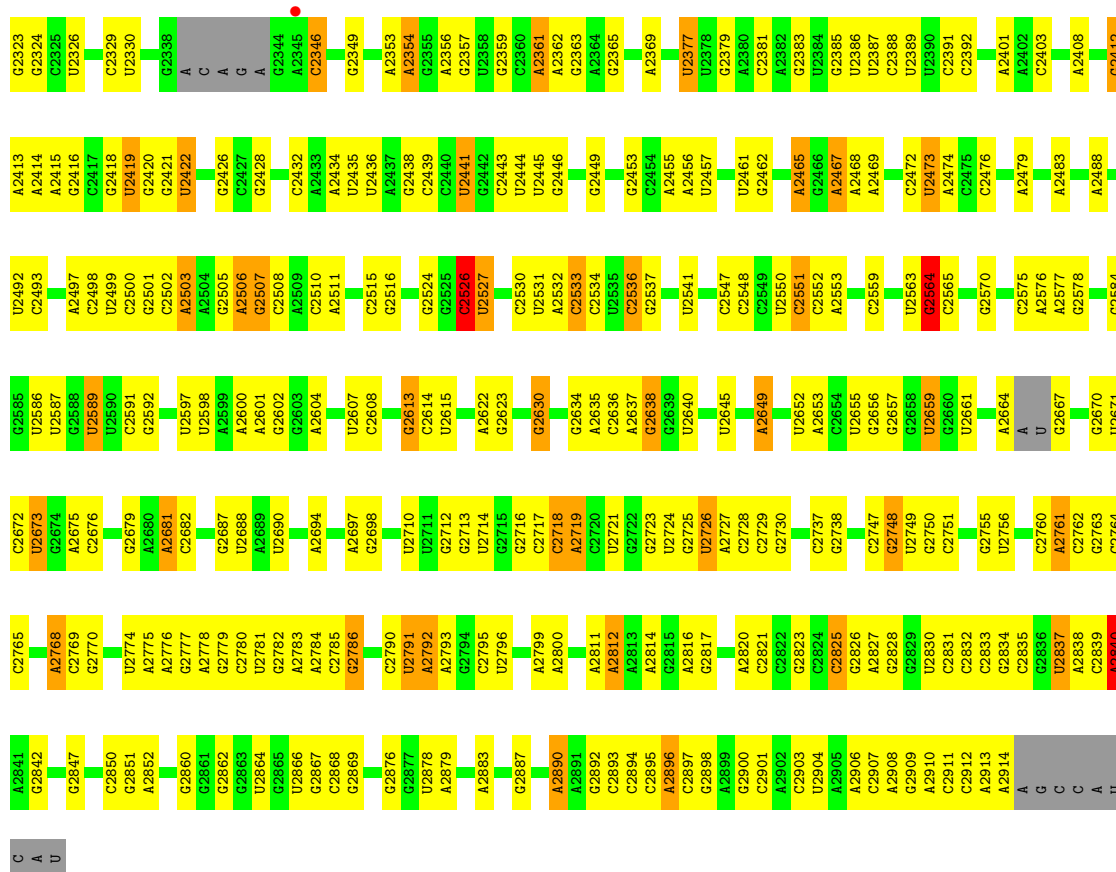
### 3 Residue-property plots

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

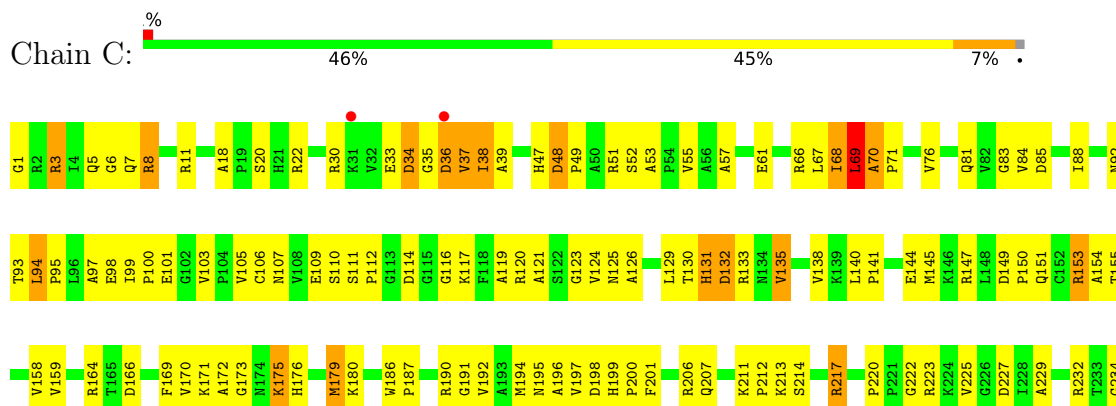
- Molecule 1: 23S rRNA



|   |       |       |       |       |       |       |       |       |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G | U2107 | A2015 | A1931 | G1827 | C1734 | A1656 | C1549 | G1441 | G1348 | A1246 | A1173 | U1095 | A1014 |
| U | G2110 | A1934 | A1934 | G1828 | C1735 | A1657 | G1555 | A1442 | G1349 | A1247 | A1174 | U1096 | C1015 |
| A | G2113 | C2023 | C1935 | A1929 | A1737 | A1658 | G1556 | U1445 | U1350 | A1248 | G1175 | A1097 | U1016 |
| C | C2114 | A2030 | C1936 | C1830 | C1738 | A1659 | A1559 | U1446 | G1351 | C1250 | C1176 | A1098 |       |
| C | U2115 | G2030 | C1940 | C1834 | U1741 | A1661 | U     | U1447 | A1352 | C1251 | A1177 | G1099 |       |
| G | U2116 | G2033 | A1941 | U1835 | U1742 | C1662 | A1561 | C1450 | C1353 | A1252 | U1180 | C1102 | C1019 |
| C | U2117 | U2034 | C1942 | A1836 | A1746 | C1666 | G1562 | G1451 | A1357 | C1253 | A1181 | C1103 | A1020 |
| G | U2120 | C2035 | C1943 | A1839 | A1746 | A1667 | G1563 | G1452 | A1358 | A1261 | C1182 | A1109 | A1022 |
| C | G2121 | A2038 | G1947 | A1840 | U1748 | U1668 | C1564 | G1453 | U1359 | C1262 | C1183 | G1110 | G1023 |
| U | A2122 | A2039 | G1948 | A1841 | U1748 | A1669 | C1565 | G1456 | C1360 | C1263 | C1185 | G1111 | G1024 |
| A | A2123 | C2040 | A1842 | A1840 | U1749 | G1670 |       | C1457 | C1361 | U1264 | U1186 | G1112 | C1025 |
| C | G2128 | G2041 | G1951 | A1843 | C1750 | C1675 | A1572 | U1457 | U1362 | U1265 | A1187 | G1113 | U1028 |
| G | U2128 | U2042 | U     | G1951 | G1752 | U1676 | C1574 | A1458 | A1368 | C1267 | A1188 | A1114 | U1029 |
| G | A2136 | U2043 | A     | U1846 | C1753 | U1677 |       | U1461 | A1369 | C1268 | A1190 | U1115 |       |
| G |       | G2044 | A     | A1847 | C1753 | A1678 | A1580 | C1462 | G1370 | G1269 | A1191 | U1116 | G1036 |
| C | A     | G2045 | C     | C1854 | U1758 | C1679 |       | A1463 | A1372 | U1270 | A1192 | A1117 | G1037 |
| C | G     | G2046 | C     | G1855 | U1759 | C1680 | G1588 | U1477 | A1372 | U1271 | A1193 | G1118 | G1038 |
| C | U     | C2047 | A     | C1856 | U1766 | A1682 | G1589 | U1478 | A1372 | C1272 | U1120 | U1120 | U1042 |
| C | G     | G2050 | U     | C1857 | U1766 | G1683 | G1592 | C1474 | A1375 | C1273 | G1197 | G1121 | C1043 |
| C | G     | G     | U     | A1857 | C1767 | G1683 | C1593 | U1478 | G1376 | U1279 | U1198 | U1122 | C1044 |
| G | U     | A2054 | A     | A1858 | C1768 | A1684 | C1594 | U1478 | C1377 |       | A1199 | A1123 | G1045 |
| U | U     | A2055 | C     | A1859 | C1769 | A1685 | C1595 | U1478 | G1378 | C1289 | A1200 | G1046 | U1047 |
| G | U     | G     | C     | U1860 | U1770 |       | U1596 | U1478 | U1380 | G1299 | C1201 | U1127 | U1048 |
| C | C     | U2063 | C     | C1861 | U1771 | G1688 | U1597 | A1486 | C1384 | G1300 | U1204 | U1130 | C1051 |
| C | A     | U2064 | U1964 | C1862 | C1772 | C1690 | A1598 | A1487 | G1385 | C1301 | U1205 | G1131 | G1052 |
| A | G     | C     | C1965 | A     | G1773 | A1691 | A1598 | U1488 |       |       | U1206 |       |       |
| C | A     | A2068 | U1966 | A1865 | A1778 | C1692 | G1601 |       |       |       | A1207 |       |       |
| C | A     | G     | U1966 | G1868 | A1779 | A1693 | C1602 | A1494 | G1389 | U1304 | C1208 | A1133 | G1055 |
| A | U     | U2069 | G1971 | A1869 | A1779 | C1693 | A1603 | C1495 | A1390 | C1305 | C1209 | A1133 | U1056 |
| U | G     | G2070 | A1972 | C1870 | A1783 | G1694 | G1604 | G1496 | G1391 | U1306 | G1210 | G1134 | A1057 |
| G | C     | C2071 | G1974 |       | U1784 | U1696 | G1605 | G1497 |       |       | G1211 |       | A1058 |
| G | A     | G2072 |       |       | U1784 |       |       |       | A1393 | U1309 | C1212 | G1137 |       |
| C | C     | G2073 |       | G1873 | C1785 | C1699 | C1613 | U1500 | C1394 | U1310 | C1213 | G1138 | G1059 |
| A | A     | A2074 | A1978 | U1874 | C1786 | C1700 | G1614 | C1507 |       | G1310 | C1213 | U1139 | C1060 |
| A | G     |       | U1979 |       | U1787 | A1701 | A1615 | C1507 | A1407 | G1311 | G1214 | C1140 |       |
| A | C     | G2079 | U1980 | G1877 | U1788 | G1701 | A1615 | U1503 | A1407 | G1312 | A1215 | C1141 | U1062 |
| C | U     | A2080 | C1981 | G1878 | G1789 | U1702 | C1617 | A1504 | U1408 | A1313 | G1216 | U1141 | G1063 |
| A | A     | A2081 | C1982 | U1879 | C1790 | U1706 |       | U1505 | G1409 | U1314 | G1217 | C1142 |       |
| U | A     | G2082 | C1982 |       | U1791 | G1706 | U1617 | U1506 |       | G1315 | U1218 |       | A1067 |
| U | A     | A2083 | G1995 | G1902 | C1792 | C1707 | U1625 | C1507 | G1416 | G1316 | U1219 | G1161 | C1068 |
| A | G     | G     | U1996 | U1903 | C1798 | C1708 | A1626 |       | U1417 |       |       | C1156 |       |
| C | G     | A     | A1997 | A1904 | C1798 | G1709 | G1627 | U1524 | U1418 | G1323 | G1224 | C1157 | G1072 |
| C | U     | C2088 | A     |       |       | A1710 |       | G1525 | C1420 | G1324 | C1225 | G1158 |       |
| U | G     | G2090 | G2001 | G1908 | A1804 |       | A1630 | A1526 | C1421 | U1326 | C1229 | G1159 | G1076 |
| G | G     | G2091 | C2002 | A1909 | G1805 | A1717 |       |       |       |       |       |       |       |
| G | G     | A2089 | U1982 | A1910 | C1805 |       |       |       |       |       |       |       |       |
| C | A     | C2089 | C2003 | A1910 | G1809 |       | C1633 | A1527 | U1422 | G1327 | A1161 | A1161 | A1079 |
| C | G     | G2092 | U2004 | A1909 | C1810 | C1720 | G1634 | A1528 | C1423 | G1328 | U1234 | G1162 | C1080 |
| G | G     | G2093 | G2005 | A1919 | G1809 | C1721 | U1635 | A1529 | A1424 | A1329 | G1163 | G1163 | A1081 |
| G | C     | A2095 | C2006 | C1920 | U1722 | G1636 | G1636 | G1425 | A1330 | A1236 | U1164 | U1164 | A1082 |
| U | A     | G2096 | A2007 | A1921 | G1814 | G1723 | A1637 | G1532 | G1426 | A1331 | U1237 | G1165 | C1083 |
| A | C     |       | U2008 | A1922 | A1815 | U1724 | A1637 | A1533 | A1427 | C1332 | C1238 | A1166 | C1084 |
| C | C     | G     | U2008 | A1922 | A1815 | U1724 | A1637 | A1533 | A1427 | C1332 | C1238 | A1166 | C1084 |
| U | U     | G2099 | C2009 | G1925 | C1816 | C1725 | A1641 | A1534 | A1427 | U1333 | G1239 | G1167 | C1085 |
| C | U     | A2100 | A2010 | G1925 | C1816 | C1725 | A1641 | A1534 | A1427 | U1333 | G1239 | G1167 | C1085 |
| C | C     | A2101 | A2011 | G1926 | G1819 | C1730 | C1642 | C1536 | A1434 | C1334 | A1242 | C1168 | A1086 |
| C | C     | G2102 | U2012 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1335 | A1243 | G1169 | G1087 |
| C | A     |       | U2012 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | U1170 | A1088 |
| C | A     |       | G2013 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
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| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 | G1820 | G1731 | C1643 | C1536 | U1435 | U1336 | C1243 | A1171 |       |
| C | A     |       | G2014 | A1927 |       |       |       |       |       |       |       |       |       |

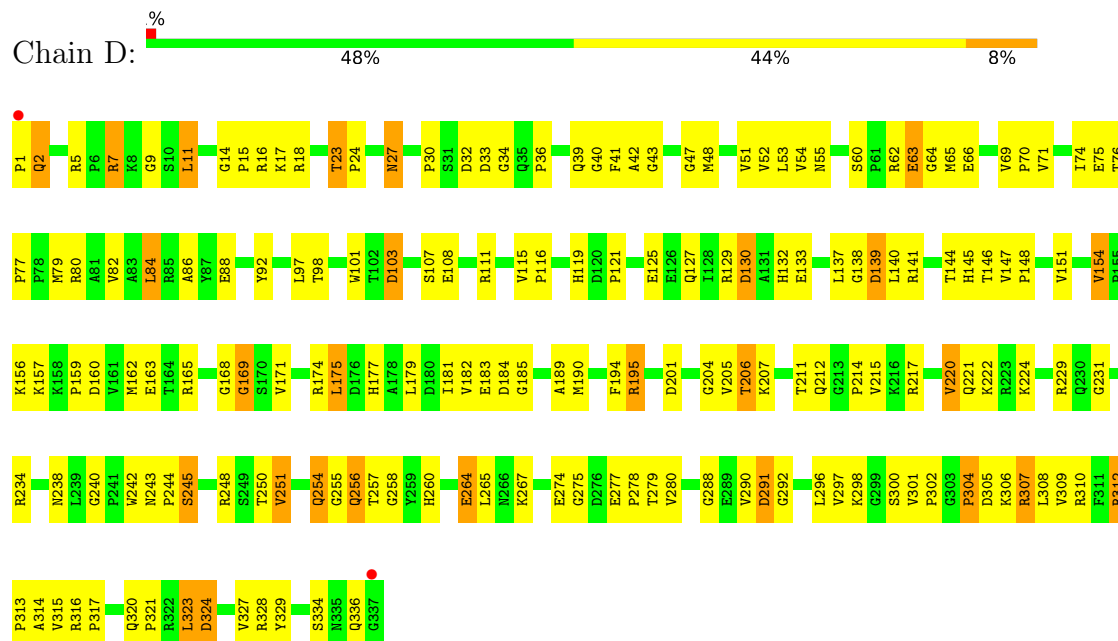


● Molecule 3: RIBOSOMAL PROTEIN L2





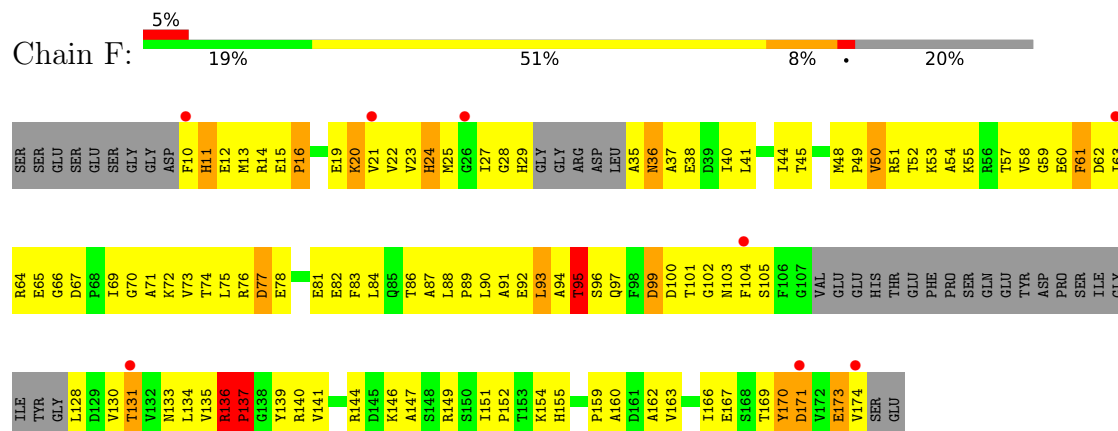
- Molecule 4: RIBOSOMAL PROTEIN L3



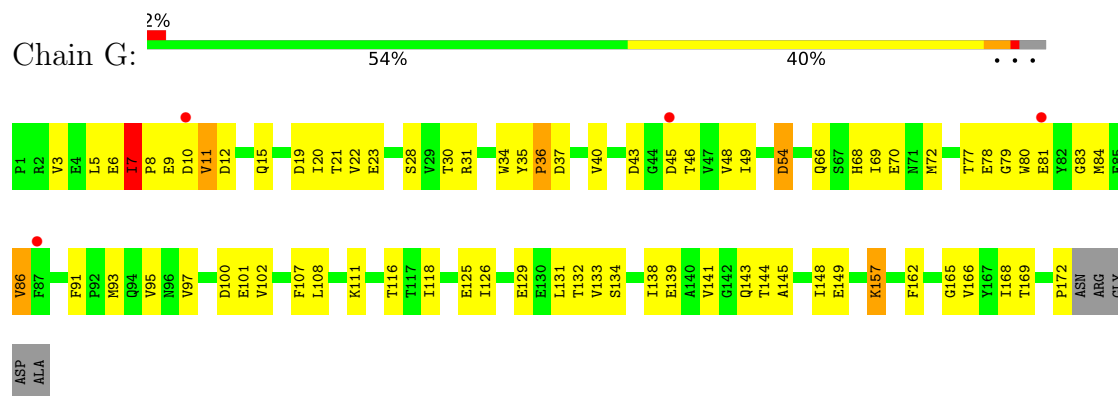
- Molecule 5: RIBOSOMAL PROTEIN L4



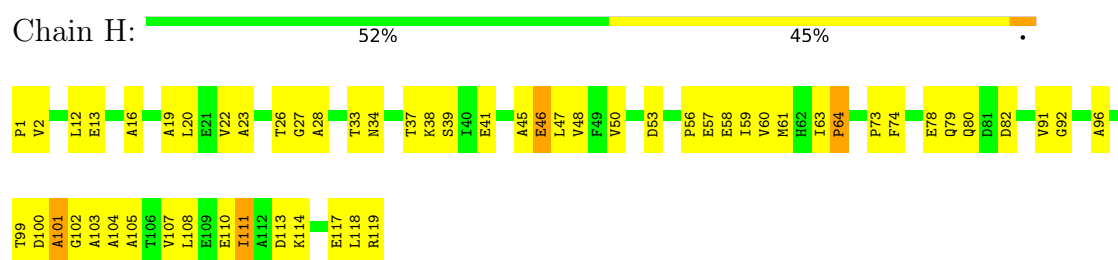
- Molecule 6: RIBOSOMAL PROTEIN L5



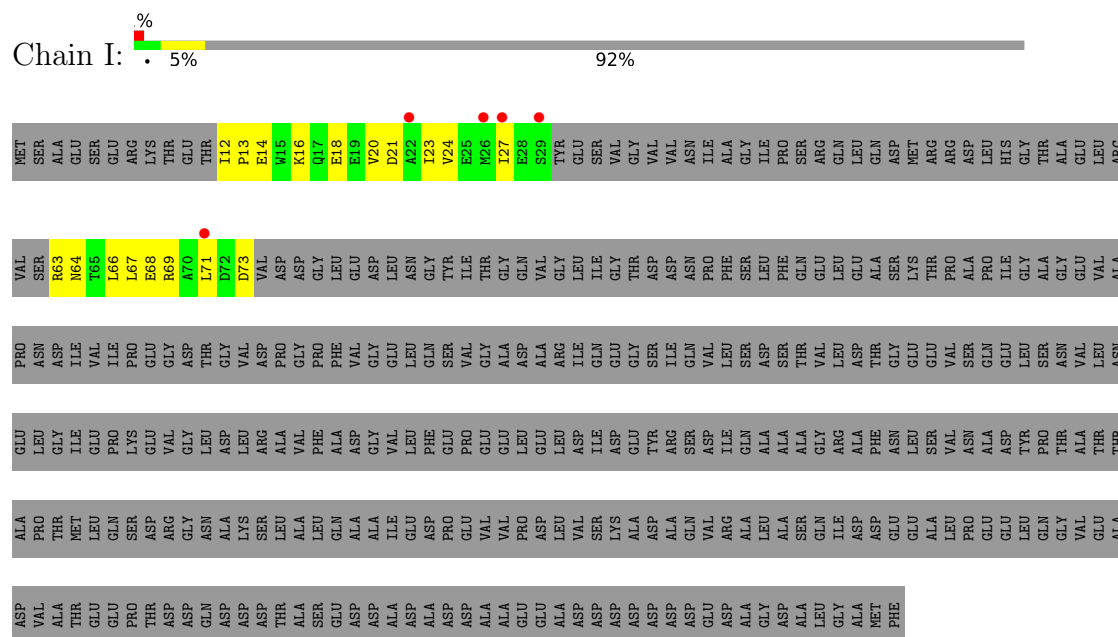
- Molecule 7: RIBOSOMAL PROTEIN L6



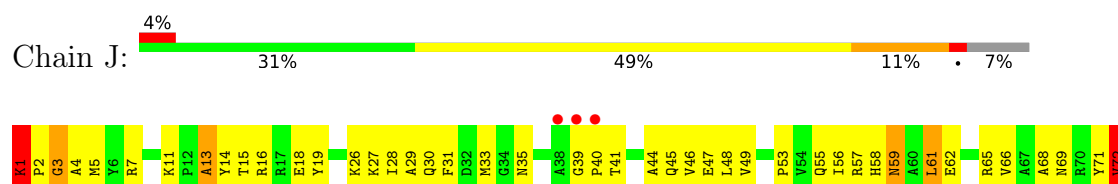
- Molecule 8: RIBOSOMAL PROTEIN L7AE

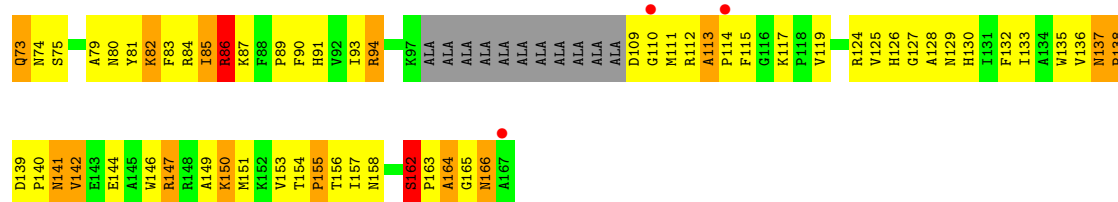


- Molecule 9: RIBOSOMAL PROTEIN L10



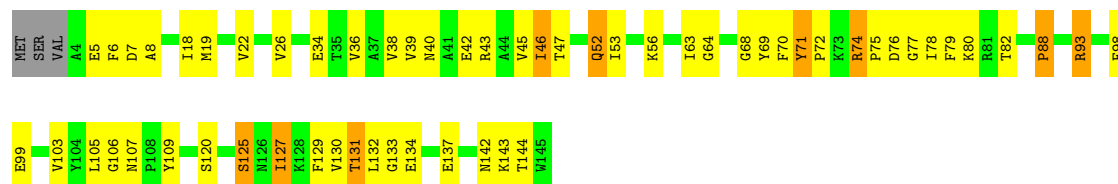
- Molecule 10: RIBOSOMAL PROTEIN L10E





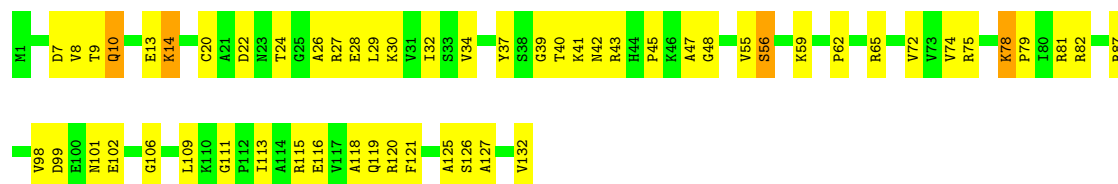
• Molecule 11: RIBOSOMAL PROTEIN L13

Chain K: 58% 34% 6%



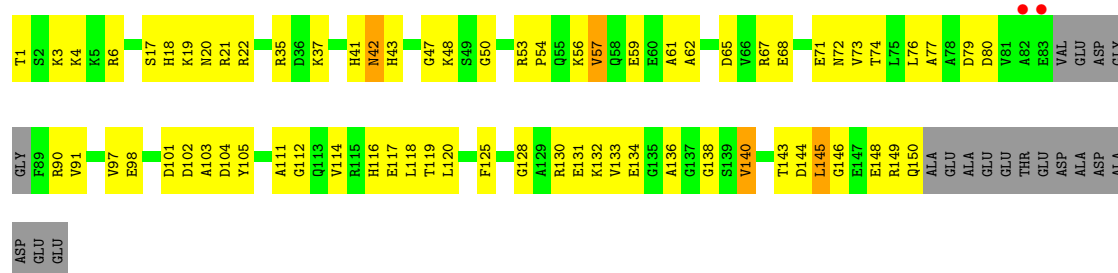
• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L: 58% 39% 1%



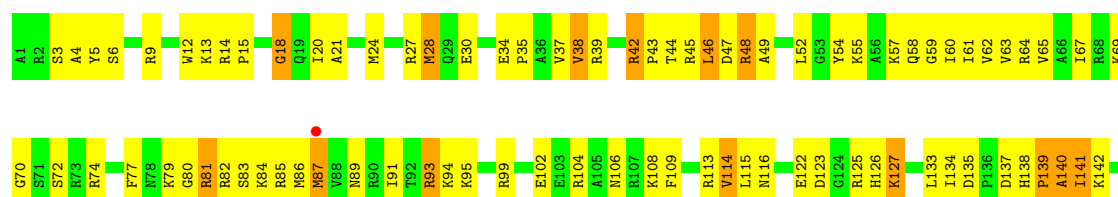
• Molecule 13: RIBOSOMAL PROTEIN L15

Chain M: 46% 40% 12%



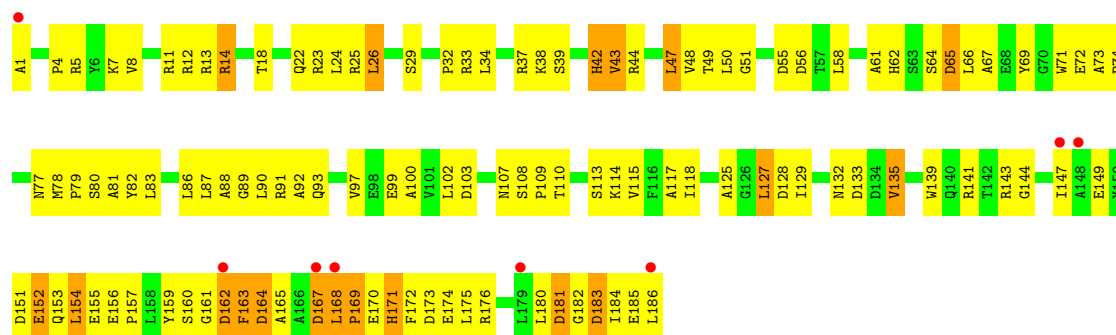
• Molecule 14: RIBOSOMAL PROTEIN L15E

Chain N: 37% 55% 8%





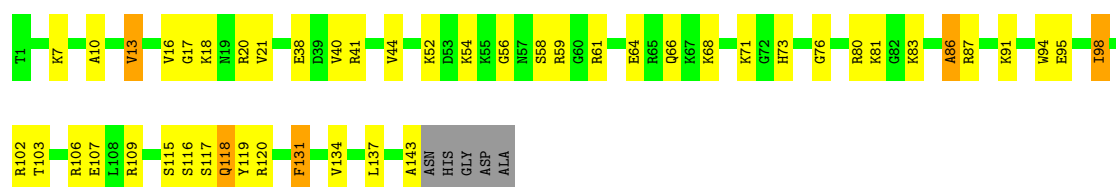
● Molecule 15: RIBOSOMAL PROTEIN L18



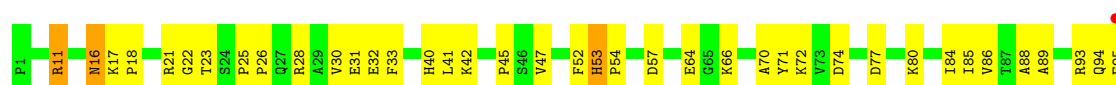
● Molecule 16: RIBOSOMAL PROTEIN L18E



● Molecule 17: RIBOSOMAL PROTEIN L19E

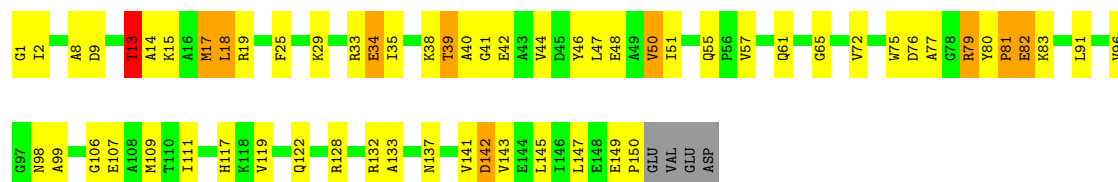


● Molecule 18: RIBOSOMAL PROTEIN L21E

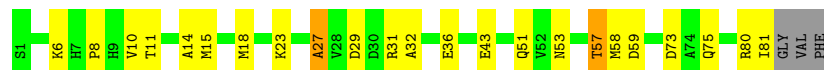


● Molecule 19: RIBOSOMAL PROTEIN L22

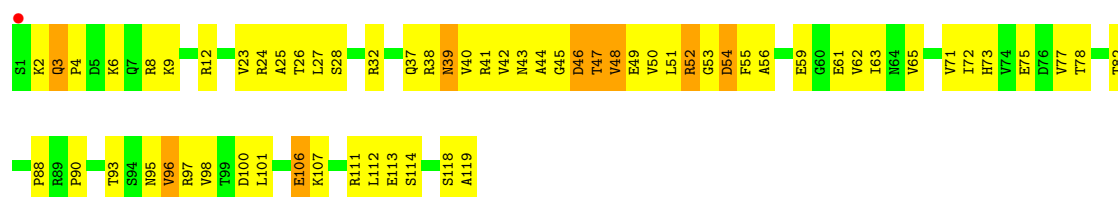




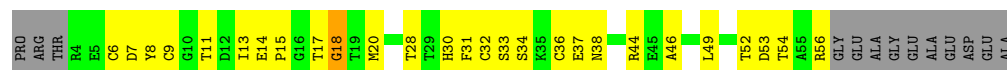
• Molecule 20: RIBOSOMAL PROTEIN L23



• Molecule 21: RIBOSOMAL PROTEIN L24



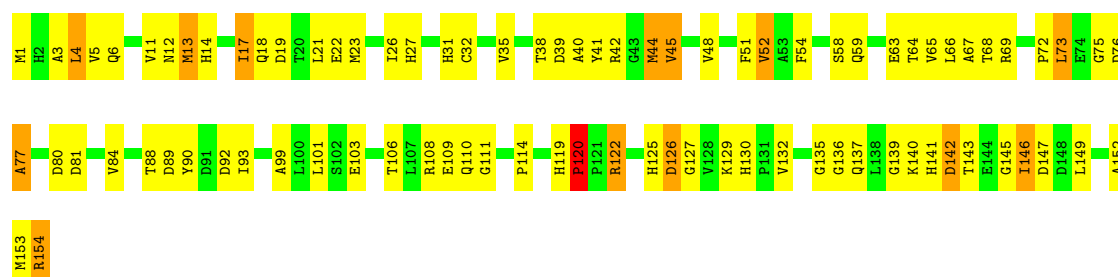
• Molecule 22: RIBOSOMAL PROTEIN L24E



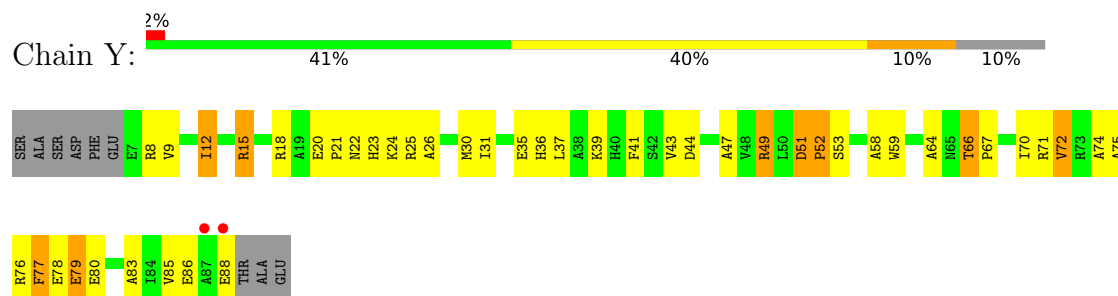
• Molecule 23: RIBOSOMAL PROTEIN L29



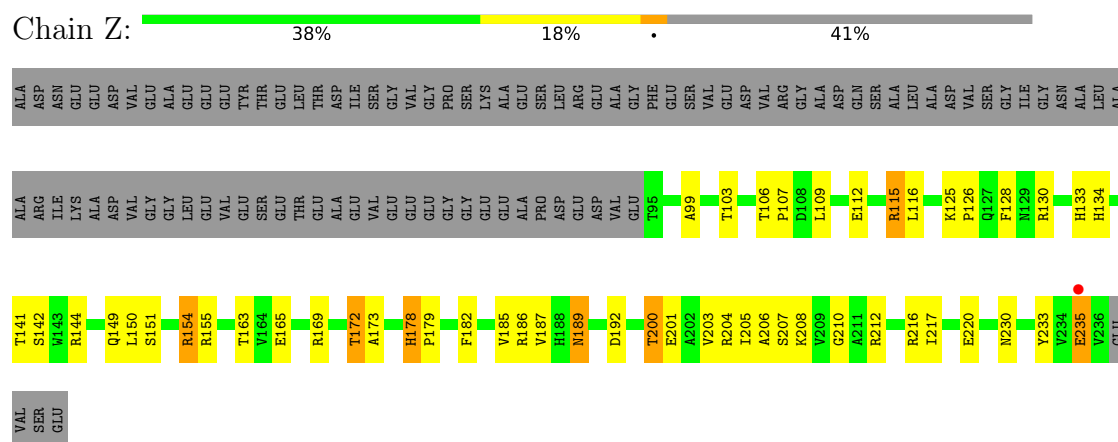
• Molecule 24: RIBOSOMAL PROTEIN L30



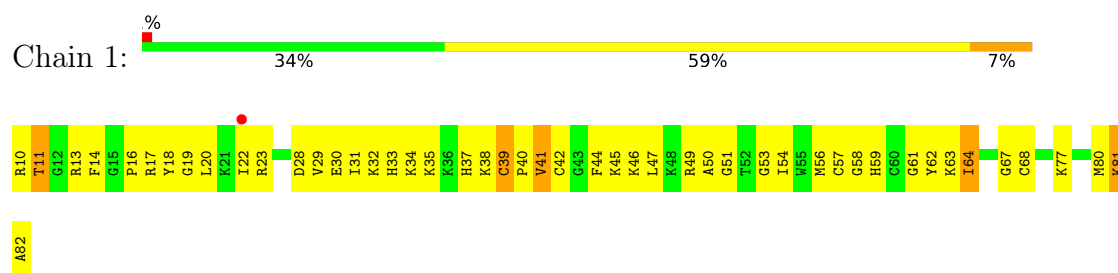
- Molecule 25: RIBOSOMAL PROTEIN L31E



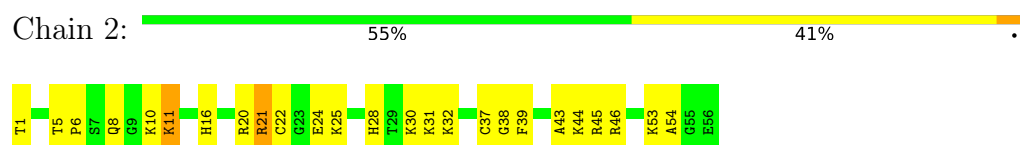
- Molecule 26: RIBOSOMAL PROTEIN L32E



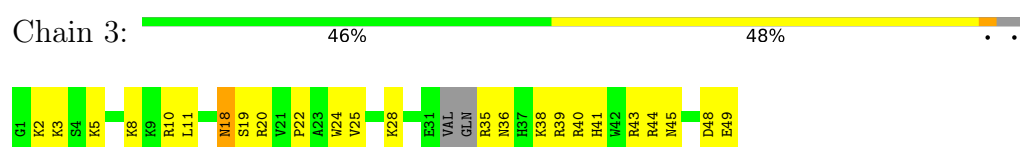
- Molecule 27: RIBOSOMAL PROTEIN L37Ae



- Molecule 28: RIBOSOMAL PROTEIN L37E



- Molecule 29: RIBOSOMAL PROTEIN L39E



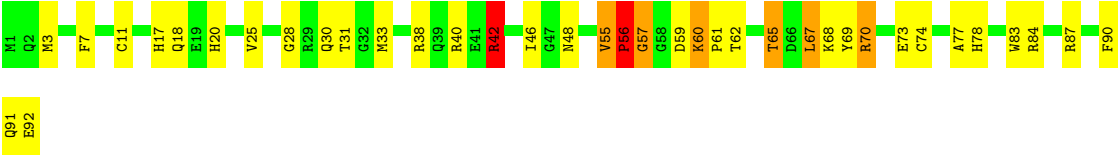
- Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 4: 

59%

33%

7%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 213.75Å 301.57Å 574.44Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.20<br>20.00 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.9 (20.00-3.20)<br>91.5 (20.00-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.19                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.27 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.214 , 0.250<br>0.198 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 60.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.511                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 74.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 98587                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CD, K, NA, CL, ZIT

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   | A     | 0.51         | 0/66076         | 0.74        | 44/103052 (0.0%)  |
| 2   | B     | 0.76         | 12/2905 (0.4%)  | 0.90        | 19/4528 (0.4%)    |
| 3   | C     | 0.61         | 0/1787          | 1.14        | 13/2409 (0.5%)    |
| 4   | D     | 0.67         | 0/2689          | 1.13        | 18/3652 (0.5%)    |
| 5   | E     | 0.63         | 0/1883          | 1.12        | 8/2551 (0.3%)     |
| 6   | F     | 0.52         | 0/1111          | 1.00        | 6/1498 (0.4%)     |
| 7   | G     | 0.62         | 0/1382          | 1.00        | 5/1880 (0.3%)     |
| 8   | H     | 0.56         | 0/896           | 0.97        | 2/1219 (0.2%)     |
| 9   | I     | 0.67         | 0/241           | 0.95        | 1/324 (0.3%)      |
| 10  | J     | 0.67         | 0/1246          | 1.37        | 17/1686 (1.0%)    |
| 11  | K     | 0.66         | 0/1135          | 1.06        | 4/1530 (0.3%)     |
| 12  | L     | 0.70         | 0/1003          | 1.20        | 7/1351 (0.5%)     |
| 13  | M     | 0.56         | 0/1126          | 1.14        | 7/1504 (0.5%)     |
| 14  | N     | 0.69         | 1/1633 (0.1%)   | 1.16        | 8/2180 (0.4%)     |
| 15  | O     | 0.57         | 0/1473          | 1.18        | 16/1999 (0.8%)    |
| 16  | P     | 0.62         | 0/873           | 1.04        | 4/1181 (0.3%)     |
| 17  | Q     | 0.60         | 1/1143 (0.1%)   | 1.03        | 5/1521 (0.3%)     |
| 18  | R     | 0.66         | 0/748           | 1.20        | 7/1005 (0.7%)     |
| 19  | S     | 0.71         | 1/1172 (0.1%)   | 1.12        | 10/1578 (0.6%)    |
| 20  | T     | 0.56         | 0/648           | 1.04        | 2/875 (0.2%)      |
| 21  | U     | 0.56         | 0/957           | 1.11        | 7/1289 (0.5%)     |
| 22  | V     | 0.60         | 0/417           | 1.04        | 1/562 (0.2%)      |
| 23  | W     | 0.55         | 0/502           | 1.04        | 3/675 (0.4%)      |
| 24  | X     | 0.75         | 3/1218 (0.2%)   | 1.06        | 5/1655 (0.3%)     |
| 25  | Y     | 0.66         | 0/664           | 1.19        | 7/895 (0.8%)      |
| 26  | Z     | 0.63         | 0/1146          | 1.06        | 4/1536 (0.3%)     |
| 27  | 1     | 0.59         | 0/575           | 1.06        | 2/763 (0.3%)      |
| 28  | 2     | 0.67         | 0/437           | 1.13        | 3/578 (0.5%)      |
| 29  | 3     | 0.54         | 0/398           | 0.83        | 0/527             |
| 30  | 4     | 0.60         | 0/771           | 1.08        | 7/1024 (0.7%)     |
| All | All   | 0.55         | 18/98255 (0.0%) | 0.86        | 242/147027 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 141                 |
| 2   | B     | 0                   | 5                   |
| All | All   | 1                   | 146                 |

All (18) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 3023 | U    | O5'-C5' | 10.10 | 1.57        | 1.42     |
| 2   | B     | 3025 | G    | O3'-P   | 8.55  | 1.74        | 1.61     |
| 2   | B     | 3025 | G    | C4'-O4' | 8.47  | 1.58        | 1.45     |
| 2   | B     | 3023 | U    | C2'-O2' | 7.66  | 1.53        | 1.42     |
| 2   | B     | 3003 | A    | C5'-C4' | 6.80  | 1.61        | 1.51     |
| 2   | B     | 3026 | C    | P-OP2   | -6.37 | 1.36        | 1.49     |
| 24  | X     | 13   | MET  | SD-CE   | -6.28 | 1.63        | 1.79     |
| 2   | B     | 3022 | G    | O5'-C5' | -6.00 | 1.33        | 1.42     |
| 2   | B     | 3026 | C    | P-O5'   | -5.84 | 1.50        | 1.59     |
| 17  | Q     | 13   | VAL  | CA-CB   | 5.79  | 1.61        | 1.54     |
| 24  | X     | 44   | MET  | SD-CE   | -5.74 | 1.65        | 1.79     |
| 2   | B     | 3025 | G    | C2'-C1' | 5.72  | 1.61        | 1.53     |
| 14  | N     | 28   | MET  | SD-CE   | 5.66  | 1.93        | 1.79     |
| 24  | X     | 132  | VAL  | CA-CB   | -5.65 | 1.47        | 1.54     |
| 2   | B     | 3025 | G    | O4'-C1' | 5.64  | 1.50        | 1.41     |
| 2   | B     | 3003 | A    | O5'-C5' | -5.24 | 1.34        | 1.42     |
| 19  | S     | 17   | MET  | SD-CE   | -5.15 | 1.66        | 1.79     |
| 2   | B     | 3024 | U    | O4'-C1' | 5.12  | 1.49        | 1.41     |

All (242) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | A     | 1164 | U    | OP1-P-O3'   | -14.96 | 63.13       | 108.00   |
| 10  | J     | 74   | ASN  | N-CA-C      | -14.67 | 93.12       | 114.39   |
| 1   | A     | 1563 | G    | C2'-C3'-O3' | 14.62  | 131.43      | 109.50   |
| 1   | A     | 1164 | U    | OP2-P-O3'   | -13.88 | 66.37       | 108.00   |
| 10  | J     | 141  | ASN  | N-CA-C      | -12.46 | 97.78       | 113.23   |
| 1   | A     | 1979 | G    | C2'-C3'-O3' | 11.14  | 126.21      | 109.50   |
| 2   | B     | 3023 | U    | P-O5'-C5'   | 11.04  | 137.46      | 120.90   |
| 14  | N     | 141  | ILE  | N-CA-C      | -10.86 | 102.47      | 111.81   |
| 15  | O     | 135  | VAL  | N-CA-C      | -10.29 | 103.07      | 113.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 3025 | G    | C3'-C2'-O2' | 9.96  | 125.64      | 110.70   |
| 1   | A     | 1942 | A    | C5'-C4'-C3' | 9.66  | 130.49      | 116.00   |
| 14  | N     | 139  | PRO  | N-CA-C      | -9.65 | 97.54       | 111.33   |
| 6   | F     | 136  | ARG  | CA-C-N      | 9.44  | 131.64      | 119.84   |
| 6   | F     | 136  | ARG  | C-N-CA      | 9.44  | 131.64      | 119.84   |
| 10  | J     | 1    | LYS  | CA-C-N      | 8.67  | 128.60      | 119.85   |
| 10  | J     | 1    | LYS  | C-N-CA      | 8.67  | 128.60      | 119.85   |
| 18  | R     | 17   | LYS  | N-CA-C      | -8.59 | 98.92       | 109.83   |
| 12  | L     | 111  | GLY  | CA-C-N      | 8.51  | 128.38      | 120.21   |
| 12  | L     | 111  | GLY  | C-N-CA      | 8.51  | 128.38      | 120.21   |
| 3   | C     | 48   | ASP  | CA-C-N      | 8.40  | 128.52      | 119.28   |
| 3   | C     | 48   | ASP  | C-N-CA      | 8.40  | 128.52      | 119.28   |
| 15  | O     | 133  | ASP  | N-CA-C      | 8.34  | 121.42      | 111.33   |
| 3   | C     | 70   | ALA  | N-CA-C      | 8.34  | 120.16      | 109.65   |
| 30  | 4     | 55   | VAL  | CA-C-N      | 8.30  | 130.21      | 119.84   |
| 30  | 4     | 55   | VAL  | C-N-CA      | 8.30  | 130.21      | 119.84   |
| 7   | G     | 11   | VAL  | N-CA-C      | 8.21  | 121.92      | 109.20   |
| 11  | K     | 71   | TYR  | CA-C-N      | 8.17  | 128.10      | 119.85   |
| 11  | K     | 71   | TYR  | C-N-CA      | 8.17  | 128.10      | 119.85   |
| 10  | J     | 155  | PRO  | N-CA-C      | 8.09  | 123.88      | 111.34   |
| 25  | Y     | 51   | ASP  | CA-C-N      | 8.04  | 128.80      | 119.47   |
| 25  | Y     | 51   | ASP  | C-N-CA      | 8.04  | 128.80      | 119.47   |
| 25  | Y     | 22   | ASN  | N-CA-C      | 7.97  | 120.97      | 111.33   |
| 21  | U     | 52   | ARG  | N-CA-C      | 7.96  | 123.76      | 113.18   |
| 13  | M     | 145  | LEU  | N-CA-C      | -7.74 | 102.92      | 111.36   |
| 1   | A     | 1563 | G    | C4'-C3'-O3' | 7.67  | 120.90      | 109.40   |
| 12  | L     | 78   | LYS  | CA-C-N      | 7.63  | 127.64      | 119.78   |
| 12  | L     | 78   | LYS  | C-N-CA      | 7.63  | 127.64      | 119.78   |
| 2   | B     | 3039 | U    | N1-C1'-C2'  | 7.60  | 123.40      | 112.00   |
| 4   | D     | 157  | LYS  | N-CA-C      | -7.53 | 104.70      | 114.04   |
| 10  | J     | 156  | THR  | N-CA-C      | -7.49 | 99.39       | 110.48   |
| 13  | M     | 57   | VAL  | N-CA-C      | -7.48 | 105.55      | 112.43   |
| 3   | C     | 222  | GLY  | N-CA-C      | -7.43 | 105.10      | 113.79   |
| 12  | L     | 8    | VAL  | N-CA-C      | 7.42  | 119.29      | 108.53   |
| 4   | D     | 23   | THR  | CA-C-N      | 7.35  | 127.35      | 119.78   |
| 4   | D     | 23   | THR  | C-N-CA      | 7.35  | 127.35      | 119.78   |
| 2   | B     | 3024 | U    | C4'-C3'-O3' | 7.35  | 124.02      | 113.00   |
| 15  | O     | 169  | PRO  | N-CA-C      | -7.23 | 104.50      | 114.27   |
| 5   | E     | 175  | LYS  | N-CA-C      | 7.23  | 119.64      | 110.24   |
| 1   | A     | 1592 | G    | N9-C1'-C2'  | 7.21  | 122.81      | 112.00   |
| 24  | X     | 75   | GLY  | N-CA-C      | 7.15  | 120.98      | 112.33   |
| 15  | O     | 14   | ARG  | N-CA-C      | -7.07 | 103.26      | 110.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 3039 | U    | C4'-C3'-O3' | -7.00 | 102.50      | 113.00   |
| 20  | T     | 57   | THR  | N-CA-C      | 6.98  | 120.82      | 110.48   |
| 3   | C     | 213  | LYS  | N-CA-C      | 6.98  | 121.06      | 112.54   |
| 4   | D     | 151  | VAL  | CA-C-N      | 6.96  | 126.21      | 118.97   |
| 4   | D     | 151  | VAL  | C-N-CA      | 6.96  | 126.21      | 118.97   |
| 2   | B     | 3026 | C    | C3'-C2'-O2' | 6.93  | 121.10      | 110.70   |
| 5   | E     | 78   | ARG  | N-CA-C      | 6.92  | 118.70      | 108.60   |
| 21  | U     | 3    | GLN  | CA-C-N      | 6.90  | 128.47      | 119.84   |
| 21  | U     | 3    | GLN  | C-N-CA      | 6.90  | 128.47      | 119.84   |
| 21  | U     | 54   | ASP  | N-CA-C      | -6.90 | 104.12      | 112.54   |
| 5   | E     | 64   | GLY  | N-CA-C      | 6.85  | 120.91      | 113.58   |
| 15  | O     | 153  | GLN  | N-CA-C      | -6.84 | 103.41      | 112.72   |
| 10  | J     | 147  | ARG  | N-CA-C      | -6.84 | 103.84      | 111.71   |
| 14  | N     | 89   | ASN  | N-CA-C      | 6.83  | 118.80      | 111.36   |
| 19  | S     | 50   | VAL  | N-CA-C      | -6.81 | 104.02      | 110.42   |
| 6   | F     | 100  | ASP  | N-CA-C      | -6.80 | 104.95      | 113.18   |
| 13  | M     | 47   | GLY  | N-CA-C      | 6.79  | 119.05      | 111.85   |
| 4   | D     | 323  | LEU  | N-CA-C      | 6.76  | 119.03      | 110.24   |
| 2   | B     | 3025 | G    | C1'-C2'-O2' | -6.76 | 98.27       | 108.40   |
| 28  | 2     | 21   | ARG  | N-CA-C      | 6.71  | 119.58      | 111.40   |
| 19  | S     | 137  | ASN  | N-CA-C      | 6.68  | 120.34      | 110.46   |
| 23  | W     | 42   | ASN  | CA-C-N      | 6.67  | 128.18      | 119.84   |
| 23  | W     | 42   | ASN  | C-N-CA      | 6.67  | 128.18      | 119.84   |
| 20  | T     | 27   | ALA  | N-CA-C      | -6.67 | 97.86       | 108.73   |
| 2   | B     | 3024 | U    | P-O5'-C5'   | 6.65  | 130.88      | 120.90   |
| 4   | D     | 222  | LYS  | N-CA-C      | -6.61 | 100.18      | 110.42   |
| 7   | G     | 7    | ILE  | CA-C-N      | 6.56  | 126.52      | 119.76   |
| 7   | G     | 7    | ILE  | C-N-CA      | 6.56  | 126.52      | 119.76   |
| 4   | D     | 154  | VAL  | N-CA-C      | 6.55  | 113.52      | 107.56   |
| 30  | 4     | 60   | LYS  | N-CA-C      | -6.50 | 101.32      | 110.29   |
| 24  | X     | 143  | THR  | N-CA-C      | -6.49 | 104.29      | 111.82   |
| 19  | S     | 34   | GLU  | N-CA-C      | 6.48  | 118.42      | 111.36   |
| 15  | O     | 117  | ALA  | N-CA-C      | -6.46 | 104.17      | 111.14   |
| 28  | 2     | 11   | LYS  | N-CA-C      | 6.43  | 119.62      | 109.39   |
| 3   | C     | 198  | ASP  | N-CA-C      | 6.43  | 121.12      | 113.28   |
| 1   | A     | 1738 | C    | O4'-C4'-C3' | -6.42 | 97.58       | 104.00   |
| 24  | X     | 120  | PRO  | N-CA-C      | -6.38 | 104.35      | 110.47   |
| 2   | B     | 3024 | U    | C5'-C4'-O4' | 6.36  | 119.34      | 109.80   |
| 18  | R     | 47   | VAL  | CA-C-N      | 6.35  | 126.10      | 119.05   |
| 18  | R     | 47   | VAL  | C-N-CA      | 6.35  | 126.10      | 119.05   |
| 7   | G     | 48   | VAL  | N-CA-C      | 6.34  | 116.99      | 108.11   |
| 17  | Q     | 86   | ALA  | N-CA-C      | -6.34 | 103.67      | 111.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | D     | 265  | LEU  | N-CA-C      | 6.31  | 118.86      | 110.53   |
| 2   | B     | 3002 | U    | C4'-C3'-O3' | 6.30  | 118.86      | 109.40   |
| 13  | M     | 43   | HIS  | N-CA-C      | -6.30 | 98.72       | 109.24   |
| 19  | S     | 79   | ARG  | N-CA-C      | 6.30  | 116.60      | 108.34   |
| 19  | S     | 18   | LEU  | N-CA-C      | -6.30 | 99.64       | 109.72   |
| 1   | A     | 1723 | G    | C4'-C3'-O3' | -6.29 | 103.57      | 113.00   |
| 10  | J     | 113  | ALA  | CA-C-N      | 6.28  | 126.82      | 120.04   |
| 10  | J     | 113  | ALA  | C-N-CA      | 6.28  | 126.82      | 120.04   |
| 22  | V     | 18   | GLY  | N-CA-C      | 6.27  | 119.92      | 112.33   |
| 4   | D     | 220  | VAL  | N-CA-C      | -6.26 | 103.14      | 110.21   |
| 28  | 2     | 43   | ALA  | N-CA-C      | -6.23 | 104.57      | 111.36   |
| 5   | E     | 179  | GLY  | N-CA-C      | -6.21 | 105.01      | 113.27   |
| 15  | O     | 13   | ARG  | N-CA-C      | -6.21 | 105.83      | 113.41   |
| 1   | A     | 1450 | C    | C2'-C3'-O3' | -6.15 | 104.47      | 113.70   |
| 26  | Z     | 115  | ARG  | N-CA-C      | -6.11 | 104.55      | 111.14   |
| 25  | Y     | 79   | GLU  | N-CA-C      | 6.10  | 120.56      | 113.18   |
| 21  | U     | 78   | THR  | N-CA-C      | 6.08  | 118.65      | 109.41   |
| 19  | S     | 142  | ASP  | N-CA-C      | -6.07 | 100.30      | 109.95   |
| 6   | F     | 77   | ASP  | CB-CA-C     | -6.05 | 109.61      | 116.63   |
| 30  | 4     | 67   | LEU  | N-CA-C      | 6.05  | 119.08      | 109.81   |
| 10  | J     | 162  | SER  | CA-C-N      | -6.05 | 112.28      | 119.84   |
| 10  | J     | 162  | SER  | C-N-CA      | -6.05 | 112.28      | 119.84   |
| 19  | S     | 13   | THR  | N-CA-C      | 6.03  | 119.06      | 108.75   |
| 1   | A     | 2291 | A    | N9-C1'-C2'  | 6.01  | 121.02      | 112.00   |
| 3   | C     | 5    | GLN  | N-CA-C      | 6.00  | 118.59      | 111.33   |
| 30  | 4     | 42   | ARG  | N-CA-C      | 5.98  | 117.47      | 111.07   |
| 4   | D     | 242  | TRP  | N-CA-C      | -5.98 | 104.68      | 111.14   |
| 10  | J     | 13   | ALA  | N-CA-C      | -5.98 | 101.00      | 109.96   |
| 15  | O     | 171  | HIS  | N-CA-C      | -5.97 | 104.85      | 111.71   |
| 16  | P     | 50   | ARG  | N-CA-C      | 5.95  | 119.72      | 112.23   |
| 1   | A     | 921  | G    | N9-C1'-C2'  | 5.93  | 120.89      | 112.00   |
| 10  | J     | 137  | ASN  | N-CA-C      | -5.88 | 101.56      | 110.39   |
| 2   | B     | 3022 | G    | N9-C1'-C2'  | 5.88  | 120.82      | 112.00   |
| 1   | A     | 920  | C    | C2'-C3'-O3' | -5.88 | 104.89      | 113.70   |
| 16  | P     | 96   | VAL  | N-CA-C      | 5.85  | 117.18      | 108.46   |
| 4   | D     | 147  | VAL  | CA-C-N      | 5.85  | 126.26      | 119.47   |
| 4   | D     | 147  | VAL  | C-N-CA      | 5.85  | 126.26      | 119.47   |
| 11  | K     | 88   | PRO  | N-CA-C      | -5.83 | 104.61      | 112.48   |
| 4   | D     | 175  | LEU  | N-CA-C      | -5.83 | 104.83      | 111.07   |
| 1   | A     | 2096 | A    | C4'-C3'-O3' | -5.82 | 104.27      | 113.00   |
| 15  | O     | 102  | LEU  | N-CA-C      | 5.81  | 117.77      | 108.41   |
| 3   | C     | 68   | ILE  | N-CA-C      | 5.80  | 117.10      | 108.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | O     | 51   | GLY  | CA-C-N      | 5.80  | 125.49      | 119.05   |
| 15  | O     | 51   | GLY  | C-N-CA      | 5.80  | 125.49      | 119.05   |
| 27  | 1     | 32   | LYS  | N-CA-C      | -5.79 | 104.97      | 111.28   |
| 3   | C     | 135  | VAL  | N-CA-C      | 5.79  | 117.09      | 108.46   |
| 3   | C     | 8    | ARG  | N-CA-C      | -5.79 | 104.94      | 112.23   |
| 4   | D     | 324  | ASP  | CA-C-N      | 5.77  | 125.53      | 119.76   |
| 4   | D     | 324  | ASP  | C-N-CA      | 5.77  | 125.53      | 119.76   |
| 16  | P     | 82   | SER  | N-CA-C      | -5.75 | 102.93      | 110.53   |
| 9   | I     | 14   | GLU  | N-CA-C      | 5.73  | 117.61      | 111.36   |
| 24  | X     | 17   | ILE  | N-CA-C      | -5.73 | 105.50      | 111.58   |
| 1   | A     | 1723 | G    | N9-C1'-C2'  | 5.69  | 120.53      | 112.00   |
| 8   | H     | 111  | ILE  | N-CA-C      | -5.68 | 104.98      | 110.72   |
| 1   | A     | 138  | U    | C2'-C3'-O3' | -5.66 | 105.21      | 113.70   |
| 10  | J     | 110  | GLY  | N-CA-C      | -5.66 | 99.77       | 113.18   |
| 1   | A     | 1819 | G    | C5'-C4'-C3' | 5.65  | 124.47      | 116.00   |
| 1   | A     | 1877 | G    | N9-C1'-C2'  | 5.63  | 120.44      | 112.00   |
| 1   | A     | 2526 | C    | N1-C1'-C2'  | 5.60  | 120.40      | 112.00   |
| 1   | A     | 2419 | U    | N1-C1'-C2'  | 5.60  | 120.40      | 112.00   |
| 1   | A     | 2667 | G    | O5'-C5'-C4' | 5.57  | 119.85      | 111.50   |
| 1   | A     | 1504 | A    | N9-C1'-C2'  | 5.56  | 120.34      | 112.00   |
| 1   | A     | 1358 | A    | C4'-C3'-O3' | -5.55 | 104.67      | 113.00   |
| 2   | B     | 3024 | U    | O5'-P-OP2   | 5.54  | 124.60      | 108.00   |
| 16  | P     | 69   | VAL  | N-CA-C      | 5.53  | 115.85      | 108.11   |
| 18  | R     | 84   | ILE  | N-CA-C      | 5.52  | 115.90      | 108.17   |
| 1   | A     | 834  | G    | C2'-C3'-O3' | -5.52 | 105.42      | 113.70   |
| 15  | O     | 168  | LEU  | N-CA-C      | 5.51  | 120.65      | 108.64   |
| 1   | A     | 206  | G    | C5'-C4'-C3' | -5.50 | 107.76      | 116.00   |
| 2   | B     | 3025 | G    | C2'-C3'-O3' | 5.50  | 121.95      | 113.70   |
| 2   | B     | 3023 | U    | C3'-C2'-O2' | 5.49  | 118.93      | 110.70   |
| 1   | A     | 129  | A    | C2'-C3'-O3' | 5.48  | 121.92      | 113.70   |
| 1   | A     | 2835 | C    | C4'-C3'-O3' | -5.48 | 104.78      | 113.00   |
| 1   | A     | 2726 | U    | N1-C1'-C2'  | 5.46  | 120.19      | 112.00   |
| 7   | G     | 157  | LYS  | N-CA-C      | 5.46  | 118.16      | 109.81   |
| 13  | M     | 102  | ASP  | N-CA-C      | -5.43 | 106.97      | 113.21   |
| 2   | B     | 3023 | U    | C5'-C4'-C3' | 5.42  | 124.12      | 116.00   |
| 3   | C     | 38   | ILE  | N-CA-C      | 5.41  | 116.23      | 108.93   |
| 30  | 4     | 59   | ASP  | N-CA-C      | 5.41  | 118.05      | 109.50   |
| 24  | X     | 126  | ASP  | N-CA-C      | 5.40  | 119.58      | 113.15   |
| 1   | A     | 959  | C    | C4'-C3'-O3' | -5.40 | 104.90      | 113.00   |
| 19  | S     | 57   | VAL  | CB-CA-C     | -5.40 | 104.57      | 110.78   |
| 6   | F     | 151  | ILE  | N-CA-C      | 5.38  | 114.22      | 108.95   |
| 14  | N     | 127  | LYS  | N-CA-C      | -5.38 | 98.80       | 108.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | S     | 122  | GLN  | N-CA-C      | -5.37 | 100.35      | 108.67   |
| 2   | B     | 3103 | A    | C4'-C3'-C2' | -5.36 | 97.24       | 102.60   |
| 4   | D     | 47   | GLY  | N-CA-C      | 5.35  | 118.07      | 110.74   |
| 1   | A     | 2012 | U    | N1-C1'-C2'  | 5.33  | 119.99      | 112.00   |
| 14  | N     | 114  | VAL  | N-CA-C      | 5.33  | 115.96      | 109.30   |
| 15  | O     | 8    | VAL  | CA-C-N      | 5.32  | 126.49      | 119.84   |
| 15  | O     | 8    | VAL  | C-N-CA      | 5.32  | 126.49      | 119.84   |
| 1   | A     | 2096 | A    | N9-C1'-C2'  | 5.32  | 119.97      | 112.00   |
| 1   | A     | 874  | A    | C4'-C3'-O3' | -5.31 | 105.04      | 113.00   |
| 17  | Q     | 56   | GLY  | N-CA-C      | -5.30 | 102.74      | 111.38   |
| 12  | L     | 14   | LYS  | N-CA-C      | -5.29 | 102.78      | 110.24   |
| 14  | N     | 42   | ARG  | CA-C-N      | 5.29  | 125.54      | 119.83   |
| 14  | N     | 42   | ARG  | C-N-CA      | 5.29  | 125.54      | 119.83   |
| 1   | A     | 1205 | U    | C3'-C2'-O2' | 5.26  | 118.58      | 110.70   |
| 1   | A     | 1450 | C    | C4'-C3'-O3' | 5.25  | 120.88      | 113.00   |
| 2   | B     | 3065 | A    | N9-C1'-C2'  | 5.25  | 119.87      | 112.00   |
| 10  | J     | 3    | GLY  | N-CA-C      | -5.25 | 107.81      | 114.16   |
| 10  | J     | 86   | ARG  | N-CA-C      | 5.25  | 118.94      | 112.54   |
| 17  | Q     | 95   | GLU  | N-CA-C      | -5.23 | 105.58      | 111.28   |
| 1   | A     | 2313 | C    | C4'-C3'-C2' | -5.22 | 97.38       | 102.60   |
| 14  | N     | 70   | GLY  | N-CA-C      | 5.21  | 118.37      | 111.70   |
| 1   | A     | 1120 | U    | C5'-C4'-C3' | -5.21 | 108.19      | 116.00   |
| 1   | A     | 2291 | A    | C4'-C3'-O3' | -5.21 | 105.19      | 113.00   |
| 3   | C     | 110  | SER  | N-CA-C      | -5.21 | 105.29      | 111.69   |
| 11  | K     | 68   | GLY  | N-CA-C      | 5.20  | 119.15      | 112.18   |
| 17  | Q     | 118  | GLN  | N-CA-C      | -5.20 | 105.69      | 111.36   |
| 13  | M     | 42   | ASN  | N-CA-C      | 5.20  | 118.89      | 111.92   |
| 18  | R     | 86   | VAL  | N-CA-C      | 5.20  | 115.21      | 108.35   |
| 25  | Y     | 53   | SER  | N-CA-C      | -5.17 | 105.53      | 111.07   |
| 5   | E     | 80   | VAL  | N-CA-C      | 5.17  | 114.65      | 108.96   |
| 12  | L     | 56   | SER  | N-CA-C      | -5.17 | 101.34      | 109.50   |
| 5   | E     | 215  | ALA  | N-CA-C      | 5.16  | 117.64      | 111.71   |
| 25  | Y     | 12   | ILE  | N-CA-C      | 5.16  | 112.97      | 107.76   |
| 27  | 1     | 39   | CYS  | N-CA-C      | 5.15  | 115.53      | 109.60   |
| 1   | A     | 1721 | C    | N1-C1'-C2'  | 5.14  | 119.71      | 112.00   |
| 19  | S     | 141  | VAL  | N-CA-C      | 5.12  | 115.96      | 108.53   |
| 26  | Z     | 230  | ASN  | CA-C-N      | 5.12  | 125.10      | 120.03   |
| 26  | Z     | 230  | ASN  | C-N-CA      | 5.12  | 125.10      | 120.03   |
| 15  | O     | 165  | ALA  | N-CA-C      | -5.10 | 107.12      | 113.55   |
| 15  | O     | 42   | HIS  | N-CA-C      | 5.10  | 116.42      | 109.18   |
| 6   | F     | 137  | PRO  | N-CA-C      | 5.09  | 122.96      | 112.47   |
| 18  | R     | 53   | HIS  | CA-C-N      | 5.09  | 126.20      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | R     | 53   | HIS  | C-N-CA      | 5.09  | 126.20      | 119.84   |
| 17  | Q     | 131  | PHE  | N-CA-C      | 5.08  | 116.69      | 108.41   |
| 1   | A     | 2864 | U    | C4'-C3'-O3' | -5.08 | 105.39      | 113.00   |
| 2   | B     | 3023 | U    | OP2-P-O3'   | -5.07 | 92.78       | 108.00   |
| 1   | A     | 2564 | G    | N9-C1'-C2'  | 5.07  | 119.60      | 112.00   |
| 1   | A     | 1204 | C    | C3'-C2'-O2' | 5.07  | 118.30      | 110.70   |
| 1   | A     | 1079 | A    | N9-C1'-C2'  | 5.06  | 119.59      | 112.00   |
| 8   | H     | 118  | LEU  | N-CA-C      | -5.06 | 107.17      | 113.19   |
| 25  | Y     | 80   | GLU  | N-CA-C      | -5.06 | 107.09      | 114.12   |
| 5   | E     | 201  | SER  | N-CA-C      | 5.05  | 116.71      | 108.63   |
| 21  | U     | 46   | ASP  | N-CA-C      | 5.04  | 117.04      | 110.43   |
| 30  | 4     | 70   | ARG  | N-CA-C      | 5.04  | 116.95      | 108.73   |
| 10  | J     | 7    | ARG  | N-CA-C      | 5.04  | 118.53      | 112.38   |
| 1   | A     | 1730 | G    | C5'-C4'-C3' | 5.04  | 122.75      | 115.20   |
| 2   | B     | 3003 | A    | C4'-C3'-C2' | -5.03 | 97.57       | 102.60   |
| 23  | W     | 64   | GLY  | N-CA-C      | -5.03 | 107.87      | 115.32   |
| 26  | Z     | 178  | HIS  | N-CA-C      | -5.03 | 103.13      | 110.08   |
| 1   | A     | 2615 | U    | N1-C1'-C2'  | 5.03  | 119.55      | 112.00   |
| 4   | D     | 130  | ASP  | N-CA-C      | -5.03 | 105.88      | 111.36   |
| 3   | C     | 166  | ASP  | N-CA-C      | 5.02  | 117.64      | 111.82   |
| 21  | U     | 106  | GLU  | N-CA-C      | -5.02 | 105.70      | 111.07   |
| 13  | M     | 37   | LYS  | N-CA-C      | 5.01  | 116.12      | 108.30   |
| 5   | E     | 167  | ASP  | N-CA-C      | -5.01 | 105.82      | 111.28   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | A     | 1563 | G    | C3'  |

All (146) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1005 | A    | Sidechain |
| 1   | A     | 1036 | G    | Sidechain |
| 1   | A     | 1038 | G    | Sidechain |
| 1   | A     | 1118 | A    | Sidechain |
| 1   | A     | 112  | G    | Sidechain |
| 1   | A     | 1127 | C    | Sidechain |
| 1   | A     | 1134 | G    | Sidechain |
| 1   | A     | 1156 | C    | Sidechain |
| 1   | A     | 1206 | U    | Sidechain |
| 1   | A     | 1234 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1264 | U    | Sidechain |
| 1   | A     | 1305 | C    | Sidechain |
| 1   | A     | 1314 | U    | Sidechain |
| 1   | A     | 1348 | A    | Sidechain |
| 1   | A     | 1349 | G    | Sidechain |
| 1   | A     | 1350 | U    | Sidechain |
| 1   | A     | 1371 | U    | Sidechain |
| 1   | A     | 1379 | A    | Sidechain |
| 1   | A     | 1390 | A    | Sidechain |
| 1   | A     | 1417 | G    | Sidechain |
| 1   | A     | 1447 | U    | Sidechain |
| 1   | A     | 146  | U    | Sidechain |
| 1   | A     | 147  | G    | Sidechain |
| 1   | A     | 1470 | A    | Sidechain |
| 1   | A     | 1635 | U    | Sidechain |
| 1   | A     | 1677 | U    | Sidechain |
| 1   | A     | 1685 | A    | Sidechain |
| 1   | A     | 1688 | G    | Sidechain |
| 1   | A     | 1694 | G    | Sidechain |
| 1   | A     | 1696 | U    | Sidechain |
| 1   | A     | 171  | C    | Sidechain |
| 1   | A     | 1720 | C    | Sidechain |
| 1   | A     | 1736 | A    | Sidechain |
| 1   | A     | 1737 | A    | Sidechain |
| 1   | A     | 1758 | U    | Sidechain |
| 1   | A     | 1809 | G    | Sidechain |
| 1   | A     | 1819 | G    | Sidechain |
| 1   | A     | 1823 | G    | Sidechain |
| 1   | A     | 1828 | G    | Sidechain |
| 1   | A     | 1829 | A    | Sidechain |
| 1   | A     | 1835 | U    | Sidechain |
| 1   | A     | 1839 | A    | Sidechain |
| 1   | A     | 1846 | U    | Sidechain |
| 1   | A     | 1860 | U    | Sidechain |
| 1   | A     | 1861 | C    | Sidechain |
| 1   | A     | 1865 | A    | Sidechain |
| 1   | A     | 1877 | G    | Sidechain |
| 1   | A     | 1878 | G    | Sidechain |
| 1   | A     | 1908 | G    | Sidechain |
| 1   | A     | 1922 | A    | Sidechain |
| 1   | A     | 194  | A    | Sidechain |
| 1   | A     | 1972 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1978 | A    | Sidechain |
| 1   | A     | 20   | G    | Sidechain |
| 1   | A     | 2023 | G    | Sidechain |
| 1   | A     | 2035 | C    | Sidechain |
| 1   | A     | 2047 | C    | Sidechain |
| 1   | A     | 2088 | C    | Sidechain |
| 1   | A     | 2110 | G    | Sidechain |
| 1   | A     | 2115 | U    | Sidechain |
| 1   | A     | 2117 | U    | Sidechain |
| 1   | A     | 2123 | A    | Sidechain |
| 1   | A     | 2263 | G    | Sidechain |
| 1   | A     | 2293 | G    | Sidechain |
| 1   | A     | 2300 | A    | Sidechain |
| 1   | A     | 2306 | U    | Sidechain |
| 1   | A     | 2313 | C    | Sidechain |
| 1   | A     | 2316 | G    | Sidechain |
| 1   | A     | 2377 | U    | Sidechain |
| 1   | A     | 2381 | C    | Sidechain |
| 1   | A     | 24   | G    | Sidechain |
| 1   | A     | 2412 | G    | Sidechain |
| 1   | A     | 2439 | C    | Sidechain |
| 1   | A     | 2441 | U    | Sidechain |
| 1   | A     | 2444 | U    | Sidechain |
| 1   | A     | 246  | G    | Sidechain |
| 1   | A     | 2465 | A    | Sidechain |
| 1   | A     | 2473 | U    | Sidechain |
| 1   | A     | 2479 | A    | Sidechain |
| 1   | A     | 2492 | U    | Sidechain |
| 1   | A     | 2493 | C    | Sidechain |
| 1   | A     | 2503 | A    | Sidechain |
| 1   | A     | 2506 | A    | Sidechain |
| 1   | A     | 2530 | C    | Sidechain |
| 1   | A     | 2551 | C    | Sidechain |
| 1   | A     | 2564 | G    | Sidechain |
| 1   | A     | 257  | G    | Sidechain |
| 1   | A     | 2607 | U    | Sidechain |
| 1   | A     | 2622 | A    | Sidechain |
| 1   | A     | 2623 | G    | Sidechain |
| 1   | A     | 2630 | G    | Sidechain |
| 1   | A     | 2640 | U    | Sidechain |
| 1   | A     | 2659 | U    | Sidechain |
| 1   | A     | 2673 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 2675 | A    | Sidechain |
| 1   | A     | 2774 | U    | Sidechain |
| 1   | A     | 2790 | C    | Sidechain |
| 1   | A     | 2793 | A    | Sidechain |
| 1   | A     | 2837 | U    | Sidechain |
| 1   | A     | 2840 | A    | Sidechain |
| 1   | A     | 2842 | G    | Sidechain |
| 1   | A     | 2887 | G    | Sidechain |
| 1   | A     | 33   | G    | Sidechain |
| 1   | A     | 333  | G    | Sidechain |
| 1   | A     | 336  | G    | Sidechain |
| 1   | A     | 391  | U    | Sidechain |
| 1   | A     | 396  | U    | Sidechain |
| 1   | A     | 397  | A    | Sidechain |
| 1   | A     | 407  | A    | Sidechain |
| 1   | A     | 436  | A    | Sidechain |
| 1   | A     | 458  | G    | Sidechain |
| 1   | A     | 474  | C    | Sidechain |
| 1   | A     | 481  | U    | Sidechain |
| 1   | A     | 482  | G    | Sidechain |
| 1   | A     | 502  | A    | Sidechain |
| 1   | A     | 515  | C    | Sidechain |
| 1   | A     | 517  | U    | Sidechain |
| 1   | A     | 518  | G    | Sidechain |
| 1   | A     | 539  | G    | Sidechain |
| 1   | A     | 548  | U    | Sidechain |
| 1   | A     | 552  | A    | Sidechain |
| 1   | A     | 565  | A    | Sidechain |
| 1   | A     | 619  | U    | Sidechain |
| 1   | A     | 631  | A    | Sidechain |
| 1   | A     | 636  | G    | Sidechain |
| 1   | A     | 639  | A    | Sidechain |
| 1   | A     | 657  | G    | Sidechain |
| 1   | A     | 678  | G    | Sidechain |
| 1   | A     | 755  | G    | Sidechain |
| 1   | A     | 766  | A    | Sidechain |
| 1   | A     | 781  | C    | Sidechain |
| 1   | A     | 815  | U    | Sidechain |
| 1   | A     | 817  | G    | Sidechain |
| 1   | A     | 844  | A    | Sidechain |
| 1   | A     | 871  | G    | Sidechain |
| 1   | A     | 878  | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 891  | G    | Sidechain |
| 1   | A     | 898  | G    | Sidechain |
| 1   | A     | 903  | U    | Sidechain |
| 1   | A     | 919  | U    | Sidechain |
| 1   | A     | 954  | U    | Sidechain |
| 2   | B     | 3022 | G    | Sidechain |
| 2   | B     | 3024 | U    | Sidechain |
| 2   | B     | 3052 | A    | Sidechain |
| 2   | B     | 3065 | A    | Sidechain |
| 2   | B     | 3094 | G    | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 59017 | 0        | 29803    | 1172    | 0            |
| 2   | B     | 2600  | 0        | 1326     | 84      | 0            |
| 3   | C     | 1754  | 0        | 1763     | 136     | 0            |
| 4   | D     | 2624  | 0        | 2533     | 190     | 0            |
| 5   | E     | 1858  | 0        | 1816     | 130     | 0            |
| 6   | F     | 1094  | 0        | 1085     | 148     | 0            |
| 7   | G     | 1357  | 0        | 1266     | 91      | 0            |
| 8   | H     | 885   | 0        | 854      | 66      | 0            |
| 9   | I     | 240   | 0        | 231      | 28      | 0            |
| 10  | J     | 1215  | 0        | 1215     | 157     | 0            |
| 11  | K     | 1119  | 0        | 1098     | 70      | 0            |
| 12  | L     | 993   | 0        | 1027     | 59      | 0            |
| 13  | M     | 1114  | 0        | 1072     | 70      | 0            |
| 14  | N     | 1605  | 0        | 1676     | 172     | 0            |
| 15  | O     | 1444  | 0        | 1401     | 150     | 0            |
| 16  | P     | 864   | 0        | 873      | 48      | 0            |
| 17  | Q     | 1133  | 0        | 1127     | 51      | 0            |
| 18  | R     | 734   | 0        | 728      | 30      | 0            |
| 19  | S     | 1149  | 0        | 1122     | 66      | 0            |
| 20  | T     | 641   | 0        | 605      | 23      | 0            |
| 21  | U     | 949   | 0        | 923      | 58      | 0            |
| 22  | V     | 410   | 0        | 364      | 36      | 0            |
| 23  | W     | 499   | 0        | 511      | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | X     | 1195  | 0        | 1137     | 103     | 0            |
| 25  | Y     | 654   | 0        | 653      | 48      | 0            |
| 26  | Z     | 1130  | 0        | 1133     | 62      | 0            |
| 27  | 1     | 563   | 0        | 597      | 55      | 0            |
| 28  | 2     | 430   | 0        | 426      | 32      | 0            |
| 29  | 3     | 393   | 0        | 406      | 31      | 0            |
| 30  | 4     | 755   | 0        | 728      | 42      | 0            |
| 31  | A     | 52    | 0        | 72       | 2       | 0            |
| 32  | 1     | 1     | 0        | 0        | 0       | 0            |
| 32  | 4     | 1     | 0        | 0        | 0       | 0            |
| 32  | A     | 109   | 0        | 0        | 1       | 0            |
| 32  | B     | 1     | 0        | 0        | 0       | 0            |
| 32  | C     | 1     | 0        | 0        | 0       | 0            |
| 32  | D     | 1     | 0        | 0        | 0       | 0            |
| 32  | L     | 1     | 0        | 0        | 0       | 0            |
| 32  | U     | 1     | 0        | 0        | 0       | 0            |
| 32  | Z     | 1     | 0        | 0        | 0       | 0            |
| 33  | A     | 2     | 0        | 0        | 0       | 0            |
| 34  | A     | 71    | 0        | 0        | 0       | 0            |
| 34  | B     | 2     | 0        | 0        | 0       | 0            |
| 34  | C     | 1     | 0        | 0        | 0       | 0            |
| 34  | E     | 1     | 0        | 0        | 0       | 0            |
| 34  | J     | 2     | 0        | 0        | 0       | 0            |
| 34  | K     | 1     | 0        | 0        | 0       | 0            |
| 34  | M     | 1     | 0        | 0        | 0       | 0            |
| 34  | N     | 1     | 0        | 0        | 0       | 0            |
| 34  | R     | 1     | 0        | 0        | 0       | 0            |
| 34  | S     | 3     | 0        | 0        | 0       | 0            |
| 34  | T     | 1     | 0        | 0        | 0       | 0            |
| 34  | U     | 1     | 0        | 0        | 0       | 0            |
| 35  | 4     | 1     | 0        | 0        | 0       | 0            |
| 35  | A     | 9     | 0        | 0        | 3       | 0            |
| 35  | C     | 1     | 0        | 0        | 0       | 0            |
| 35  | D     | 1     | 0        | 0        | 0       | 0            |
| 35  | K     | 4     | 0        | 0        | 5       | 0            |
| 35  | L     | 1     | 0        | 0        | 0       | 0            |
| 35  | N     | 1     | 0        | 0        | 2       | 0            |
| 35  | O     | 1     | 0        | 0        | 2       | 0            |
| 35  | P     | 1     | 0        | 0        | 0       | 0            |
| 35  | R     | 1     | 0        | 0        | 0       | 0            |
| 35  | S     | 1     | 0        | 0        | 0       | 0            |
| 36  | 1     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36  | 2     | 1     | 0        | 0        | 0       | 0            |
| 36  | 4     | 1     | 0        | 0        | 0       | 0            |
| 36  | P     | 1     | 0        | 0        | 0       | 0            |
| 36  | V     | 1     | 0        | 0        | 0       | 0            |
| 37  | 1     | 38    | 0        | 0        | 9       | 0            |
| 37  | 2     | 57    | 0        | 0        | 5       | 0            |
| 37  | 3     | 39    | 0        | 0        | 4       | 0            |
| 37  | 4     | 72    | 0        | 0        | 12      | 0            |
| 37  | A     | 5898  | 0        | 0        | 233     | 0            |
| 37  | B     | 140   | 0        | 0        | 15      | 0            |
| 37  | C     | 129   | 0        | 0        | 24      | 0            |
| 37  | D     | 152   | 0        | 0        | 27      | 0            |
| 37  | E     | 169   | 0        | 0        | 34      | 0            |
| 37  | F     | 52    | 0        | 0        | 19      | 0            |
| 37  | G     | 42    | 0        | 0        | 14      | 0            |
| 37  | H     | 28    | 0        | 0        | 10      | 0            |
| 37  | I     | 21    | 0        | 0        | 6       | 0            |
| 37  | J     | 81    | 0        | 0        | 18      | 0            |
| 37  | K     | 56    | 0        | 0        | 6       | 0            |
| 37  | L     | 61    | 0        | 0        | 12      | 0            |
| 37  | M     | 81    | 0        | 0        | 19      | 0            |
| 37  | N     | 129   | 0        | 0        | 22      | 0            |
| 37  | O     | 68    | 0        | 0        | 21      | 0            |
| 37  | P     | 45    | 0        | 0        | 13      | 0            |
| 37  | Q     | 69    | 0        | 0        | 6       | 0            |
| 37  | R     | 56    | 0        | 0        | 3       | 0            |
| 37  | S     | 89    | 0        | 0        | 8       | 0            |
| 37  | T     | 36    | 0        | 0        | 4       | 0            |
| 37  | U     | 39    | 0        | 0        | 5       | 0            |
| 37  | V     | 27    | 0        | 0        | 5       | 0            |
| 37  | W     | 15    | 0        | 0        | 3       | 0            |
| 37  | X     | 73    | 0        | 0        | 6       | 0            |
| 37  | Y     | 30    | 0        | 0        | 8       | 0            |
| 37  | Z     | 93    | 0        | 0        | 15      | 0            |
| All | All   | 98587 | 0        | 59571    | 3149    | 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 21.

All (3149) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1160:G:H5'    | 1:A:1161:A:H5'    | 1.22                     | 1.15              |
| 6:F:25:MET:HE2    | 6:F:41:LEU:HG     | 1.21                     | 1.15              |
| 25:Y:37:LEU:HD13  | 25:Y:85:VAL:HG21  | 1.26                     | 1.13              |
| 1:A:1134:G:H4'    | 10:J:151:MET:HE1  | 1.32                     | 1.11              |
| 21:U:71:VAL:HG11  | 21:U:90:PRO:HB3   | 1.33                     | 1.11              |
| 19:S:99:ALA:HB1   | 19:S:109:MET:HE1  | 1.22                     | 1.10              |
| 10:J:86:ARG:NH1   | 10:J:133:ILE:HG13 | 1.67                     | 1.10              |
| 1:A:871:G:H5'     | 1:A:871:G:H8      | 1.14                     | 1.07              |
| 23:W:12:THR:HG22  | 23:W:15:GLU:HG3   | 1.34                     | 1.07              |
| 27:1:10:ARG:HA    | 37:1:8415:HOH:O   | 1.55                     | 1.07              |
| 5:E:236:THR:HG22  | 5:E:239:ALA:H     | 1.11                     | 1.06              |
| 1:A:156:C:H5''    | 14:N:171:ARG:HD3  | 1.35                     | 1.05              |
| 1:A:871:G:H5'     | 1:A:871:G:C8      | 1.89                     | 1.05              |
| 2:B:3023:U:H5''   | 2:B:3024:U:OP2    | 1.55                     | 1.04              |
| 11:K:19:MET:HE3   | 11:K:132:LEU:HD11 | 1.34                     | 1.04              |
| 2:B:3076:G:H3'    | 2:B:3077:A:H5''   | 1.38                     | 1.04              |
| 1:A:541:C:H2'     | 1:A:542:A:H5''    | 1.38                     | 1.03              |
| 29:3:39:ARG:HG2   | 37:3:3143:HOH:O   | 1.57                     | 1.03              |
| 15:O:47:LEU:HD11  | 15:O:127:LEU:HD21 | 1.41                     | 1.02              |
| 1:A:542:A:H5'     | 1:A:542:A:H8      | 1.22                     | 1.02              |
| 10:J:162:SER:HB2  | 10:J:163:PRO:HD3  | 1.40                     | 1.01              |
| 4:D:321:PRO:HA    | 37:D:8662:HOH:O   | 1.61                     | 1.00              |
| 10:J:45:GLN:HB3   | 10:J:163:PRO:HD2  | 1.40                     | 0.99              |
| 4:D:162:MET:HE1   | 4:D:308:LEU:HD21  | 1.41                     | 0.99              |
| 10:J:86:ARG:HH11  | 10:J:133:ILE:HG13 | 0.85                     | 0.99              |
| 10:J:165:GLY:HA3  | 37:J:8401:HOH:O   | 1.61                     | 0.99              |
| 10:J:26:LYS:HD2   | 10:J:28:ILE:HD12  | 1.45                     | 0.98              |
| 2:B:3056:A:H2'    | 2:B:3057:A:H5''   | 1.44                     | 0.98              |
| 12:L:29:LEU:HB3   | 12:L:55:VAL:HG11  | 1.44                     | 0.98              |
| 14:N:35:PRO:HG2   | 14:N:38:VAL:HG23  | 1.43                     | 0.98              |
| 14:N:164:THR:HG22 | 14:N:167:GLY:H    | 1.24                     | 0.98              |
| 1:A:962:C:H1'     | 15:O:5:ARG:NH1    | 1.80                     | 0.97              |
| 1:A:1474:C:H6     | 1:A:1474:C:H5'    | 1.28                     | 0.97              |
| 4:D:140:LEU:HA    | 37:D:8583:HOH:O   | 1.63                     | 0.97              |
| 12:L:10:GLN:NE2   | 12:L:10:GLN:H     | 1.63                     | 0.97              |
| 13:M:79:ASP:HB3   | 37:M:8432:HOH:O   | 1.65                     | 0.96              |
| 1:A:1751:G:H2'    | 1:A:1752:G:H5''   | 1.44                     | 0.96              |
| 14:N:87:MET:HG2   | 30:4:46:ILE:HG21  | 1.45                     | 0.96              |
| 6:F:134:LEU:HD11  | 6:F:166:ILE:HD11  | 1.48                     | 0.95              |
| 17:Q:115:SER:H    | 17:Q:118:GLN:HE21 | 0.95                     | 0.95              |
| 5:E:5:ILE:HD11    | 5:E:16:VAL:HG23   | 1.48                     | 0.94              |
| 24:X:149:LEU:HG   | 24:X:153:MET:HE2  | 1.47                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1835:U:H5     | 1:A:1840:A:N7     | 1.66                     | 0.94              |
| 14:N:64:ARG:HD2   | 37:N:8585:HOH:O   | 1.66                     | 0.94              |
| 12:L:81:ARG:HB2   | 12:L:87:ARG:HH11  | 1.32                     | 0.93              |
| 1:A:871:G:H8      | 1:A:871:G:C5'     | 1.82                     | 0.93              |
| 14:N:102:GLU:OE1  | 14:N:164:THR:HG21 | 1.69                     | 0.93              |
| 10:J:142:VAL:HG13 | 37:J:8383:HOH:O   | 1.69                     | 0.92              |
| 10:J:4:ALA:HB3    | 37:J:8367:HOH:O   | 1.69                     | 0.92              |
| 2:B:3006:C:H5''   | 15:O:37:ARG:NH1   | 1.83                     | 0.92              |
| 5:E:236:THR:HG21  | 37:E:8370:HOH:O   | 1.70                     | 0.92              |
| 1:A:960:G:H4'     | 37:A:7000:HOH:O   | 1.68                     | 0.92              |
| 1:A:1667:A:H5'    | 1:A:1667:A:H8     | 1.32                     | 0.92              |
| 14:N:24:MET:HE3   | 14:N:28:MET:HE3   | 1.49                     | 0.91              |
| 10:J:2:PRO:HB2    | 37:J:8367:HOH:O   | 1.69                     | 0.91              |
| 12:L:10:GLN:H     | 12:L:10:GLN:HE21  | 0.95                     | 0.91              |
| 1:A:856:G:H2'     | 37:A:5003:HOH:O   | 1.71                     | 0.91              |
| 14:N:87:MET:HB3   | 30:4:46:ILE:HD13  | 1.51                     | 0.91              |
| 27:1:46:LYS:HD3   | 27:1:59:HIS:HB2   | 1.52                     | 0.90              |
| 24:X:88:THR:HB    | 37:X:6679:HOH:O   | 1.72                     | 0.90              |
| 3:C:211:LYS:HB3   | 3:C:212:PRO:HD2   | 1.54                     | 0.90              |
| 24:X:137:GLN:HE21 | 24:X:141:HIS:HE1  | 1.16                     | 0.90              |
| 11:K:76:ASP:HA    | 37:K:5907:HOH:O   | 1.69                     | 0.90              |
| 26:Z:187:VAL:HG23 | 26:Z:192:ASP:HB2  | 1.52                     | 0.90              |
| 7:G:84:MET:HE1    | 7:G:148:ILE:CD1   | 2.01                     | 0.89              |
| 19:S:8:ALA:HB1    | 19:S:13:THR:HG21  | 1.54                     | 0.89              |
| 10:J:29:ALA:HB3   | 10:J:65:ARG:HH12  | 1.37                     | 0.89              |
| 1:A:1372:A:H3'    | 37:A:6759:HOH:O   | 1.71                     | 0.89              |
| 1:A:1119:G:H22    | 1:A:1246:A:H2     | 1.20                     | 0.89              |
| 37:A:3259:HOH:O   | 14:N:79:LYS:HD3   | 1.71                     | 0.89              |
| 5:E:115:LEU:HD13  | 5:E:223:LEU:HD21  | 1.54                     | 0.89              |
| 5:E:127:ARG:NH2   | 5:E:225:PRO:HG2   | 1.87                     | 0.89              |
| 37:A:4432:HOH:O   | 14:N:14:ARG:HG2   | 1.72                     | 0.89              |
| 14:N:94:LYS:HE3   | 37:N:8581:HOH:O   | 1.73                     | 0.88              |
| 6:F:64:ARG:HG2    | 6:F:67:ASP:HB3    | 1.56                     | 0.88              |
| 14:N:35:PRO:CG    | 14:N:38:VAL:HG23  | 2.02                     | 0.88              |
| 15:O:144:GLY:O    | 15:O:147:ILE:HG22 | 1.72                     | 0.88              |
| 37:A:3362:HOH:O   | 14:N:189:VAL:HG21 | 1.74                     | 0.88              |
| 12:L:10:GLN:HE21  | 12:L:10:GLN:N     | 1.72                     | 0.88              |
| 24:X:88:THR:HG22  | 24:X:89:ASP:H     | 1.37                     | 0.88              |
| 29:3:41:HIS:H     | 29:3:45:ASN:HD22  | 1.21                     | 0.88              |
| 22:V:14:GLU:OE1   | 22:V:15:PRO:HD2   | 1.73                     | 0.87              |
| 10:J:86:ARG:HH11  | 10:J:133:ILE:CG1  | 1.80                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:115:SER:H    | 17:Q:118:GLN:NE2  | 1.73                     | 0.87              |
| 5:E:246:ARG:HB3   | 5:E:246:ARG:NH1   | 1.90                     | 0.87              |
| 1:A:645:U:OP2     | 13:M:4:LYS:HE2    | 1.72                     | 0.87              |
| 1:A:870:G:H2'     | 1:A:871:G:H5''    | 1.53                     | 0.87              |
| 15:O:7:LYS:HE3    | 18:R:21:ARG:O     | 1.73                     | 0.87              |
| 1:A:2274:A:N3     | 14:N:86:MET:HE1   | 1.90                     | 0.86              |
| 10:J:150:LYS:HE2  | 37:J:8385:HOH:O   | 1.76                     | 0.86              |
| 1:A:2717:C:H2'    | 1:A:2718:C:H5''   | 1.56                     | 0.86              |
| 6:F:105:SER:HB2   | 6:F:131:THR:HG23  | 1.56                     | 0.86              |
| 13:M:68:GLU:HA    | 37:M:8417:HOH:O   | 1.73                     | 0.86              |
| 3:C:7:GLN:O       | 37:C:8515:HOH:O   | 1.92                     | 0.86              |
| 1:A:2506:A:HO2'   | 1:A:2507:G:H8     | 0.89                     | 0.86              |
| 1:A:1209:C:H4'    | 37:A:4854:HOH:O   | 1.76                     | 0.86              |
| 4:D:162:MET:HE2   | 4:D:310:ARG:HD3   | 1.56                     | 0.86              |
| 1:A:1166:A:H1'    | 1:A:1192:A:C2     | 2.10                     | 0.86              |
| 1:A:2586:U:H3     | 1:A:2592:G:H22    | 1.23                     | 0.86              |
| 5:E:104:ASP:HA    | 5:E:107:ARG:HH12  | 1.38                     | 0.86              |
| 1:A:506:G:H22     | 1:A:509:A:C5'     | 1.89                     | 0.85              |
| 6:F:154:LYS:H     | 6:F:154:LYS:HD2   | 1.38                     | 0.85              |
| 27:I:49:ARG:HD2   | 37:I:8429:HOH:O   | 1.75                     | 0.85              |
| 1:A:236:A:H4'     | 1:A:237:G:H5'     | 1.59                     | 0.85              |
| 37:A:3303:HOH:O   | 14:N:157:LEU:HD11 | 1.75                     | 0.85              |
| 10:J:26:LYS:HG2   | 10:J:28:ILE:H     | 1.39                     | 0.85              |
| 8:H:58:GLU:HG3    | 8:H:61:MET:HE2    | 1.59                     | 0.85              |
| 1:A:541:C:C2'     | 1:A:542:A:H5''    | 2.07                     | 0.85              |
| 1:A:1116:U:H3     | 1:A:1246:A:H62    | 1.21                     | 0.85              |
| 5:E:78:ARG:HG3    | 5:E:78:ARG:HH11   | 1.39                     | 0.85              |
| 10:J:162:SER:HB2  | 10:J:163:PRO:CD   | 2.06                     | 0.85              |
| 14:N:52:LEU:HD11  | 37:N:8615:HOH:O   | 1.75                     | 0.84              |
| 2:B:3023:U:C5'    | 2:B:3024:U:OP2    | 2.24                     | 0.84              |
| 5:E:246:ARG:HB3   | 5:E:246:ARG:HH11  | 1.41                     | 0.84              |
| 20:T:57:THR:HG22  | 20:T:59:ASP:H     | 1.40                     | 0.84              |
| 25:Y:15:ARG:HB3   | 25:Y:15:ARG:HH11  | 1.42                     | 0.84              |
| 10:J:59:ASN:H     | 10:J:59:ASN:HD22  | 1.25                     | 0.84              |
| 37:A:6348:HOH:O   | 15:O:4:PRO:HD2    | 1.77                     | 0.84              |
| 7:G:84:MET:HE1    | 7:G:148:ILE:HD12  | 1.60                     | 0.84              |
| 7:G:100:ASP:HB2   | 37:G:2789:HOH:O   | 1.77                     | 0.84              |
| 30:4:60:LYS:HG3   | 30:4:61:PRO:HD2   | 1.59                     | 0.84              |
| 1:A:545:G:H5'     | 1:A:545:G:H8      | 1.43                     | 0.83              |
| 4:D:264:GLU:HG2   | 4:D:267:LYS:HE2   | 1.59                     | 0.83              |
| 14:N:164:THR:HG23 | 14:N:165:SER:N    | 1.94                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:214:U:H5'     | 37:A:5719:HOH:O   | 1.77                     | 0.83              |
| 4:D:86:ALA:HA     | 37:D:8583:HOH:O   | 1.78                     | 0.83              |
| 19:S:44:VAL:O     | 19:S:48:GLU:HG3   | 1.78                     | 0.83              |
| 14:N:61:ILE:HG13  | 37:N:8622:HOH:O   | 1.78                     | 0.83              |
| 25:Y:78:GLU:HG2   | 25:Y:79:GLU:H     | 1.42                     | 0.83              |
| 24:X:122:ARG:HH21 | 24:X:154:ARG:HD2  | 1.41                     | 0.83              |
| 10:J:59:ASN:HD22  | 10:J:59:ASN:N     | 1.77                     | 0.82              |
| 12:L:81:ARG:HB2   | 12:L:87:ARG:NH1   | 1.94                     | 0.82              |
| 1:A:1116:U:HO2'   | 1:A:1118:A:H2     | 0.83                     | 0.82              |
| 7:G:20:ILE:HD11   | 7:G:40:VAL:HG11   | 1.61                     | 0.82              |
| 7:G:97:VAL:HG12   | 37:G:4191:HOH:O   | 1.80                     | 0.82              |
| 3:C:88:ILE:HD13   | 3:C:100:PRO:HD3   | 1.61                     | 0.82              |
| 10:J:49:VAL:O     | 10:J:157:ILE:HG23 | 1.79                     | 0.82              |
| 1:A:962:C:H1'     | 15:O:5:ARG:HH12   | 1.45                     | 0.82              |
| 5:E:236:THR:HG22  | 5:E:239:ALA:N     | 1.95                     | 0.82              |
| 13:M:133:VAL:HA   | 37:M:8445:HOH:O   | 1.76                     | 0.82              |
| 1:A:1603:A:H5'    | 1:A:1605:G:O4'    | 1.78                     | 0.82              |
| 23:W:1:THR:HG23   | 23:W:2:VAL:H      | 1.44                     | 0.82              |
| 4:D:212:GLN:HB2   | 4:D:257:THR:HG21  | 1.61                     | 0.81              |
| 4:D:62:ARG:HA     | 4:D:65:MET:HE3    | 1.61                     | 0.81              |
| 16:P:47:ARG:HH11  | 16:P:47:ARG:HG3   | 1.45                     | 0.81              |
| 6:F:20:LYS:HA     | 6:F:75:LEU:O      | 1.81                     | 0.81              |
| 25:Y:30:MET:HE1   | 25:Y:58:ALA:HB3   | 1.62                     | 0.81              |
| 1:A:1666:C:O2'    | 1:A:1667:A:H5''   | 1.80                     | 0.81              |
| 5:E:236:THR:HA    | 37:E:8448:HOH:O   | 1.78                     | 0.81              |
| 14:N:80:GLY:O     | 14:N:81:ARG:HD3   | 1.81                     | 0.81              |
| 15:O:49:THR:HG22  | 15:O:56:ASP:HB2   | 1.63                     | 0.81              |
| 1:A:506:G:H22     | 1:A:509:A:H5''    | 1.46                     | 0.81              |
| 1:A:1242:A:H5'    | 11:K:82:THR:HG23  | 1.60                     | 0.81              |
| 7:G:15:GLN:HG3    | 7:G:20:ILE:HG12   | 1.60                     | 0.81              |
| 20:T:51:GLN:HE21  | 20:T:53:ASN:HD21  | 1.26                     | 0.81              |
| 27:1:58:GLY:HA3   | 37:1:8439:HOH:O   | 1.81                     | 0.81              |
| 1:A:1184:C:H1'    | 37:A:7039:HOH:O   | 1.81                     | 0.80              |
| 8:H:46:GLU:O      | 8:H:73:PRO:HD2    | 1.81                     | 0.80              |
| 1:A:1160:G:H5'    | 1:A:1161:A:C5'    | 2.09                     | 0.80              |
| 1:A:2426:G:H1'    | 37:A:5671:HOH:O   | 1.79                     | 0.80              |
| 19:S:99:ALA:CB    | 19:S:109:MET:HE1  | 2.10                     | 0.80              |
| 24:X:68:THR:HG23  | 24:X:69:ARG:HG2   | 1.61                     | 0.80              |
| 6:F:146:LYS:NZ    | 15:O:107:ASN:HD21 | 1.78                     | 0.80              |
| 3:C:191:GLY:HA2   | 3:C:194:MET:HE2   | 1.62                     | 0.80              |
| 4:D:175:LEU:HD23  | 4:D:175:LEU:C     | 2.06                     | 0.80              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:Y:37:LEU:CD1  | 25:Y:85:VAL:HG21  | 2.10                     | 0.80              |
| 37:A:7026:HOH:O  | 4:D:211:THR:HG21  | 1.81                     | 0.80              |
| 12:L:14:LYS:HB2  | 12:L:45:PRO:HG2   | 1.64                     | 0.80              |
| 12:L:74:VAL:HG11 | 12:L:113:ILE:HG12 | 1.63                     | 0.80              |
| 1:A:542:A:H5'    | 1:A:542:A:C8      | 2.13                     | 0.80              |
| 1:A:1119:G:N2    | 1:A:1246:A:C2     | 2.50                     | 0.80              |
| 1:A:1205:U:H2'   | 1:A:1206:U:H5'    | 1.62                     | 0.80              |
| 1:A:1474:C:H5'   | 1:A:1474:C:C6     | 2.16                     | 0.80              |
| 1:A:1160:G:C5'   | 1:A:1161:A:H5'    | 2.08                     | 0.80              |
| 3:C:199:HIS:HD2  | 3:C:201:PHE:H     | 1.30                     | 0.80              |
| 15:O:87:LEU:HD12 | 15:O:186:LEU:HD21 | 1.63                     | 0.80              |
| 1:A:1625:U:H4'   | 37:A:4242:HOH:O   | 1.81                     | 0.79              |
| 19:S:17:MET:HE1  | 19:S:19:ARG:NH2   | 1.97                     | 0.79              |
| 10:J:27:LYS:H    | 10:J:58:HIS:HD2   | 1.27                     | 0.79              |
| 21:U:61:GLU:HG3  | 37:U:3851:HOH:O   | 1.80                     | 0.79              |
| 23:W:4:HIS:HB3   | 37:W:6622:HOH:O   | 1.83                     | 0.79              |
| 25:Y:71:ARG:HB3  | 25:Y:88:GLU:OE1   | 1.81                     | 0.79              |
| 2:B:3056:A:C2'   | 2:B:3057:A:H5''   | 2.12                     | 0.79              |
| 27:1:37:HIS:HB2  | 27:1:47:LEU:HB2   | 1.65                     | 0.79              |
| 3:C:100:PRO:HG2  | 3:C:103:VAL:HG21  | 1.64                     | 0.79              |
| 10:J:139:ASP:N   | 10:J:140:PRO:HD3  | 1.98                     | 0.79              |
| 10:J:150:LYS:HB2 | 10:J:157:ILE:HD12 | 1.63                     | 0.79              |
| 3:C:153:ARG:HB2  | 3:C:153:ARG:HH11  | 1.47                     | 0.79              |
| 19:S:9:ASP:O     | 19:S:13:THR:HB    | 1.83                     | 0.79              |
| 3:C:105:VAL:HG11 | 3:C:154:ALA:HB1   | 1.65                     | 0.79              |
| 30:4:70:ARG:HG2  | 30:4:77:ALA:HB2   | 1.63                     | 0.79              |
| 17:Q:115:SER:N   | 17:Q:118:GLN:HE21 | 1.79                     | 0.78              |
| 21:U:48:VAL:HG22 | 21:U:97:ARG:O     | 1.83                     | 0.78              |
| 27:1:38:LYS:HE2  | 27:1:45:LYS:HE2   | 1.64                     | 0.78              |
| 1:A:282:C:H1'    | 1:A:368:C:N4      | 1.98                     | 0.78              |
| 24:X:6:GLN:HB2   | 24:X:26:ILE:HD12  | 1.65                     | 0.78              |
| 1:A:1450:C:H4'   | 1:A:1451:C:OP2    | 1.83                     | 0.78              |
| 14:N:152:ARG:HG3 | 37:N:8555:HOH:O   | 1.84                     | 0.78              |
| 37:A:6446:HOH:O  | 14:N:178:LYS:HB2  | 1.83                     | 0.78              |
| 10:J:41:THR:HA   | 37:J:8398:HOH:O   | 1.83                     | 0.78              |
| 26:Z:220:GLU:HG2 | 37:Z:8137:HOH:O   | 1.82                     | 0.78              |
| 2:B:3048:C:H4'   | 15:O:141:ARG:HH21 | 1.49                     | 0.78              |
| 10:J:55:GLN:HE21 | 10:J:124:ARG:HE   | 1.30                     | 0.78              |
| 1:A:2676:C:H4'   | 11:K:70:PHE:CE1   | 2.18                     | 0.78              |
| 3:C:125:ASN:HB3  | 3:C:158:VAL:HG12  | 1.65                     | 0.77              |
| 15:O:86:LEU:HD12 | 15:O:125:ALA:HB2  | 1.65                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:164:ASP:CG   | 15:O:167:ASP:HA   | 2.09                     | 0.77              |
| 1:A:711:G:H1'     | 37:A:6665:HOH:O   | 1.84                     | 0.77              |
| 2:B:3014:G:H5'    | 2:B:3014:G:H8     | 1.49                     | 0.77              |
| 7:G:132:THR:HB    | 37:G:2227:HOH:O   | 1.84                     | 0.77              |
| 14:N:106:ASN:HD22 | 14:N:114:VAL:HG23 | 1.47                     | 0.77              |
| 15:O:113:SER:HB2  | 37:O:8559:HOH:O   | 1.83                     | 0.77              |
| 4:D:201:ASP:HB2   | 4:D:312:ARG:HD2   | 1.67                     | 0.77              |
| 24:X:122:ARG:HG2  | 24:X:122:ARG:HH11 | 1.50                     | 0.77              |
| 1:A:1947:G:OP2    | 37:A:3246:HOH:O   | 2.02                     | 0.77              |
| 5:E:1:MET:HG2     | 5:E:2:GLN:H       | 1.48                     | 0.77              |
| 10:J:137:ASN:O    | 10:J:139:ASP:N    | 2.18                     | 0.77              |
| 3:C:199:HIS:CD2   | 3:C:201:PHE:H     | 2.02                     | 0.77              |
| 9:I:23:ILE:HD13   | 9:I:67:LEU:HD23   | 1.65                     | 0.77              |
| 1:A:31:C:H4'      | 37:A:6994:HOH:O   | 1.84                     | 0.77              |
| 15:O:48:VAL:CG1   | 15:O:55:ASP:HB3   | 2.14                     | 0.77              |
| 10:J:140:PRO:HB3  | 37:J:8383:HOH:O   | 1.85                     | 0.77              |
| 14:N:87:MET:CG    | 30:4:46:ILE:HG21  | 2.14                     | 0.77              |
| 7:G:37:ASP:OD1    | 11:K:125:SER:HB3  | 1.85                     | 0.77              |
| 6:F:64:ARG:CG     | 6:F:67:ASP:HB3    | 2.15                     | 0.77              |
| 27:1:38:LYS:HG2   | 27:1:45:LYS:HG2   | 1.66                     | 0.77              |
| 1:A:1116:U:O2'    | 1:A:1118:A:H2     | 1.65                     | 0.76              |
| 1:A:1165:G:H4'    | 1:A:1174:A:O2'    | 1.85                     | 0.76              |
| 13:M:148:GLU:HA   | 37:M:8444:HOH:O   | 1.84                     | 0.76              |
| 13:M:53:ARG:HH22  | 13:M:57:VAL:HG12  | 1.50                     | 0.76              |
| 30:4:25:VAL:HG22  | 30:4:68:LYS:HG3   | 1.66                     | 0.76              |
| 1:A:288:A:H61     | 1:A:364:C:H42     | 1.34                     | 0.76              |
| 3:C:35:GLY:O      | 3:C:36:ASP:HB3    | 1.84                     | 0.76              |
| 24:X:88:THR:HG22  | 24:X:89:ASP:N     | 2.00                     | 0.76              |
| 26:Z:187:VAL:HG23 | 26:Z:192:ASP:CB   | 2.15                     | 0.76              |
| 16:P:32:ARG:O     | 16:P:32:ARG:HD3   | 1.85                     | 0.76              |
| 1:A:447:A:OP1     | 21:U:2:LYS:HG2    | 1.85                     | 0.76              |
| 1:A:284:C:H4'     | 1:A:285:A:O5'     | 1.84                     | 0.76              |
| 10:J:47:GLU:HB3   | 10:J:133:ILE:HD13 | 1.66                     | 0.76              |
| 11:K:74:ARG:HB3   | 11:K:74:ARG:HH11  | 1.49                     | 0.76              |
| 1:A:31:C:H2'      | 37:A:7262:HOH:O   | 1.85                     | 0.76              |
| 1:A:1187:U:H2'    | 37:A:6468:HOH:O   | 1.85                     | 0.76              |
| 1:A:1191:A:H3'    | 1:A:1192:A:H5''   | 1.67                     | 0.76              |
| 1:A:2054:A:N3     | 19:S:128:ARG:NH2  | 2.33                     | 0.76              |
| 24:X:154:ARG:C    | 37:X:4276:HOH:O   | 2.28                     | 0.76              |
| 1:A:1118:A:C8     | 1:A:1118:A:H3'    | 2.21                     | 0.76              |
| 26:Z:200:THR:HG22 | 26:Z:201:GLU:HG3  | 1.68                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:544:G:H2'     | 1:A:545:G:H5''    | 1.67                     | 0.76              |
| 1:A:2506:A:O2'    | 1:A:2507:G:H8     | 1.66                     | 0.76              |
| 5:E:214:THR:HG21  | 37:E:8398:HOH:O   | 1.85                     | 0.76              |
| 1:A:657:G:OP1     | 5:E:27:ARG:NH2    | 2.16                     | 0.75              |
| 37:A:4244:HOH:O   | 20:T:23:LYS:HE2   | 1.87                     | 0.75              |
| 2:B:3049:G:H5''   | 37:B:8465:HOH:O   | 1.85                     | 0.75              |
| 5:E:2:GLN:HB3     | 37:E:8336:HOH:O   | 1.86                     | 0.75              |
| 28:2:10:LYS:HG3   | 37:2:8433:HOH:O   | 1.85                     | 0.75              |
| 7:G:81:GLU:HG2    | 7:G:134:SER:HB3   | 1.67                     | 0.75              |
| 14:N:104:ARG:O    | 14:N:108:LYS:HE2  | 1.86                     | 0.75              |
| 4:D:162:MET:HE2   | 4:D:310:ARG:CD    | 2.16                     | 0.75              |
| 1:A:1151:G:OP1    | 9:I:16:LYS:NZ     | 2.20                     | 0.75              |
| 2:B:3006:C:H5''   | 15:O:37:ARG:HH12  | 1.49                     | 0.75              |
| 12:L:62:PRO:HG3   | 12:L:65:ARG:HH21  | 1.52                     | 0.75              |
| 17:Q:115:SER:OG   | 17:Q:118:GLN:HG3  | 1.85                     | 0.75              |
| 19:S:39:THR:HG23  | 19:S:107:GLU:O    | 1.85                     | 0.75              |
| 5:E:214:THR:HG23  | 37:E:8433:HOH:O   | 1.86                     | 0.75              |
| 15:O:71:TRP:CE3   | 15:O:175:LEU:HD22 | 2.22                     | 0.75              |
| 28:2:25:LYS:HG2   | 28:2:25:LYS:O     | 1.86                     | 0.75              |
| 1:A:2063:U:OP2    | 37:A:9303:HOH:O   | 2.04                     | 0.75              |
| 1:A:2676:C:H4'    | 11:K:70:PHE:HE1   | 1.51                     | 0.75              |
| 3:C:194:MET:HE3   | 3:C:199:HIS:HB2   | 1.68                     | 0.75              |
| 26:Z:133:HIS:HD2  | 37:Z:8169:HOH:O   | 1.70                     | 0.75              |
| 4:D:238:ASN:HD22  | 4:D:240:GLY:H     | 1.34                     | 0.74              |
| 5:E:5:ILE:HD11    | 5:E:16:VAL:CG2    | 2.17                     | 0.74              |
| 22:V:14:GLU:O     | 22:V:17:THR:HB    | 1.86                     | 0.74              |
| 24:X:137:GLN:HE21 | 24:X:141:HIS:CE1  | 2.05                     | 0.74              |
| 1:A:21:G:H5'      | 19:S:2:ILE:HA     | 1.70                     | 0.74              |
| 1:A:188:C:H5''    | 14:N:163:LEU:HD21 | 1.70                     | 0.74              |
| 1:A:2533:C:H6     | 1:A:2533:C:H5'    | 1.51                     | 0.74              |
| 1:A:2690:U:O2'    | 7:G:111:LYS:HE3   | 1.87                     | 0.74              |
| 2:B:3023:U:H3'    | 37:B:8478:HOH:O   | 1.86                     | 0.74              |
| 12:L:74:VAL:CG1   | 12:L:113:ILE:HG12 | 2.18                     | 0.74              |
| 21:U:55:PHE:HB2   | 37:U:6384:HOH:O   | 1.86                     | 0.74              |
| 1:A:2717:C:C2'    | 1:A:2718:C:H5''   | 2.17                     | 0.74              |
| 1:A:1234:U:N3     | 4:D:244:PRO:HB3   | 2.02                     | 0.74              |
| 17:Q:143:ALA:HA   | 37:Q:2178:HOH:O   | 1.87                     | 0.74              |
| 30:4:73:GLU:HB3   | 37:4:8561:HOH:O   | 1.87                     | 0.74              |
| 1:A:560:C:H42     | 1:A:597:A:H61     | 1.36                     | 0.74              |
| 4:D:307:ARG:HH11  | 4:D:307:ARG:HB2   | 1.51                     | 0.74              |
| 1:A:871:G:C8      | 1:A:871:G:C5'     | 2.62                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2637:A:H5'    | 37:A:8857:HOH:O   | 1.87                     | 0.73              |
| 4:D:42:ALA:HB1    | 4:D:308:LEU:HD11  | 1.68                     | 0.73              |
| 6:F:27:ILE:HG22   | 6:F:28:GLY:H      | 1.52                     | 0.73              |
| 1:A:1751:G:C2'    | 1:A:1752:G:H5''   | 2.18                     | 0.73              |
| 37:A:4797:HOH:O   | 12:L:39:GLY:HA2   | 1.88                     | 0.73              |
| 14:N:38:VAL:O     | 14:N:63:VAL:HG13  | 1.87                     | 0.73              |
| 1:A:1667:A:H5'    | 1:A:1667:A:C8     | 2.21                     | 0.73              |
| 3:C:121:ALA:O     | 3:C:124:VAL:HG22  | 1.86                     | 0.73              |
| 21:U:47:THR:HB    | 21:U:100:ASP:HB3  | 1.69                     | 0.73              |
| 1:A:2812:A:H2     | 1:A:2814:A:H62    | 1.33                     | 0.73              |
| 4:D:41:PHE:CD1    | 4:D:79:MET:HE2    | 2.23                     | 0.73              |
| 6:F:95:THR:C      | 6:F:97:GLN:H      | 1.96                     | 0.73              |
| 10:J:141:ASN:HA   | 37:J:8369:HOH:O   | 1.88                     | 0.73              |
| 1:A:2851:G:O2'    | 1:A:2852:A:H5'    | 1.87                     | 0.73              |
| 24:X:88:THR:HG23  | 24:X:110:GLN:NE2  | 2.03                     | 0.73              |
| 1:A:1118:A:H3'    | 1:A:1118:A:H8     | 1.53                     | 0.73              |
| 1:A:1164:U:H3     | 1:A:1192:A:H2     | 1.36                     | 0.73              |
| 1:A:2508:C:H2'    | 37:A:6330:HOH:O   | 1.89                     | 0.73              |
| 4:D:195:ARG:HG2   | 4:D:323:LEU:HD22  | 1.71                     | 0.73              |
| 13:M:67:ARG:O     | 13:M:71:GLU:HG3   | 1.88                     | 0.73              |
| 17:Q:38:GLU:HA    | 17:Q:41:ARG:HH11  | 1.53                     | 0.73              |
| 1:A:289:G:H22     | 1:A:363:A:H2      | 1.37                     | 0.73              |
| 11:K:99:GLU:HA    | 37:K:7377:HOH:O   | 1.87                     | 0.73              |
| 14:N:84:LYS:HE2   | 37:N:8575:HOH:O   | 1.89                     | 0.73              |
| 1:A:2638:G:H1'    | 37:A:7334:HOH:O   | 1.87                     | 0.73              |
| 8:H:63:ILE:HB     | 8:H:64:PRO:HD3    | 1.71                     | 0.73              |
| 27:I:40:PRO:HD3   | 27:I:47:LEU:HD11  | 1.71                     | 0.73              |
| 37:A:5369:HOH:O   | 14:N:170:CYS:SG   | 2.47                     | 0.72              |
| 4:D:82:VAL:O      | 4:D:82:VAL:HG12   | 1.88                     | 0.72              |
| 13:M:143:THR:HG22 | 13:M:144:ASP:N    | 2.04                     | 0.72              |
| 14:N:104:ARG:O    | 14:N:108:LYS:HG2  | 1.89                     | 0.72              |
| 15:O:83:LEU:HD13  | 15:O:175:LEU:HD23 | 1.72                     | 0.72              |
| 20:T:57:THR:HG22  | 20:T:59:ASP:N     | 2.02                     | 0.72              |
| 25:Y:25:ARG:HD2   | 37:Y:3861:HOH:O   | 1.87                     | 0.72              |
| 1:A:346:U:H4'     | 37:A:6416:HOH:O   | 1.88                     | 0.72              |
| 6:F:49:PRO:HG3    | 37:F:5828:HOH:O   | 1.88                     | 0.72              |
| 6:F:95:THR:O      | 6:F:97:GLN:N      | 2.17                     | 0.72              |
| 1:A:450:C:OP1     | 5:E:184:ARG:NH2   | 2.18                     | 0.72              |
| 1:A:559:U:H6      | 1:A:559:U:H5'     | 1.53                     | 0.72              |
| 5:E:107:ARG:NH1   | 5:E:107:ARG:HB3   | 2.04                     | 0.72              |
| 11:K:19:MET:HE2   | 11:K:79:PHE:HA    | 1.70                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:19:MET:HE1   | 11:K:78:ILE:HG22  | 1.71                     | 0.72              |
| 37:A:4523:HOH:O   | 2:B:3103:A:H4'    | 1.89                     | 0.72              |
| 6:F:88:LEU:HB2    | 6:F:89:PRO:HD3    | 1.71                     | 0.72              |
| 24:X:122:ARG:NH2  | 24:X:154:ARG:HD2  | 2.03                     | 0.72              |
| 2:B:3006:C:OP1    | 15:O:37:ARG:NH1   | 2.22                     | 0.72              |
| 9:I:12:ILE:N      | 9:I:13:PRO:HD3    | 2.03                     | 0.72              |
| 14:N:87:MET:CB    | 30:4:46:ILE:HD13  | 2.18                     | 0.72              |
| 1:A:1134:G:C4'    | 10:J:151:MET:HE1  | 2.15                     | 0.72              |
| 1:A:2780:C:H1'    | 7:G:143:GLN:HE21  | 1.53                     | 0.72              |
| 3:C:95:PRO:HG2    | 3:C:98:GLU:HG2    | 1.72                     | 0.72              |
| 6:F:136:ARG:HD2   | 6:F:155:HIS:O     | 1.89                     | 0.72              |
| 26:Z:141:THR:HG23 | 37:Z:8175:HOH:O   | 1.89                     | 0.72              |
| 7:G:84:MET:HE1    | 7:G:148:ILE:HD13  | 1.72                     | 0.72              |
| 15:O:164:ASP:OD2  | 15:O:167:ASP:HA   | 1.90                     | 0.72              |
| 10:J:47:GLU:HB3   | 10:J:133:ILE:CD1  | 2.18                     | 0.71              |
| 1:A:2716:G:H5''   | 4:D:206:THR:HG21  | 1.71                     | 0.71              |
| 5:E:132:ASP:HB3   | 37:E:8360:HOH:O   | 1.90                     | 0.71              |
| 8:H:96:ALA:HA     | 37:H:3111:HOH:O   | 1.90                     | 0.71              |
| 13:M:114:VAL:HG11 | 37:M:8445:HOH:O   | 1.90                     | 0.71              |
| 20:T:51:GLN:NE2   | 20:T:53:ASN:HD21  | 1.88                     | 0.71              |
| 1:A:1684:A:H1'    | 29:3:43:ARG:HH22  | 1.55                     | 0.71              |
| 14:N:74:ARG:HH11  | 14:N:74:ARG:HG3   | 1.55                     | 0.71              |
| 26:Z:200:THR:HG22 | 26:Z:201:GLU:CG   | 2.21                     | 0.71              |
| 1:A:1118:A:H62    | 1:A:1244:U:H3     | 1.39                     | 0.71              |
| 10:J:26:LYS:HD2   | 10:J:28:ILE:CD1   | 2.20                     | 0.71              |
| 1:A:281:U:H2'     | 1:A:282:C:O4'     | 1.90                     | 0.71              |
| 5:E:140:VAL:HB    | 37:E:8448:HOH:O   | 1.89                     | 0.71              |
| 7:G:84:MET:HE2    | 7:G:133:VAL:CG2   | 2.20                     | 0.71              |
| 20:T:51:GLN:HE21  | 20:T:53:ASN:ND2   | 1.88                     | 0.71              |
| 1:A:603:A:H5''    | 1:A:604:G:OP1     | 1.90                     | 0.71              |
| 4:D:36:PRO:HA     | 4:D:168:GLY:CA    | 2.21                     | 0.71              |
| 5:E:27:ARG:HG3    | 5:E:29:ASP:OD1    | 1.89                     | 0.71              |
| 19:S:18:LEU:HD12  | 19:S:143:VAL:HG11 | 1.72                     | 0.71              |
| 25:Y:72:VAL:HG22  | 25:Y:85:VAL:HG12  | 1.73                     | 0.71              |
| 1:A:2779:G:H21    | 7:G:143:GLN:NE2   | 1.89                     | 0.71              |
| 10:J:162:SER:CB   | 10:J:163:PRO:HD3  | 2.19                     | 0.71              |
| 13:M:53:ARG:NH2   | 13:M:57:VAL:HG12  | 2.05                     | 0.71              |
| 14:N:38:VAL:C     | 14:N:63:VAL:HG13  | 2.15                     | 0.71              |
| 14:N:164:THR:HG22 | 14:N:167:GLY:N    | 2.04                     | 0.71              |
| 15:O:183:ASP:OD2  | 15:O:186:LEU:HD12 | 1.90                     | 0.71              |
| 30:4:70:ARG:HD3   | 37:4:8539:HOH:O   | 1.90                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:25:MET:HE2   | 6:F:41:LEU:CG     | 2.12                     | 0.70              |
| 7:G:11:VAL:HG12  | 7:G:12:ASP:N      | 2.04                     | 0.70              |
| 1:A:541:C:H2'    | 1:A:542:A:C5'     | 2.18                     | 0.70              |
| 1:A:1185:U:H2'   | 1:A:1186:C:C6     | 2.26                     | 0.70              |
| 21:U:48:VAL:HG22 | 21:U:97:ARG:C     | 2.15                     | 0.70              |
| 27:1:62:TYR:CE2  | 27:1:64:ILE:HG23  | 2.26                     | 0.70              |
| 4:D:36:PRO:HA    | 4:D:168:GLY:HA3   | 1.73                     | 0.70              |
| 1:A:2044:G:OP1   | 25:Y:23:HIS:HE1   | 1.73                     | 0.70              |
| 6:F:55:LYS:HA    | 37:F:6752:HOH:O   | 1.91                     | 0.70              |
| 2:B:3039:U:H1'   | 2:B:3044:A:H61    | 1.57                     | 0.70              |
| 1:A:2890:A:H1'   | 22:V:56:ARG:NH2   | 2.07                     | 0.70              |
| 4:D:221:GLN:HE22 | 12:L:42:ASN:HD22  | 1.39                     | 0.70              |
| 1:A:1666:C:H2'   | 1:A:1667:A:H5'    | 1.73                     | 0.70              |
| 37:A:5870:HOH:O  | 6:F:99:ASP:HA     | 1.90                     | 0.70              |
| 2:B:3026:C:P     | 37:B:8441:HOH:O   | 2.48                     | 0.70              |
| 6:F:23:VAL:HG23  | 6:F:23:VAL:O      | 1.92                     | 0.70              |
| 24:X:4:LEU:HD23  | 24:X:54:PHE:HB3   | 1.72                     | 0.70              |
| 1:A:2768:A:H2'   | 1:A:2769:C:O4'    | 1.91                     | 0.69              |
| 2:B:3035:C:H5''  | 37:B:8455:HOH:O   | 1.91                     | 0.69              |
| 24:X:5:VAL:HG11  | 24:X:153:MET:HE1  | 1.73                     | 0.69              |
| 1:A:2346:C:O2'   | 6:F:52:THR:HG21   | 1.92                     | 0.69              |
| 1:A:2812:A:N7    | 37:A:7092:HOH:O   | 2.24                     | 0.69              |
| 3:C:105:VAL:CG1  | 3:C:154:ALA:HB1   | 2.21                     | 0.69              |
| 8:H:91:VAL:HG12  | 8:H:92:GLY:H      | 1.57                     | 0.69              |
| 3:C:173:GLY:O    | 3:C:176:HIS:HB3   | 1.91                     | 0.69              |
| 6:F:35:ALA:N     | 37:F:5576:HOH:O   | 2.24                     | 0.69              |
| 7:G:107:PHE:CE2  | 7:G:108:LEU:HD13  | 2.28                     | 0.69              |
| 15:O:71:TRP:HE3  | 15:O:175:LEU:HD22 | 1.56                     | 0.69              |
| 1:A:21:G:C5'     | 19:S:2:ILE:HA     | 2.22                     | 0.69              |
| 1:A:381:G:H5''   | 37:A:3894:HOH:O   | 1.92                     | 0.69              |
| 35:A:8513:CL:CL  | 37:A:4259:HOH:O   | 2.46                     | 0.69              |
| 12:L:22:ASP:HB2  | 37:L:5264:HOH:O   | 1.92                     | 0.69              |
| 14:N:60:ILE:C    | 14:N:61:ILE:HD12  | 2.17                     | 0.69              |
| 1:A:1127:C:H2'   | 1:A:1128:U:H5'    | 1.72                     | 0.69              |
| 23:W:64:GLY:O    | 23:W:65:ASP:HB2   | 1.91                     | 0.69              |
| 1:A:1080:C:H4'   | 1:A:1081:A:OP1    | 1.92                     | 0.69              |
| 1:A:1441:G:O2'   | 1:A:1442:A:H5'    | 1.93                     | 0.69              |
| 1:A:2301:A:H5''  | 1:A:2302:A:H5'    | 1.73                     | 0.69              |
| 10:J:130:HIS:CD2 | 10:J:133:ILE:HD11 | 2.27                     | 0.69              |
| 11:K:107:ASN:ND2 | 11:K:109:TYR:H    | 1.90                     | 0.69              |
| 1:A:1328:A:N7    | 1:A:1329:A:C5     | 2.61                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:N:30:GLU:O    | 14:N:34:GLU:HG3   | 1.92                     | 0.69              |
| 16:P:87:THR:O    | 16:P:91:GLN:HG3   | 1.93                     | 0.69              |
| 7:G:7:ILE:HD11   | 7:G:11:VAL:C      | 2.18                     | 0.69              |
| 14:N:164:THR:CG2 | 14:N:165:SER:N    | 2.55                     | 0.69              |
| 1:A:282:C:H1'    | 1:A:368:C:H42     | 1.58                     | 0.69              |
| 1:A:1170:U:O2'   | 1:A:1172:G:N7     | 2.24                     | 0.69              |
| 5:E:129:HIS:HE1  | 5:E:231:ARG:HA    | 1.58                     | 0.69              |
| 1:A:1835:U:C5    | 1:A:1840:A:N7     | 2.55                     | 0.68              |
| 14:N:34:GLU:HB3  | 14:N:35:PRO:HD2   | 1.75                     | 0.68              |
| 1:A:1973:A:H5'   | 1:A:1973:A:H8     | 1.57                     | 0.68              |
| 1:A:1862:C:H1'   | 37:A:6790:HOH:O   | 1.92                     | 0.68              |
| 4:D:297:VAL:HB   | 37:D:8607:HOH:O   | 1.93                     | 0.68              |
| 21:U:63:ILE:HD11 | 21:U:75:GLU:HB2   | 1.75                     | 0.68              |
| 1:A:820:G:O2'    | 1:A:856:G:H4'     | 1.94                     | 0.68              |
| 1:A:1160:G:N3    | 37:A:5210:HOH:O   | 2.26                     | 0.68              |
| 10:J:139:ASP:HA  | 37:J:8373:HOH:O   | 1.93                     | 0.68              |
| 4:D:75:GLU:C     | 4:D:77:PRO:HD3    | 2.19                     | 0.68              |
| 6:F:69:ILE:HG22  | 6:F:69:ILE:O      | 1.93                     | 0.68              |
| 11:K:88:PRO:HA   | 35:K:8502:CL:CL   | 2.30                     | 0.68              |
| 37:A:3935:HOH:O  | 16:P:37:ARG:HG3   | 1.94                     | 0.68              |
| 14:N:139:PRO:O   | 14:N:140:ALA:HB3  | 1.93                     | 0.68              |
| 23:W:8:ILE:HA    | 23:W:11:MET:HE3   | 1.74                     | 0.68              |
| 1:A:2420:G:O2'   | 1:A:2421:G:H5'    | 1.94                     | 0.68              |
| 10:J:84:ARG:NH2  | 10:J:135:TRP:HH2  | 1.91                     | 0.68              |
| 23:W:58:THR:O    | 23:W:62:GLU:HG3   | 1.94                     | 0.68              |
| 25:Y:76:ARG:HH11 | 25:Y:76:ARG:HG3   | 1.58                     | 0.68              |
| 1:A:2414:A:H2'   | 1:A:2415:A:C8     | 2.28                     | 0.68              |
| 2:B:3028:U:H2'   | 2:B:3029:C:C6     | 2.29                     | 0.68              |
| 22:V:9:CYS:HA    | 22:V:52:THR:HG23  | 1.74                     | 0.68              |
| 26:Z:189:ASN:HA  | 26:Z:217:ILE:HD11 | 1.74                     | 0.68              |
| 1:A:1209:C:H2'   | 1:A:1210:G:H8     | 1.59                     | 0.68              |
| 26:Z:186:ARG:HG2 | 26:Z:186:ARG:HH11 | 1.59                     | 0.68              |
| 15:O:80:SER:HB2  | 37:O:8536:HOH:O   | 1.93                     | 0.67              |
| 27:1:19:GLY:O    | 27:1:23:ARG:HG2   | 1.93                     | 0.67              |
| 6:F:25:MET:HE1   | 6:F:37:ALA:O      | 1.93                     | 0.67              |
| 10:J:3:GLY:HA2   | 10:J:57:ARG:HH12  | 1.57                     | 0.67              |
| 12:L:62:PRO:HG3  | 12:L:65:ARG:NH2   | 2.09                     | 0.67              |
| 23:W:39:ALA:N    | 23:W:40:PRO:HD2   | 2.09                     | 0.67              |
| 5:E:104:ASP:HA   | 5:E:107:ARG:NH1   | 2.08                     | 0.67              |
| 1:A:2265:U:H2'   | 1:A:2266:A:C8     | 2.30                     | 0.67              |
| 8:H:110:GLU:HG2  | 37:H:6926:HOH:O   | 1.95                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1003:U:O2    | 10:J:90:PHE:HZ   | 1.78                     | 0.67              |
| 1:A:1119:G:N2    | 1:A:1246:A:H2    | 1.91                     | 0.67              |
| 1:A:2064:U:OP1   | 37:A:9929:HOH:O  | 2.12                     | 0.67              |
| 6:F:38:GLU:OE2   | 6:F:51:ARG:CZ    | 2.43                     | 0.67              |
| 8:H:50:VAL:HG13  | 8:H:60:VAL:HG11  | 1.77                     | 0.67              |
| 10:J:46:VAL:HG12 | 10:J:146:TRP:HZ3 | 1.59                     | 0.67              |
| 12:L:55:VAL:HG12 | 12:L:56:SER:N    | 2.08                     | 0.67              |
| 3:C:131:HIS:O    | 3:C:132:ASP:HB2  | 1.93                     | 0.67              |
| 5:E:129:HIS:CE1  | 5:E:231:ARG:HA   | 2.30                     | 0.67              |
| 6:F:99:ASP:HB2   | 6:F:103:ASN:HB2  | 1.77                     | 0.67              |
| 8:H:53:ASP:OD1   | 8:H:80:GLN:HB2   | 1.94                     | 0.67              |
| 1:A:1733:A:H4'   | 4:D:212:GLN:HA   | 1.75                     | 0.67              |
| 10:J:55:GLN:NE2  | 10:J:124:ARG:HE  | 1.93                     | 0.67              |
| 24:X:65:VAL:HA   | 24:X:68:THR:HG22 | 1.77                     | 0.67              |
| 25:Y:71:ARG:HD3  | 37:Y:2171:HOH:O  | 1.95                     | 0.67              |
| 1:A:1594:C:OP2   | 17:Q:120:ARG:HD2 | 1.94                     | 0.67              |
| 14:N:138:HIS:ND1 | 14:N:139:PRO:O   | 2.22                     | 0.67              |
| 19:S:39:THR:HB   | 19:S:42:GLU:HG3  | 1.76                     | 0.67              |
| 26:Z:235:GLU:H   | 26:Z:235:GLU:CD  | 2.03                     | 0.67              |
| 1:A:506:G:H22    | 1:A:509:A:H5'    | 1.60                     | 0.67              |
| 1:A:1119:G:H2'   | 11:K:52:GLN:NE2  | 2.09                     | 0.67              |
| 5:E:233:THR:HG22 | 5:E:234:VAL:N    | 2.08                     | 0.67              |
| 8:H:39:SER:HB3   | 8:H:45:ALA:HB2   | 1.77                     | 0.67              |
| 8:H:99:THR:HA    | 37:H:3461:HOH:O  | 1.95                     | 0.67              |
| 19:S:106:GLY:HA2 | 19:S:109:MET:HE3 | 1.77                     | 0.67              |
| 1:A:1919:A:H4'   | 37:A:4419:HOH:O  | 1.95                     | 0.66              |
| 1:A:2004:U:H4'   | 37:A:4881:HOH:O  | 1.94                     | 0.66              |
| 1:A:2578:G:H5'   | 1:A:2578:G:H8    | 1.60                     | 0.66              |
| 2:B:3023:U:C4'   | 2:B:3024:U:OP2   | 2.39                     | 0.66              |
| 3:C:194:MET:HE3  | 3:C:199:HIS:CB   | 2.25                     | 0.66              |
| 11:K:133:GLY:O   | 11:K:137:GLU:HG3 | 1.95                     | 0.66              |
| 20:T:80:ARG:NH1  | 37:T:8346:HOH:O  | 2.28                     | 0.66              |
| 24:X:21:LEU:HD22 | 24:X:26:ILE:HD11 | 1.75                     | 0.66              |
| 26:Z:187:VAL:CG2 | 26:Z:192:ASP:HB2 | 2.26                     | 0.66              |
| 1:A:69:A:H5'     | 1:A:69:A:H8      | 1.60                     | 0.66              |
| 1:A:885:G:OP2    | 37:A:8984:HOH:O  | 2.14                     | 0.66              |
| 37:A:7154:HOH:O  | 27:1:31:ILE:HG13 | 1.95                     | 0.66              |
| 3:C:192:VAL:HB   | 37:C:8596:HOH:O  | 1.94                     | 0.66              |
| 4:D:71:VAL:HG11  | 4:D:296:LEU:HB3  | 1.76                     | 0.66              |
| 14:N:139:PRO:O   | 14:N:140:ALA:CB  | 2.43                     | 0.66              |
| 1:A:870:G:C2'    | 1:A:871:G:H5''   | 2.23                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1328:A:OP1    | 26:Z:169:ARG:HD2 | 1.94                     | 0.66              |
| 1:A:1213:C:O2'    | 1:A:1214:G:H5'   | 1.96                     | 0.66              |
| 1:A:1847:A:OP1    | 3:C:175:LYS:HG3  | 1.96                     | 0.66              |
| 1:A:2391:C:OP1    | 37:A:8913:HOH:O  | 2.14                     | 0.66              |
| 4:D:41:PHE:HB3    | 4:D:190:MET:HE1  | 1.76                     | 0.66              |
| 6:F:57:THR:HG23   | 6:F:63:ILE:HG22  | 1.77                     | 0.66              |
| 25:Y:25:ARG:NH1   | 37:Y:3861:HOH:O  | 2.29                     | 0.66              |
| 26:Z:212:ARG:HD2  | 37:Z:8186:HOH:O  | 1.95                     | 0.66              |
| 1:A:2361:A:H5''   | 37:A:8601:HOH:O  | 1.94                     | 0.66              |
| 3:C:36:ASP:OD2    | 3:C:85:ASP:HB2   | 1.95                     | 0.66              |
| 3:C:200:PRO:O     | 37:C:8589:HOH:O  | 2.14                     | 0.66              |
| 23:W:12:THR:HG22  | 23:W:15:GLU:CG   | 2.18                     | 0.66              |
| 1:A:2587:U:H2'    | 1:A:2589:U:H5''  | 1.78                     | 0.66              |
| 4:D:190:MET:HE2   | 4:D:194:PHE:CD1  | 2.30                     | 0.66              |
| 10:J:14:TYR:H     | 10:J:91:HIS:CE1  | 2.13                     | 0.66              |
| 1:A:2630:G:O6     | 3:C:206:ARG:NH2  | 2.28                     | 0.66              |
| 37:A:7029:HOH:O   | 5:E:188:ARG:HD2  | 1.95                     | 0.66              |
| 3:C:76:VAL:HG23   | 27:1:63:LYS:HB3  | 1.77                     | 0.66              |
| 11:K:93:ARG:HB3   | 11:K:93:ARG:HH11 | 1.59                     | 0.66              |
| 14:N:87:MET:CB    | 30:4:46:ILE:HG21 | 2.25                     | 0.66              |
| 29:3:41:HIS:H     | 29:3:45:ASN:ND2  | 1.94                     | 0.66              |
| 1:A:204:A:H2'     | 1:A:205:U:H5'    | 1.77                     | 0.66              |
| 1:A:1330:A:H5''   | 1:A:1331:A:OP2   | 1.95                     | 0.66              |
| 1:A:2064:U:H5'    | 1:A:2652:U:O3'   | 1.96                     | 0.66              |
| 2:B:3029:C:H2'    | 2:B:3030:C:H5'   | 1.77                     | 0.66              |
| 22:V:20:MET:HE2   | 22:V:30:HIS:NE2  | 2.11                     | 0.66              |
| 1:A:428:G:OP1     | 37:A:5799:HOH:O  | 2.13                     | 0.66              |
| 1:A:1159:G:P      | 37:A:3869:HOH:O  | 2.53                     | 0.66              |
| 6:F:97:GLN:HG2    | 6:F:97:GLN:O     | 1.96                     | 0.66              |
| 11:K:107:ASN:HD21 | 11:K:109:TYR:HB2 | 1.61                     | 0.66              |
| 14:N:157:LEU:HB3  | 14:N:160:PHE:HD1 | 1.60                     | 0.66              |
| 29:3:41:HIS:N     | 29:3:45:ASN:HD22 | 1.92                     | 0.66              |
| 1:A:681:G:H5'     | 1:A:681:G:N3     | 2.11                     | 0.65              |
| 1:A:2488:A:H61    | 1:A:2534:C:H42   | 1.43                     | 0.65              |
| 4:D:18:ARG:HG3    | 4:D:256:GLN:HG3  | 1.77                     | 0.65              |
| 25:Y:15:ARG:HB3   | 25:Y:15:ARG:NH1  | 2.10                     | 0.65              |
| 25:Y:25:ARG:HG2   | 37:Y:5356:HOH:O  | 1.96                     | 0.65              |
| 27:1:28:ASP:O     | 27:1:31:ILE:HG22 | 1.96                     | 0.65              |
| 1:A:2719:A:C2     | 4:D:70:PRO:HG3   | 2.31                     | 0.65              |
| 17:Q:59:ARG:NH2   | 17:Q:66:GLN:HE22 | 1.95                     | 0.65              |
| 1:A:629:A:N7      | 37:A:9440:HOH:O  | 2.30                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1119:G:H8    | 11:K:52:GLN:HE22 | 1.44                     | 0.65              |
| 6:F:135:VAL:HG22 | 6:F:136:ARG:H    | 1.61                     | 0.65              |
| 10:J:35:ASN:ND2  | 10:J:80:ASN:HA   | 2.11                     | 0.65              |
| 1:A:69:A:H5'     | 1:A:69:A:C8      | 2.31                     | 0.65              |
| 4:D:175:LEU:HD23 | 4:D:175:LEU:O    | 1.96                     | 0.65              |
| 26:Z:216:ARG:HD3 | 37:Z:8157:HOH:O  | 1.95                     | 0.65              |
| 1:A:2064:U:H4'   | 1:A:2653:A:OP1   | 1.97                     | 0.65              |
| 37:B:8473:HOH:O  | 15:O:23:ARG:HD3  | 1.96                     | 0.65              |
| 6:F:19:GLU:O     | 6:F:20:LYS:HG2   | 1.96                     | 0.65              |
| 10:J:151:MET:HA  | 10:J:151:MET:HE3 | 1.79                     | 0.65              |
| 14:N:59:GLY:HA3  | 14:N:141:ILE:CD1 | 2.26                     | 0.65              |
| 23:W:44:GLY:O    | 23:W:48:GLU:HG2  | 1.96                     | 0.65              |
| 1:A:299:U:H5'    | 37:A:6908:HOH:O  | 1.97                     | 0.65              |
| 1:A:316:A:H5'    | 21:U:54:ASP:OD2  | 1.97                     | 0.65              |
| 4:D:145:HIS:HD2  | 4:D:146:THR:O    | 1.78                     | 0.65              |
| 7:G:6:GLU:HA     | 7:G:46:THR:HG22  | 1.77                     | 0.65              |
| 8:H:91:VAL:HG12  | 8:H:92:GLY:N     | 2.11                     | 0.65              |
| 3:C:105:VAL:HG12 | 3:C:106:CYS:N    | 2.12                     | 0.65              |
| 1:A:131:A:OP2    | 37:A:9746:HOH:O  | 2.14                     | 0.65              |
| 1:A:2502:C:C2'   | 1:A:2503:A:H5'   | 2.27                     | 0.65              |
| 1:A:2821:C:H4'   | 4:D:116:PRO:HB3  | 1.76                     | 0.65              |
| 22:V:52:THR:HG22 | 22:V:54:THR:H    | 1.62                     | 0.65              |
| 1:A:2536:C:OP1   | 37:A:9702:HOH:O  | 2.12                     | 0.65              |
| 4:D:2:GLN:HA     | 37:D:8622:HOH:O  | 1.96                     | 0.65              |
| 6:F:41:LEU:HA    | 6:F:44:ILE:HG22  | 1.79                     | 0.65              |
| 10:J:57:ARG:O    | 10:J:61:LEU:HD22 | 1.97                     | 0.65              |
| 10:J:71:TYR:C    | 10:J:73:GLN:H    | 2.05                     | 0.65              |
| 1:A:545:G:H5'    | 1:A:545:G:C8     | 2.30                     | 0.65              |
| 2:B:3014:G:H5'   | 2:B:3014:G:C8    | 2.30                     | 0.65              |
| 35:K:8501:CL:CL  | 37:K:4038:HOH:O  | 2.51                     | 0.65              |
| 24:X:4:LEU:HD22  | 24:X:52:VAL:HG21 | 1.79                     | 0.65              |
| 24:X:72:PRO:HG2  | 24:X:77:ALA:HB3  | 1.78                     | 0.65              |
| 1:A:1130:U:H2'   | 1:A:1131:G:O4'   | 1.97                     | 0.64              |
| 1:A:1377:C:H6    | 1:A:1377:C:H5'   | 1.62                     | 0.64              |
| 1:A:2908:A:H2'   | 1:A:2909:G:O4'   | 1.97                     | 0.64              |
| 6:F:37:ALA:O     | 6:F:40:ILE:HG12  | 1.97                     | 0.64              |
| 6:F:174:VAL:HG13 | 37:F:6555:HOH:O  | 1.96                     | 0.64              |
| 20:T:58:MET:SD   | 29:3:8:LYS:HE3   | 2.37                     | 0.64              |
| 1:A:272:A:H3'    | 37:A:7105:HOH:O  | 1.98                     | 0.64              |
| 4:D:125:GLU:O    | 4:D:129:ARG:HG3  | 1.96                     | 0.64              |
| 12:L:74:VAL:HG12 | 12:L:75:ARG:HG3  | 1.78                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:X:88:THR:HG23 | 24:X:110:GLN:HE21 | 1.63                     | 0.64              |
| 30:4:69:TYR:HB2  | 30:4:78:HIS:CE1   | 2.32                     | 0.64              |
| 1:A:1329:A:N1    | 35:A:8513:CL:CL   | 2.67                     | 0.64              |
| 5:E:78:ARG:HG3   | 5:E:78:ARG:NH1    | 2.08                     | 0.64              |
| 14:N:87:MET:HB3  | 30:4:46:ILE:HG21  | 1.79                     | 0.64              |
| 17:Q:38:GLU:HA   | 17:Q:41:ARG:NH1   | 2.12                     | 0.64              |
| 27:1:61:GLY:HA3  | 37:1:8427:HOH:O   | 1.97                     | 0.64              |
| 3:C:125:ASN:CB   | 3:C:158:VAL:HG12  | 2.27                     | 0.64              |
| 5:E:236:THR:CG2  | 5:E:239:ALA:H     | 2.00                     | 0.64              |
| 11:K:80:LYS:HE2  | 11:K:98:PHE:CZ    | 2.32                     | 0.64              |
| 15:O:143:ARG:HA  | 15:O:172:PHE:CD2  | 2.33                     | 0.64              |
| 1:A:282:C:O2'    | 1:A:283:U:H5'     | 1.98                     | 0.64              |
| 10:J:3:GLY:HA2   | 10:J:57:ARG:NH1   | 2.12                     | 0.64              |
| 15:O:43:VAL:HG11 | 15:O:81:ALA:HA    | 1.79                     | 0.64              |
| 15:O:159:TYR:HB3 | 15:O:162:ASP:HB2  | 1.80                     | 0.64              |
| 25:Y:15:ARG:HH11 | 25:Y:15:ARG:CB    | 2.10                     | 0.64              |
| 1:A:558:C:O2'    | 1:A:559:U:H5''    | 1.98                     | 0.64              |
| 1:A:1874:U:H2'   | 3:C:120:ARG:HG3   | 1.79                     | 0.64              |
| 4:D:16:ARG:NE    | 37:D:8556:HOH:O   | 2.11                     | 0.64              |
| 13:M:136:ALA:HB3 | 37:M:8445:HOH:O   | 1.97                     | 0.64              |
| 21:U:52:ARG:HB2  | 21:U:95:ASN:HB3   | 1.80                     | 0.64              |
| 4:D:179:LEU:O    | 4:D:183:GLU:HG2   | 1.98                     | 0.64              |
| 4:D:258:GLY:H    | 4:D:260:HIS:CE1   | 2.14                     | 0.64              |
| 17:Q:103:THR:HA  | 17:Q:106:ARG:NH1  | 2.12                     | 0.64              |
| 1:A:182:G:H5'    | 37:A:4731:HOH:O   | 1.98                     | 0.64              |
| 1:A:2783:A:H3'   | 37:A:4807:HOH:O   | 1.98                     | 0.64              |
| 11:K:88:PRO:CA   | 35:K:8502:CL:CL   | 2.83                     | 0.64              |
| 1:A:821:U:O2'    | 1:A:822:C:H5'     | 1.98                     | 0.64              |
| 5:E:129:HIS:CE1  | 5:E:232:LEU:H     | 2.16                     | 0.64              |
| 5:E:180:SER:HB2  | 37:E:8442:HOH:O   | 1.97                     | 0.64              |
| 6:F:23:VAL:HG22  | 6:F:73:VAL:HB     | 1.80                     | 0.64              |
| 14:N:172:GLY:O   | 14:N:183:VAL:HG11 | 1.98                     | 0.64              |
| 1:A:1741:U:H5'   | 1:A:1742:A:OP1    | 1.97                     | 0.63              |
| 2:B:3092:G:H2'   | 2:B:3093:A:C8     | 2.34                     | 0.63              |
| 19:S:18:LEU:HB2  | 19:S:143:VAL:HG12 | 1.79                     | 0.63              |
| 24:X:41:TYR:O    | 24:X:45:VAL:HG13  | 1.98                     | 0.63              |
| 1:A:2748:G:H2'   | 37:A:7117:HOH:O   | 1.97                     | 0.63              |
| 6:F:64:ARG:CD    | 6:F:67:ASP:HB3    | 2.28                     | 0.63              |
| 1:A:2547:C:OP2   | 4:D:5:ARG:NH1     | 2.31                     | 0.63              |
| 5:E:219:ASN:O    | 5:E:222:ASP:OD1   | 2.16                     | 0.63              |
| 25:Y:71:ARG:CD   | 37:Y:2171:HOH:O   | 2.47                     | 0.63              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 30:4:65:THR:HG23 | 30:4:67:LEU:HG     | 1.80                     | 0.63              |
| 23:W:39:ALA:C    | 23:W:41:GLU:H      | 2.06                     | 0.63              |
| 26:Z:99:ALA:HB2  | 26:Z:233:TYR:CZ    | 2.33                     | 0.63              |
| 1:A:1441:G:H1'   | 37:A:7340:HOH:O    | 1.98                     | 0.63              |
| 1:A:2270:G:H4'   | 3:C:223:ARG:HH12   | 1.63                     | 0.63              |
| 1:A:1015:C:H2'   | 1:A:1016:U:H6      | 1.63                     | 0.63              |
| 1:A:2502:C:H2'   | 1:A:2503:A:H5'     | 1.80                     | 0.63              |
| 3:C:94:LEU:N     | 3:C:94:LEU:HD23    | 2.13                     | 0.63              |
| 4:D:48:MET:N     | 37:D:8560:HOH:O    | 2.31                     | 0.63              |
| 5:E:242:GLU:HG3  | 37:E:8378:HOH:O    | 1.97                     | 0.63              |
| 14:N:81:ARG:HG3  | 14:N:85:ARG:HB2    | 1.81                     | 0.63              |
| 1:A:281:U:H3'    | 37:A:6777:HOH:O    | 1.99                     | 0.63              |
| 1:A:1878:G:H1'   | 37:A:5700:HOH:O    | 1.97                     | 0.63              |
| 1:A:2363:G:O3'   | 18:R:11:ARG:NH1    | 2.32                     | 0.63              |
| 6:F:146:LYS:HZ3  | 15:O:107:ASN:HD21  | 1.44                     | 0.63              |
| 12:L:81:ARG:HD3  | 12:L:87:ARG:NH1    | 2.14                     | 0.63              |
| 21:U:65:VAL:HG22 | 21:U:72:ILE:HG22   | 1.81                     | 0.63              |
| 21:U:71:VAL:HG11 | 21:U:90:PRO:CB     | 2.20                     | 0.63              |
| 1:A:1735:C:O2'   | 1:A:1736:A:H5'     | 1.99                     | 0.63              |
| 1:A:1771:U:H4'   | 27:1:20:LEU:HD21   | 1.79                     | 0.63              |
| 1:A:2419:U:H5''  | 1:A:2420:G:H5'     | 1.80                     | 0.63              |
| 1:A:2468:A:H61   | 30:4:48:ASN:HD21   | 1.45                     | 0.63              |
| 37:A:6598:HOH:O  | 3:C:211:LYS:HG2    | 1.99                     | 0.63              |
| 5:E:127:ARG:HG2  | 5:E:127:ARG:HH11   | 1.62                     | 0.63              |
| 1:A:111:C:O2'    | 28:2:20:ARG:HG2    | 1.99                     | 0.62              |
| 1:A:2349:G:OP1   | 6:F:20:LYS:NZ      | 2.28                     | 0.62              |
| 2:B:3001:U:O3'   | 2:B:3003:A:H5''    | 1.99                     | 0.62              |
| 10:J:59:ASN:H    | 10:J:59:ASN:ND2    | 1.96                     | 0.62              |
| 22:V:52:THR:HG22 | 22:V:54:THR:N      | 2.13                     | 0.62              |
| 1:A:419:A:H1'    | 1:A:1921:A:C2      | 2.34                     | 0.62              |
| 1:A:1679:C:H5'   | 37:A:8905:HOH:O    | 1.98                     | 0.62              |
| 1:A:2416:G:O2'   | 37:A:9212:HOH:O    | 2.15                     | 0.62              |
| 27:1:29:VAL:O    | 27:1:33:HIS:HB2    | 1.99                     | 0.62              |
| 4:D:62:ARG:CA    | 4:D:65:MET:HE3     | 2.30                     | 0.62              |
| 5:E:12:THR:HB    | 37:E:8438:HOH:O    | 1.98                     | 0.62              |
| 23:W:42:ASN:HB3  | 37:W:7247:HOH:O    | 1.99                     | 0.62              |
| 1:A:755:G:O2'    | 1:A:756:A:H5'      | 1.99                     | 0.62              |
| 1:A:1503:U:H2'   | 1:A:1504:A:O4'     | 1.98                     | 0.62              |
| 13:M:125:PHE:CZ  | 13:M:140:VAL:HG13  | 2.34                     | 0.62              |
| 1:A:2099:G:N2    | 31:A:8600:ZIT:H181 | 2.14                     | 0.62              |
| 1:A:2383:G:N3    | 37:A:6280:HOH:O    | 2.31                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:139:VAL:HG13 | 37:E:8445:HOH:O   | 1.98                     | 0.62              |
| 25:Y:31:ILE:O    | 25:Y:35:GLU:HG3   | 2.00                     | 0.62              |
| 1:A:960:G:H2'    | 1:A:960:G:N3      | 2.15                     | 0.62              |
| 4:D:62:ARG:HA    | 4:D:65:MET:CE     | 2.28                     | 0.62              |
| 6:F:144:ARG:NH2  | 37:F:3839:HOH:O   | 2.32                     | 0.62              |
| 8:H:19:ALA:O     | 8:H:22:VAL:HG22   | 2.00                     | 0.62              |
| 14:N:186:SER:OG  | 14:N:189:VAL:HG12 | 1.99                     | 0.62              |
| 19:S:18:LEU:HG   | 19:S:91:LEU:HD13  | 1.82                     | 0.62              |
| 1:A:542:A:H8     | 1:A:542:A:C5'     | 2.07                     | 0.62              |
| 3:C:53:ALA:HB3   | 37:C:8609:HOH:O   | 2.00                     | 0.62              |
| 12:L:115:ARG:HG3 | 12:L:116:GLU:N    | 2.14                     | 0.62              |
| 13:M:133:VAL:HB  | 37:M:8431:HOH:O   | 1.99                     | 0.62              |
| 15:O:33:ARG:NH1  | 15:O:103:ASP:OD2  | 2.31                     | 0.62              |
| 15:O:151:ASP:O   | 15:O:154:LEU:HB2  | 2.00                     | 0.62              |
| 15:O:154:LEU:O   | 15:O:155:GLU:HB3  | 1.98                     | 0.62              |
| 22:V:37:GLU:HB3  | 37:V:408:HOH:O    | 1.98                     | 0.62              |
| 26:Z:107:PRO:HB3 | 26:Z:182:PHE:CE2  | 2.34                     | 0.62              |
| 4:D:195:ARG:HD2  | 4:D:324:ASP:OD1   | 2.00                     | 0.62              |
| 11:K:19:MET:CE   | 11:K:132:LEU:HD11 | 2.20                     | 0.62              |
| 11:K:74:ARG:O    | 11:K:78:ILE:HG12  | 1.99                     | 0.62              |
| 22:V:13:ILE:HG12 | 22:V:32:CYS:HB3   | 1.80                     | 0.62              |
| 1:A:1701:A:H5'   | 37:A:5859:HOH:O   | 1.99                     | 0.62              |
| 1:A:1701:A:H4'   | 1:A:1702:U:H5''   | 1.80                     | 0.62              |
| 1:A:1789:G:O6    | 17:Q:73:HIS:HE1   | 1.83                     | 0.62              |
| 2:B:3013:A:O2'   | 2:B:3014:G:H5''   | 2.00                     | 0.62              |
| 3:C:109:GLU:HG2  | 3:C:116:GLY:H     | 1.65                     | 0.62              |
| 4:D:30:PRO:HB2   | 4:D:39:GLN:NE2    | 2.15                     | 0.62              |
| 7:G:166:VAL:HG12 | 37:G:3134:HOH:O   | 1.98                     | 0.62              |
| 8:H:2:VAL:HG22   | 8:H:57:GLU:OE1    | 2.00                     | 0.62              |
| 24:X:81:ASP:OD1  | 24:X:92:ASP:HB2   | 2.00                     | 0.62              |
| 1:A:2526:C:O2'   | 1:A:2527:U:H5'    | 2.00                     | 0.62              |
| 14:N:12:TRP:CE2  | 14:N:20:ILE:HD11  | 2.35                     | 0.62              |
| 24:X:54:PHE:CZ   | 24:X:140:LYS:HB2  | 2.35                     | 0.62              |
| 25:Y:21:PRO:HG2  | 25:Y:24:LYS:HD3   | 1.81                     | 0.62              |
| 1:A:396:U:H1'    | 37:A:7204:HOH:O   | 1.99                     | 0.61              |
| 1:A:1116:U:O2'   | 1:A:1118:A:C2     | 2.46                     | 0.61              |
| 37:A:3767:HOH:O  | 26:Z:186:ARG:HD2  | 1.99                     | 0.61              |
| 15:O:12:ARG:HD3  | 15:O:18:THR:OG1   | 2.00                     | 0.61              |
| 15:O:61:ALA:HB3  | 15:O:88:ALA:HB2   | 1.82                     | 0.61              |
| 27:1:13:ARG:NH1  | 27:1:14:PHE:CE2   | 2.68                     | 0.61              |
| 1:A:1003:U:O2    | 10:J:90:PHE:CZ    | 2.53                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1306:U:OP1   | 5:E:184:ARG:HD2  | 2.00                     | 0.61              |
| 4:D:141:ARG:HG2  | 4:D:165:ARG:HA   | 1.82                     | 0.61              |
| 5:E:236:THR:H    | 5:E:239:ALA:HB3  | 1.65                     | 0.61              |
| 4:D:204:GLY:HA3  | 37:D:8658:HOH:O  | 1.99                     | 0.61              |
| 5:E:118:THR:O    | 5:E:136:VAL:HG13 | 2.01                     | 0.61              |
| 10:J:33:MET:HB2  | 10:J:83:PHE:HB3  | 1.82                     | 0.61              |
| 25:Y:41:PHE:O    | 25:Y:43:VAL:HG23 | 2.00                     | 0.61              |
| 1:A:1329:A:H2    | 37:A:4259:HOH:O  | 1.83                     | 0.61              |
| 1:A:2694:A:H4'   | 7:G:91:PHE:CE1   | 2.35                     | 0.61              |
| 6:F:44:ILE:HG23  | 6:F:45:THR:HG23  | 1.82                     | 0.61              |
| 9:I:12:ILE:N     | 9:I:13:PRO:CD    | 2.64                     | 0.61              |
| 10:J:53:PRO:HG3  | 10:J:127:GLY:H   | 1.64                     | 0.61              |
| 11:K:45:VAL:HG23 | 11:K:130:VAL:O   | 2.01                     | 0.61              |
| 15:O:78:MET:HB2  | 15:O:79:PRO:HD3  | 1.82                     | 0.61              |
| 20:T:81:ILE:HG23 | 37:T:8337:HOH:O  | 2.00                     | 0.61              |
| 1:A:1200:A:H4'   | 37:A:6912:HOH:O  | 1.99                     | 0.61              |
| 1:A:1313:A:H5'   | 26:Z:208:LYS:O   | 2.00                     | 0.61              |
| 3:C:101:GLU:OE2  | 3:C:131:HIS:HB2  | 2.00                     | 0.61              |
| 5:E:236:THR:C    | 37:E:8445:HOH:O  | 2.44                     | 0.61              |
| 6:F:99:ASP:CB    | 6:F:103:ASN:H    | 2.13                     | 0.61              |
| 10:J:144:GLU:OE1 | 10:J:144:GLU:HA  | 2.00                     | 0.61              |
| 14:N:74:ARG:HG3  | 14:N:74:ARG:NH1  | 2.15                     | 0.61              |
| 26:Z:107:PRO:HB3 | 26:Z:182:PHE:CD2 | 2.36                     | 0.61              |
| 1:A:2827:A:H2'   | 1:A:2828:G:O4'   | 1.99                     | 0.61              |
| 8:H:50:VAL:HG21  | 8:H:63:ILE:HG21  | 1.83                     | 0.61              |
| 9:I:63:ARG:N     | 37:I:2569:HOH:O  | 2.33                     | 0.61              |
| 11:K:52:GLN:HG3  | 11:K:53:ILE:N    | 2.14                     | 0.61              |
| 23:W:49:LEU:O    | 23:W:53:ILE:HG13 | 1.99                     | 0.61              |
| 30:4:62:THR:HB   | 37:4:8551:HOH:O  | 2.00                     | 0.61              |
| 1:A:1119:G:H2'   | 11:K:52:GLN:HE22 | 1.64                     | 0.61              |
| 1:A:2501:G:H1'   | 37:A:4118:HOH:O  | 2.00                     | 0.61              |
| 1:A:2710:U:H1'   | 37:A:7196:HOH:O  | 2.00                     | 0.61              |
| 4:D:51:VAL:CG2   | 4:D:327:VAL:HG13 | 2.30                     | 0.61              |
| 13:M:57:VAL:HG12 | 13:M:57:VAL:O    | 2.00                     | 0.61              |
| 1:A:1130:U:H5'   | 37:A:7245:HOH:O  | 2.00                     | 0.61              |
| 1:A:2320:U:H4'   | 1:A:2321:A:O4'   | 2.01                     | 0.61              |
| 37:A:4405:HOH:O  | 11:K:47:THR:HB   | 1.99                     | 0.61              |
| 4:D:307:ARG:HH11 | 4:D:307:ARG:CB   | 2.13                     | 0.61              |
| 5:E:237:GLU:HB2  | 37:E:8426:HOH:O  | 2.00                     | 0.61              |
| 10:J:27:LYS:N    | 10:J:58:HIS:HD2  | 1.96                     | 0.61              |
| 15:O:64:SER:C    | 15:O:66:LEU:H    | 2.09                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:Z:126:PRO:HG2 | 26:Z:128:PHE:CE1  | 2.36                     | 0.61              |
| 1:A:182:G:H4'    | 14:N:157:LEU:HD13 | 1.82                     | 0.61              |
| 1:A:184:G:H5''   | 14:N:153:THR:HG22 | 1.83                     | 0.61              |
| 1:A:558:C:H2'    | 1:A:559:U:H5'     | 1.83                     | 0.61              |
| 6:F:146:LYS:NZ   | 15:O:107:ASN:ND2  | 2.47                     | 0.61              |
| 6:F:166:ILE:HD12 | 37:F:6326:HOH:O   | 2.01                     | 0.61              |
| 13:M:104:ASP:O   | 13:M:105:TYR:HB3  | 2.00                     | 0.61              |
| 1:A:738:G:H3'    | 37:A:6619:HOH:O   | 2.00                     | 0.61              |
| 1:A:2505:G:O2'   | 1:A:2506:A:H5'    | 2.01                     | 0.61              |
| 32:A:8036:MG:MG  | 37:A:7398:HOH:O   | 1.43                     | 0.61              |
| 2:B:3002:U:OP2   | 2:B:3002:U:H4'    | 2.00                     | 0.61              |
| 3:C:153:ARG:HH11 | 3:C:153:ARG:CB    | 2.14                     | 0.61              |
| 8:H:100:ASP:HB3  | 37:H:5691:HOH:O   | 2.01                     | 0.61              |
| 14:N:87:MET:HG2  | 30:4:46:ILE:CG2   | 2.27                     | 0.61              |
| 14:N:185:PRO:HG2 | 14:N:189:VAL:HG11 | 1.81                     | 0.61              |
| 16:P:42:GLU:HB2  | 37:P:2176:HOH:O   | 2.00                     | 0.61              |
| 1:A:240:C:H4'    | 14:N:146:GLN:NE2  | 2.16                     | 0.60              |
| 37:A:4040:HOH:O  | 14:N:146:GLN:HG2  | 1.99                     | 0.60              |
| 14:N:172:GLY:C   | 14:N:183:VAL:HG11 | 2.26                     | 0.60              |
| 1:A:2081:A:H4'   | 11:K:69:TYR:CE1   | 2.35                     | 0.60              |
| 1:A:2403:C:H3'   | 37:A:4787:HOH:O   | 2.01                     | 0.60              |
| 4:D:55:ASN:HB3   | 4:D:63:GLU:HA     | 1.83                     | 0.60              |
| 16:P:26:TRP:N    | 37:P:3062:HOH:O   | 2.34                     | 0.60              |
| 22:V:52:THR:CG2  | 22:V:54:THR:HB    | 2.31                     | 0.60              |
| 24:X:130:HIS:O   | 24:X:136:GLY:HA3  | 2.01                     | 0.60              |
| 30:4:17:HIS:O    | 30:4:18:GLN:HG3   | 2.01                     | 0.60              |
| 1:A:1008:C:H5''  | 10:J:16:ARG:HH12  | 1.65                     | 0.60              |
| 1:A:1120:U:C6    | 1:A:1120:U:H5''   | 2.36                     | 0.60              |
| 1:A:1205:U:H2'   | 1:A:1206:U:C5'    | 2.30                     | 0.60              |
| 1:A:1636:G:O2'   | 1:A:1637:A:H5'    | 2.00                     | 0.60              |
| 4:D:305:ASP:O    | 4:D:306:LYS:HB2   | 2.02                     | 0.60              |
| 7:G:31:ARG:NH1   | 7:G:68:HIS:CG     | 2.70                     | 0.60              |
| 25:Y:66:THR:HG23 | 25:Y:67:PRO:HD2   | 1.82                     | 0.60              |
| 1:A:136:C:H2'    | 1:A:137:U:O4'     | 2.00                     | 0.60              |
| 1:A:2392:C:N3    | 37:A:4421:HOH:O   | 2.31                     | 0.60              |
| 3:C:190:ARG:NH2  | 3:C:207:GLN:OE1   | 2.33                     | 0.60              |
| 5:E:84:VAL:O     | 5:E:85:LYS:HB2    | 2.00                     | 0.60              |
| 6:F:65:GLU:HG3   | 37:F:6752:HOH:O   | 2.00                     | 0.60              |
| 7:G:49:ILE:HD11  | 7:G:69:ILE:HD12   | 1.83                     | 0.60              |
| 10:J:139:ASP:H   | 10:J:140:PRO:HD3  | 1.66                     | 0.60              |
| 1:A:321:A:H1'    | 37:A:6605:HOH:O   | 2.02                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1200:A:C4'    | 37:A:6912:HOH:O  | 2.49                     | 0.60              |
| 1:A:2346:C:O5'    | 1:A:2346:C:H6    | 1.83                     | 0.60              |
| 7:G:20:ILE:CD1    | 7:G:40:VAL:HG11  | 2.30                     | 0.60              |
| 7:G:23:GLU:HG2    | 7:G:28:SER:CB    | 2.32                     | 0.60              |
| 10:J:26:LYS:HG2   | 10:J:28:ILE:N    | 2.15                     | 0.60              |
| 10:J:53:PRO:HA    | 10:J:125:VAL:O   | 2.02                     | 0.60              |
| 10:J:136:VAL:HG22 | 10:J:137:ASN:O   | 2.01                     | 0.60              |
| 1:A:212:A:O4'     | 1:A:214:U:C6     | 2.55                     | 0.60              |
| 1:A:1151:G:OP1    | 9:I:63:ARG:NH1   | 2.35                     | 0.60              |
| 1:A:2672:C:H1'    | 37:A:6256:HOH:O  | 2.01                     | 0.60              |
| 4:D:66:GLU:OE1    | 4:D:328:ARG:HD2  | 2.02                     | 0.60              |
| 6:F:93:LEU:HB3    | 6:F:97:GLN:OE1   | 2.02                     | 0.60              |
| 20:T:43:GLU:HB3   | 37:T:8344:HOH:O  | 2.01                     | 0.60              |
| 25:Y:78:GLU:CG    | 25:Y:79:GLU:H    | 2.14                     | 0.60              |
| 1:A:285:A:H2'     | 1:A:286:U:O4'    | 2.02                     | 0.60              |
| 1:A:1187:U:O2'    | 1:A:1189:A:H2    | 1.85                     | 0.60              |
| 1:A:1834:C:H2'    | 1:A:1840:A:N6    | 2.17                     | 0.60              |
| 1:A:2121:G:OP2    | 37:A:3095:HOH:O  | 2.17                     | 0.60              |
| 1:A:2756:U:H3     | 1:A:2896:A:H2    | 1.46                     | 0.60              |
| 11:K:131:THR:HG22 | 11:K:134:GLU:H   | 1.65                     | 0.60              |
| 24:X:149:LEU:CG   | 24:X:153:MET:HE2 | 2.25                     | 0.60              |
| 6:F:101:THR:HG22  | 37:F:7400:HOH:O  | 2.01                     | 0.60              |
| 27:1:30:GLU:HA    | 27:1:33:HIS:HB3  | 1.84                     | 0.60              |
| 4:D:301:VAL:HG13  | 4:D:302:PRO:HD2  | 1.83                     | 0.60              |
| 7:G:101:GLU:HB2   | 7:G:116:THR:O    | 2.02                     | 0.60              |
| 10:J:58:HIS:HA    | 10:J:61:LEU:HD23 | 1.83                     | 0.60              |
| 15:O:37:ARG:NE    | 37:O:8534:HOH:O  | 2.34                     | 0.60              |
| 1:A:2768:A:O2'    | 1:A:2769:C:H5'   | 2.02                     | 0.59              |
| 3:C:69:LEU:HD21   | 3:C:120:ARG:HB3  | 1.82                     | 0.59              |
| 13:M:53:ARG:NH2   | 13:M:57:VAL:CG1  | 2.65                     | 0.59              |
| 14:N:52:LEU:HD21  | 37:N:8615:HOH:O  | 2.02                     | 0.59              |
| 14:N:69:LYS:HG2   | 14:N:127:LYS:HG3 | 1.82                     | 0.59              |
| 21:U:24:ARG:HH21  | 21:U:39:ASN:HD22 | 1.48                     | 0.59              |
| 3:C:211:LYS:NZ    | 37:C:8574:HOH:O  | 2.35                     | 0.59              |
| 7:G:157:LYS:NZ    | 37:G:2401:HOH:O  | 2.35                     | 0.59              |
| 8:H:28:ALA:HB3    | 8:H:99:THR:O     | 2.02                     | 0.59              |
| 27:1:53:GLY:HA2   | 27:1:67:GLY:O    | 2.01                     | 0.59              |
| 1:A:1766:U:O2     | 1:A:1778:A:H5'   | 2.02                     | 0.59              |
| 6:F:135:VAL:HG21  | 6:F:139:TYR:CD1  | 2.38                     | 0.59              |
| 15:O:169:PRO:O    | 15:O:172:PHE:HB3 | 2.02                     | 0.59              |
| 24:X:139:GLY:O    | 24:X:141:HIS:HD2 | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2256:G:O2'    | 1:A:2257:G:H5'    | 2.02                     | 0.59              |
| 4:D:168:GLY:N     | 4:D:174:ARG:HD3   | 2.17                     | 0.59              |
| 4:D:175:LEU:C     | 4:D:175:LEU:CD2   | 2.75                     | 0.59              |
| 5:E:104:ASP:O     | 5:E:108:GLN:HG3   | 2.03                     | 0.59              |
| 8:H:58:GLU:OE1    | 14:N:27:ARG:NH2   | 2.31                     | 0.59              |
| 14:N:113:ARG:NH2  | 14:N:156:ARG:HG2  | 2.18                     | 0.59              |
| 26:Z:185:VAL:HG12 | 37:Z:8158:HOH:O   | 2.00                     | 0.59              |
| 1:A:1058:A:H2'    | 1:A:1060:C:H5''   | 1.83                     | 0.59              |
| 1:A:1159:G:H21    | 1:A:1189:A:H8     | 1.49                     | 0.59              |
| 1:A:1165:G:OP1    | 1:A:1165:G:H3'    | 2.03                     | 0.59              |
| 1:A:2434:A:O3'    | 30:4:28:GLY:HA3   | 2.03                     | 0.59              |
| 1:A:2694:A:H4'    | 7:G:91:PHE:HE1    | 1.66                     | 0.59              |
| 2:B:3107:C:C5     | 37:B:8437:HOH:O   | 2.52                     | 0.59              |
| 4:D:207:LYS:HG2   | 4:D:304:PRO:HB3   | 1.84                     | 0.59              |
| 4:D:314:ALA:HB3   | 4:D:317:PRO:HG3   | 1.85                     | 0.59              |
| 20:T:53:ASN:ND2   | 37:T:8323:HOH:O   | 2.35                     | 0.59              |
| 1:A:151:A:C2      | 1:A:442:A:C8      | 2.90                     | 0.59              |
| 1:A:2363:G:O2'    | 18:R:11:ARG:HG3   | 2.03                     | 0.59              |
| 2:B:3039:U:H1'    | 2:B:3044:A:N6     | 2.17                     | 0.59              |
| 5:E:16:VAL:HG12   | 5:E:17:ASP:N      | 2.17                     | 0.59              |
| 10:J:163:PRO:O    | 10:J:164:ALA:HB2  | 2.03                     | 0.59              |
| 1:A:544:G:C2'     | 1:A:545:G:H5''    | 2.31                     | 0.59              |
| 1:A:1249:U:H2'    | 1:A:1250:C:C6     | 2.37                     | 0.59              |
| 37:A:6798:HOH:O   | 14:N:13:LYS:HE2   | 2.03                     | 0.59              |
| 16:P:14:LEU:HD23  | 16:P:102:ILE:HD11 | 1.83                     | 0.59              |
| 37:A:8703:HOH:O   | 5:E:103:ASN:HB3   | 2.02                     | 0.59              |
| 11:K:74:ARG:HH11  | 11:K:74:ARG:CB    | 2.14                     | 0.59              |
| 1:A:156:C:H5''    | 14:N:171:ARG:CD   | 2.23                     | 0.59              |
| 1:A:263:U:O4'     | 8:H:59:ILE:HD13   | 2.02                     | 0.59              |
| 1:A:1819:G:H2'    | 1:A:1820:G:H4'    | 1.85                     | 0.59              |
| 7:G:23:GLU:HG2    | 7:G:28:SER:HB3    | 1.85                     | 0.59              |
| 12:L:74:VAL:HG13  | 12:L:113:ILE:HG23 | 1.84                     | 0.59              |
| 14:N:61:ILE:HA    | 37:N:8622:HOH:O   | 2.03                     | 0.59              |
| 28:2:28:HIS:HD2   | 28:2:31:LYS:H     | 1.50                     | 0.59              |
| 1:A:396:U:H5'     | 30:4:42:ARG:HH12  | 1.67                     | 0.59              |
| 1:A:449:A:N7      | 5:E:43:LYS:HG2    | 2.17                     | 0.59              |
| 1:A:558:C:H2'     | 1:A:559:U:C5'     | 2.33                     | 0.59              |
| 1:A:1119:G:H8     | 11:K:52:GLN:NE2   | 2.01                     | 0.59              |
| 2:B:3025:G:N2     | 37:B:8507:HOH:O   | 2.36                     | 0.59              |
| 2:B:3048:C:H4'    | 15:O:141:ARG:NH2  | 2.18                     | 0.59              |
| 3:C:33:GLU:O      | 3:C:34:ASP:HB2    | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:235:PHE:HE2   | 5:E:243:VAL:HG21  | 1.66                     | 0.59              |
| 13:M:143:THR:HG22 | 13:M:145:LEU:H    | 1.66                     | 0.59              |
| 16:P:25:VAL:HG23  | 16:P:26:TRP:N     | 2.18                     | 0.59              |
| 1:A:2769:C:C2'    | 1:A:2770:G:H5'    | 2.33                     | 0.58              |
| 1:A:2878:U:H2'    | 1:A:2879:A:O4'    | 2.03                     | 0.58              |
| 3:C:114:ASP:HB2   | 3:C:117:LYS:HE2   | 1.84                     | 0.58              |
| 5:E:1:MET:HG2     | 5:E:2:GLN:N       | 2.16                     | 0.58              |
| 14:N:146:GLN:NE2  | 37:N:8645:HOH:O   | 2.36                     | 0.58              |
| 28:2:20:ARG:HB2   | 37:2:8413:HOH:O   | 2.02                     | 0.58              |
| 1:A:157:G:H4'     | 14:N:95:LYS:HE3   | 1.85                     | 0.58              |
| 3:C:37:VAL:HG22   | 37:C:8599:HOH:O   | 2.02                     | 0.58              |
| 3:C:81:GLN:HB2    | 3:C:92:ASN:ND2    | 2.18                     | 0.58              |
| 4:D:16:ARG:NH2    | 37:D:8556:HOH:O   | 2.34                     | 0.58              |
| 28:2:21:ARG:HD2   | 28:2:37:CYS:SG    | 2.42                     | 0.58              |
| 1:A:1234:U:C4     | 4:D:244:PRO:HB3   | 2.39                     | 0.58              |
| 1:A:1423:C:O2'    | 1:A:1424:A:H5'    | 2.03                     | 0.58              |
| 37:A:9350:HOH:O   | 13:M:41:HIS:HE1   | 1.86                     | 0.58              |
| 6:F:86:THR:O      | 6:F:90:LEU:HG     | 2.03                     | 0.58              |
| 11:K:88:PRO:C     | 35:K:8502:CL:CL   | 2.83                     | 0.58              |
| 24:X:4:LEU:HD22   | 24:X:52:VAL:CG2   | 2.33                     | 0.58              |
| 26:Z:106:THR:HG23 | 26:Z:107:PRO:HD2  | 1.85                     | 0.58              |
| 1:A:566:A:H2'     | 1:A:567:U:O4'     | 2.03                     | 0.58              |
| 1:A:2256:G:C2'    | 1:A:2257:G:H5'    | 2.33                     | 0.58              |
| 14:N:12:TRP:O     | 14:N:15:PRO:HD3   | 2.02                     | 0.58              |
| 26:Z:189:ASN:HD22 | 26:Z:189:ASN:C    | 2.12                     | 0.58              |
| 1:A:1192:A:O2'    | 1:A:1193:A:OP1    | 2.21                     | 0.58              |
| 4:D:154:VAL:HG12  | 4:D:156:LYS:HG2   | 1.86                     | 0.58              |
| 6:F:50:VAL:O      | 6:F:71:ALA:HA     | 2.03                     | 0.58              |
| 8:H:28:ALA:CB     | 8:H:99:THR:HG23   | 2.32                     | 0.58              |
| 10:J:48:LEU:HG    | 10:J:157:ILE:HG21 | 1.85                     | 0.58              |
| 15:O:34:LEU:HA    | 15:O:47:LEU:HD23  | 1.86                     | 0.58              |
| 16:P:47:ARG:HG3   | 16:P:47:ARG:NH1   | 2.17                     | 0.58              |
| 24:X:21:LEU:HD22  | 24:X:26:ILE:CD1   | 2.33                     | 0.58              |
| 1:A:1182:C:H1'    | 1:A:1192:A:H8     | 1.68                     | 0.58              |
| 1:A:2834:G:OP1    | 25:Y:39:LYS:HE2   | 2.01                     | 0.58              |
| 4:D:162:MET:HG3   | 4:D:310:ARG:CZ    | 2.34                     | 0.58              |
| 22:V:11:THR:HG22  | 22:V:53:ASP:OD2   | 2.03                     | 0.58              |
| 24:X:6:GLN:HB2    | 24:X:26:ILE:CD1   | 2.32                     | 0.58              |
| 1:A:558:C:C2'     | 1:A:559:U:H5''    | 2.33                     | 0.58              |
| 6:F:54:ALA:HB2    | 6:F:69:ILE:HD12   | 1.86                     | 0.58              |
| 10:J:75:SER:C     | 10:J:79:ALA:HB2   | 2.29                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:U:101:LEU:HD13 | 21:U:112:LEU:HD11 | 1.86                     | 0.58              |
| 1:A:1559:A:H1'    | 37:A:5443:HOH:O   | 2.04                     | 0.58              |
| 4:D:14:GLY:HA2    | 4:D:15:PRO:C      | 2.29                     | 0.58              |
| 9:I:12:ILE:HA     | 37:I:4499:HOH:O   | 2.03                     | 0.58              |
| 29:3:18:ASN:HD21  | 29:3:40:ARG:H     | 1.52                     | 0.58              |
| 1:A:241:A:C2      | 1:A:378:A:H4'     | 2.39                     | 0.58              |
| 1:A:656:G:OP2     | 16:P:37:ARG:HD2   | 2.03                     | 0.58              |
| 1:A:2094:G:H4'    | 4:D:245:SER:HB3   | 1.85                     | 0.58              |
| 12:L:106:GLY:HA3  | 37:L:5264:HOH:O   | 2.02                     | 0.58              |
| 15:O:82:TYR:C     | 15:O:82:TYR:CD2   | 2.82                     | 0.58              |
| 22:V:6:CYS:C      | 22:V:8:TYR:H      | 2.12                     | 0.58              |
| 1:A:396:U:H5'     | 30:4:42:ARG:NH1   | 2.18                     | 0.58              |
| 1:A:2276:U:H2'    | 1:A:2277:U:C6     | 2.38                     | 0.58              |
| 37:A:5895:HOH:O   | 6:F:55:LYS:HB2    | 2.04                     | 0.58              |
| 37:A:7282:HOH:O   | 5:E:94:THR:HG21   | 2.04                     | 0.58              |
| 4:D:7:ARG:NH1     | 4:D:11:LEU:HD22   | 2.18                     | 0.58              |
| 5:E:107:ARG:NE    | 37:E:8454:HOH:O   | 2.25                     | 0.58              |
| 6:F:86:THR:C      | 6:F:89:PRO:HD2    | 2.28                     | 0.58              |
| 10:J:127:GLY:O    | 10:J:128:ALA:HB3  | 2.03                     | 0.58              |
| 12:L:28:GLU:HB3   | 12:L:59:LYS:HB2   | 1.86                     | 0.58              |
| 12:L:55:VAL:HG12  | 12:L:56:SER:H     | 1.68                     | 0.58              |
| 13:M:149:ARG:O    | 13:M:150:GLN:HB2  | 2.03                     | 0.58              |
| 1:A:1528:A:H2'    | 1:A:1529:G:O4'    | 2.04                     | 0.57              |
| 1:A:2721:U:H4'    | 12:L:87:ARG:HG3   | 1.86                     | 0.57              |
| 3:C:186:TRP:CG    | 3:C:187:PRO:HA    | 2.39                     | 0.57              |
| 10:J:47:GLU:CB    | 10:J:133:ILE:HD13 | 2.34                     | 0.57              |
| 19:S:119:VAL:O    | 19:S:119:VAL:HG12 | 2.03                     | 0.57              |
| 1:A:2265:U:H2'    | 1:A:2266:A:H8     | 1.67                     | 0.57              |
| 1:A:2472:C:O2'    | 1:A:2634:G:H4'    | 2.04                     | 0.57              |
| 11:K:19:MET:HE3   | 11:K:132:LEU:CD1  | 2.23                     | 0.57              |
| 19:S:18:LEU:HD12  | 19:S:143:VAL:CG1  | 2.34                     | 0.57              |
| 1:A:281:U:O2'     | 1:A:282:C:H5'     | 2.04                     | 0.57              |
| 1:A:1086:A:C6     | 24:X:11:VAL:HG11  | 2.38                     | 0.57              |
| 14:N:59:GLY:HA3   | 14:N:141:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:20:G:H21      | 19:S:117:HIS:HD2  | 1.51                     | 0.57              |
| 2:B:3107:C:H5     | 37:B:8437:HOH:O   | 1.86                     | 0.57              |
| 10:J:81:TYR:CD1   | 10:J:81:TYR:C     | 2.81                     | 0.57              |
| 25:Y:75:ALA:O     | 25:Y:83:ALA:HA    | 2.04                     | 0.57              |
| 1:A:204:A:C2'     | 1:A:205:U:H5'     | 2.33                     | 0.57              |
| 1:A:280:C:H2'     | 1:A:281:U:O4'     | 2.05                     | 0.57              |
| 1:A:336:G:OP1     | 37:A:3304:HOH:O   | 2.17                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:2:GLN:CD     | 37:D:8622:HOH:O   | 2.46                     | 0.57              |
| 13:M:145:LEU:O   | 13:M:148:GLU:HG3  | 2.03                     | 0.57              |
| 16:P:39:THR:O    | 16:P:115:ARG:NH2  | 2.37                     | 0.57              |
| 1:A:1191:A:C3'   | 1:A:1192:A:H5''   | 2.35                     | 0.57              |
| 4:D:40:GLY:O     | 37:D:8557:HOH:O   | 2.17                     | 0.57              |
| 5:E:27:ARG:HG2   | 5:E:30:LEU:HG     | 1.86                     | 0.57              |
| 9:I:64:ASN:HD22  | 9:I:64:ASN:N      | 2.02                     | 0.57              |
| 15:O:86:LEU:O    | 15:O:90:LEU:HG    | 2.05                     | 0.57              |
| 1:A:1028:U:H1'   | 37:A:3225:HOH:O   | 2.05                     | 0.57              |
| 1:A:2488:A:H1'   | 37:A:8685:HOH:O   | 2.05                     | 0.57              |
| 37:A:7029:HOH:O  | 5:E:188:ARG:CD    | 2.52                     | 0.57              |
| 37:B:8465:HOH:O  | 15:O:147:ILE:HD12 | 2.04                     | 0.57              |
| 14:N:87:MET:HB2  | 14:N:91:ILE:HD11  | 1.87                     | 0.57              |
| 15:O:100:ALA:O   | 15:O:129:ILE:HG23 | 2.04                     | 0.57              |
| 29:3:22:PRO:HG2  | 29:3:25:VAL:CG2   | 2.34                     | 0.57              |
| 1:A:283:U:H5     | 1:A:284:C:N4      | 2.02                     | 0.57              |
| 1:A:2310:G:OP2   | 10:J:114:PRO:HD2  | 2.04                     | 0.57              |
| 1:A:2866:U:C2    | 37:A:7073:HOH:O   | 2.53                     | 0.57              |
| 3:C:18:ALA:O     | 3:C:20:SER:N      | 2.34                     | 0.57              |
| 21:U:37:GLN:OE1  | 21:U:118:SER:HA   | 2.05                     | 0.57              |
| 24:X:38:THR:HG22 | 24:X:39:ASP:H     | 1.69                     | 0.57              |
| 1:A:629:A:C2     | 1:A:2074:A:C2     | 2.93                     | 0.57              |
| 1:A:1730:G:H5'   | 1:A:1731:C:C5     | 2.40                     | 0.57              |
| 3:C:94:LEU:HG    | 3:C:99:ILE:HD11   | 1.87                     | 0.57              |
| 7:G:69:ILE:HA    | 7:G:72:MET:CE     | 2.35                     | 0.57              |
| 8:H:58:GLU:HA    | 8:H:61:MET:HE2    | 1.87                     | 0.57              |
| 10:J:65:ARG:CZ   | 37:J:8387:HOH:O   | 2.53                     | 0.57              |
| 19:S:82:GLU:HG3  | 19:S:83:LYS:N     | 2.19                     | 0.57              |
| 20:T:29:ASP:OD1  | 20:T:31:ARG:NH1   | 2.38                     | 0.57              |
| 1:A:2415:A:C2    | 15:O:25:ARG:HB3   | 2.40                     | 0.57              |
| 1:A:2502:C:H4'   | 10:J:151:MET:SD   | 2.45                     | 0.57              |
| 1:A:2657:G:OP1   | 4:D:17:LYS:HB2    | 2.05                     | 0.57              |
| 1:A:2769:C:H2'   | 1:A:2770:G:O4'    | 2.05                     | 0.57              |
| 37:A:6281:HOH:O  | 26:Z:165:GLU:HB3  | 2.04                     | 0.57              |
| 4:D:168:GLY:O    | 4:D:169:GLY:O     | 2.22                     | 0.57              |
| 6:F:23:VAL:HG21  | 6:F:45:THR:HG21   | 1.87                     | 0.57              |
| 1:A:21:G:H4'     | 19:S:2:ILE:HG22   | 1.87                     | 0.56              |
| 1:A:1244:U:OP1   | 11:K:18:ILE:HD13  | 2.05                     | 0.56              |
| 1:A:2256:G:H2'   | 1:A:2257:G:H5'    | 1.87                     | 0.56              |
| 1:A:2748:G:H5'   | 37:A:7117:HOH:O   | 2.05                     | 0.56              |
| 2:B:3006:C:C5'   | 15:O:37:ARG:NH1   | 2.62                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1:GLY:N       | 37:C:8611:HOH:O   | 2.28                     | 0.56              |
| 4:D:280:VAL:CG1   | 4:D:334:SER:HA    | 2.35                     | 0.56              |
| 6:F:22:VAL:HG22   | 6:F:74:THR:HG22   | 1.87                     | 0.56              |
| 10:J:166:ASN:N    | 10:J:166:ASN:HD22 | 2.02                     | 0.56              |
| 11:K:77:GLY:O     | 11:K:78:ILE:C     | 2.48                     | 0.56              |
| 1:A:1266:U:H4'    | 26:Z:115:ARG:HH21 | 1.70                     | 0.56              |
| 1:A:1474:C:H6     | 1:A:1474:C:C5'    | 2.11                     | 0.56              |
| 1:A:2635:A:O2'    | 1:A:2636:C:H5'    | 2.05                     | 0.56              |
| 2:B:3020:G:O2'    | 2:B:3021:G:H5'    | 2.05                     | 0.56              |
| 7:G:93:MET:HE1    | 7:G:165:GLY:N     | 2.20                     | 0.56              |
| 1:A:183:A:O2'     | 1:A:184:G:H5'     | 2.06                     | 0.56              |
| 1:A:200:U:H2'     | 37:A:3028:HOH:O   | 2.04                     | 0.56              |
| 1:A:371:U:H2'     | 1:A:372:A:H8      | 1.70                     | 0.56              |
| 1:A:1753:C:O2     | 4:D:229:ARG:NH2   | 2.38                     | 0.56              |
| 1:A:2659:U:H4'    | 19:S:76:ASP:HB3   | 1.87                     | 0.56              |
| 37:A:4118:HOH:O   | 10:J:151:MET:HE2  | 2.05                     | 0.56              |
| 37:A:4544:HOH:O   | 10:J:57:ARG:HG3   | 2.05                     | 0.56              |
| 37:A:5094:HOH:O   | 4:D:298:LYS:HD3   | 2.04                     | 0.56              |
| 4:D:138:GLY:O     | 4:D:139:ASP:O     | 2.23                     | 0.56              |
| 4:D:329:TYR:CE2   | 22:V:15:PRO:HG2   | 2.40                     | 0.56              |
| 13:M:143:THR:CG2  | 13:M:144:ASP:N    | 2.68                     | 0.56              |
| 16:P:25:VAL:O     | 16:P:29:VAL:HG23  | 2.04                     | 0.56              |
| 23:W:56:ILE:O     | 23:W:60:GLN:HG3   | 2.05                     | 0.56              |
| 1:A:168:C:O2'     | 1:A:169:A:H5'     | 2.05                     | 0.56              |
| 1:A:1333:U:H2'    | 1:A:1334:C:C6     | 2.41                     | 0.56              |
| 1:A:1909:A:H2'    | 1:A:1910:A:C8     | 2.39                     | 0.56              |
| 4:D:254:GLN:HG2   | 4:D:255:GLY:N     | 2.19                     | 0.56              |
| 7:G:172:PRO:HB3   | 37:G:6931:HOH:O   | 2.06                     | 0.56              |
| 8:H:110:GLU:O     | 8:H:114:LYS:HG3   | 2.05                     | 0.56              |
| 10:J:44:ALA:HA    | 10:J:163:PRO:O    | 2.06                     | 0.56              |
| 13:M:143:THR:HG22 | 13:M:144:ASP:H    | 1.71                     | 0.56              |
| 26:Z:144:ARG:NE   | 37:Z:8197:HOH:O   | 2.39                     | 0.56              |
| 1:A:175:G:H2'     | 14:N:192:ALA:HB3  | 1.87                     | 0.56              |
| 1:A:328:U:O4'     | 5:E:202:THR:HG22  | 2.05                     | 0.56              |
| 1:A:775:G:OP1     | 28:2:16:HIS:HE1   | 1.89                     | 0.56              |
| 1:A:797:A:C4'     | 27:1:10:ARG:N     | 2.69                     | 0.56              |
| 1:A:2713:G:O2'    | 1:A:2714:U:H5'    | 2.05                     | 0.56              |
| 4:D:7:ARG:HG2     | 4:D:7:ARG:HH11    | 1.69                     | 0.56              |
| 5:E:79:ARG:O      | 5:E:87:ARG:HG2    | 2.06                     | 0.56              |
| 6:F:163:VAL:HA    | 37:F:6326:HOH:O   | 2.04                     | 0.56              |
| 10:J:11:LYS:NZ    | 37:J:8335:HOH:O   | 2.39                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:34:VAL:HB   | 37:L:7169:HOH:O  | 2.06                     | 0.56              |
| 15:O:89:GLY:O    | 15:O:92:ALA:HB3  | 2.06                     | 0.56              |
| 24:X:110:GLN:NE2 | 24:X:110:GLN:HA  | 2.20                     | 0.56              |
| 1:A:450:C:H4'    | 5:E:46:TYR:CE1   | 2.41                     | 0.56              |
| 1:A:1699:C:H4'   | 37:A:6017:HOH:O  | 2.06                     | 0.56              |
| 1:A:2011:A:P     | 37:A:5537:HOH:O  | 2.63                     | 0.56              |
| 5:E:107:ARG:HB3  | 5:E:107:ARG:HH11 | 1.70                     | 0.56              |
| 14:N:162:GLY:HA2 | 37:N:8519:HOH:O  | 2.04                     | 0.56              |
| 26:Z:189:ASN:ND2 | 26:Z:192:ASP:H   | 2.04                     | 0.56              |
| 1:A:154:C:C2     | 1:A:155:C:C5     | 2.93                     | 0.56              |
| 1:A:1393:A:H2'   | 1:A:1394:C:C6    | 2.41                     | 0.56              |
| 1:A:2780:C:H1'   | 7:G:143:GLN:NE2  | 2.20                     | 0.56              |
| 1:A:2830:U:H3'   | 37:A:4804:HOH:O  | 2.05                     | 0.56              |
| 6:F:25:MET:CE    | 6:F:37:ALA:HB1   | 2.36                     | 0.56              |
| 8:H:99:THR:O     | 8:H:99:THR:HG23  | 2.05                     | 0.56              |
| 22:V:46:ALA:HB1  | 22:V:52:THR:HG21 | 1.88                     | 0.56              |
| 1:A:661:G:C5     | 1:A:686:A:C2     | 2.93                     | 0.56              |
| 1:A:1137:G:H1'   | 37:A:3455:HOH:O  | 2.05                     | 0.56              |
| 37:A:4628:HOH:O  | 17:Q:68:LYS:HD3  | 2.06                     | 0.56              |
| 2:B:3041:C:O4'   | 6:F:50:VAL:HG23  | 2.06                     | 0.56              |
| 1:A:1189:A:H1'   | 1:A:1209:C:C1'   | 2.36                     | 0.56              |
| 4:D:215:VAL:HB   | 4:D:234:ARG:HH12 | 1.71                     | 0.56              |
| 6:F:11:HIS:O     | 6:F:12:GLU:HB3   | 2.05                     | 0.56              |
| 10:J:27:LYS:H    | 10:J:58:HIS:CD2  | 2.17                     | 0.56              |
| 14:N:191:GLY:O   | 14:N:192:ALA:HB3 | 2.06                     | 0.56              |
| 15:O:47:LEU:HD13 | 15:O:97:VAL:HG11 | 1.88                     | 0.56              |
| 16:P:7:LEU:HD22  | 37:P:5650:HOH:O  | 2.05                     | 0.56              |
| 28:2:1:THR:HB    | 37:2:8457:HOH:O  | 2.04                     | 0.56              |
| 1:A:694:A:H2'    | 1:A:695:C:H5'    | 1.87                     | 0.56              |
| 1:A:1181:A:H2'   | 1:A:1182:C:O4'   | 2.05                     | 0.56              |
| 4:D:307:ARG:HH11 | 4:D:307:ARG:CG   | 2.18                     | 0.56              |
| 5:E:95:GLU:H     | 5:E:95:GLU:CD    | 2.14                     | 0.56              |
| 25:Y:25:ARG:CZ   | 37:Y:3861:HOH:O  | 2.52                     | 0.56              |
| 1:A:135:G:OP1    | 37:A:6873:HOH:O  | 2.18                     | 0.55              |
| 1:A:485:A:N3     | 1:A:487:G:H5''   | 2.21                     | 0.55              |
| 1:A:512:G:O3'    | 1:A:513:A:H8     | 1.89                     | 0.55              |
| 1:A:952:G:H4'    | 37:A:3606:HOH:O  | 2.06                     | 0.55              |
| 1:A:2724:U:H2'   | 1:A:2725:G:O4'   | 2.05                     | 0.55              |
| 2:B:3078:G:H22   | 2:B:3102:G:H2'   | 1.71                     | 0.55              |
| 5:E:142:ASP:OD1  | 5:E:237:GLU:HB3  | 2.05                     | 0.55              |
| 6:F:44:ILE:HG12  | 6:F:83:PHE:HE1   | 1.71                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:O:38:LYS:HD2  | 15:O:114:LYS:HE3  | 1.87                     | 0.55              |
| 15:O:152:GLU:C   | 15:O:154:LEU:H    | 2.12                     | 0.55              |
| 19:S:39:THR:HB   | 19:S:42:GLU:CG    | 2.35                     | 0.55              |
| 19:S:79:ARG:C    | 19:S:81:PRO:HD3   | 2.31                     | 0.55              |
| 1:A:283:U:H5''   | 1:A:284:C:P       | 2.46                     | 0.55              |
| 1:A:558:C:H5'    | 37:A:4832:HOH:O   | 2.06                     | 0.55              |
| 1:A:1015:C:H2'   | 1:A:1016:U:C6     | 2.40                     | 0.55              |
| 1:A:1362:U:H5'   | 37:A:9849:HOH:O   | 2.05                     | 0.55              |
| 2:B:3078:G:N2    | 2:B:3102:G:H2'    | 2.22                     | 0.55              |
| 4:D:24:PRO:HG2   | 4:D:204:GLY:HA2   | 1.87                     | 0.55              |
| 4:D:146:THR:O    | 4:D:159:PRO:HB3   | 2.05                     | 0.55              |
| 6:F:36:ASN:HA    | 37:F:7500:HOH:O   | 2.06                     | 0.55              |
| 6:F:105:SER:CB   | 6:F:131:THR:HG23  | 2.33                     | 0.55              |
| 12:L:75:ARG:CZ   | 37:L:4172:HOH:O   | 2.53                     | 0.55              |
| 15:O:170:GLU:O   | 15:O:174:GLU:HG3  | 2.06                     | 0.55              |
| 21:U:4:PRO:O     | 21:U:8:ARG:HG3    | 2.05                     | 0.55              |
| 29:3:22:PRO:HG2  | 29:3:25:VAL:HG23  | 1.87                     | 0.55              |
| 1:A:877:G:H3'    | 37:A:9699:HOH:O   | 2.05                     | 0.55              |
| 1:A:1086:A:N6    | 24:X:11:VAL:HG11  | 2.22                     | 0.55              |
| 37:A:8978:HOH:O  | 14:N:94:LYS:HE2   | 2.07                     | 0.55              |
| 2:B:3069:U:OP1   | 15:O:4:PRO:HG3    | 2.05                     | 0.55              |
| 4:D:7:ARG:NH1    | 4:D:11:LEU:CD2    | 2.69                     | 0.55              |
| 18:R:32:GLU:HA   | 18:R:71:TYR:OH    | 2.06                     | 0.55              |
| 24:X:13:MET:HE2  | 24:X:18:GLN:N     | 2.21                     | 0.55              |
| 1:A:1497:G:H4'   | 1:A:1627:G:O2'    | 2.07                     | 0.55              |
| 1:A:1925:G:O2'   | 1:A:1926:G:H5'    | 2.06                     | 0.55              |
| 3:C:105:VAL:HG11 | 3:C:154:ALA:CB    | 2.36                     | 0.55              |
| 6:F:99:ASP:HB3   | 6:F:103:ASN:H     | 1.71                     | 0.55              |
| 14:N:37:VAL:HG13 | 14:N:63:VAL:HG11  | 1.87                     | 0.55              |
| 30:4:69:TYR:CB   | 30:4:78:HIS:CE1   | 2.89                     | 0.55              |
| 1:A:567:U:H5''   | 37:A:5977:HOH:O   | 2.05                     | 0.55              |
| 1:A:1176:C:H1'   | 37:A:3506:HOH:O   | 2.07                     | 0.55              |
| 37:A:4444:HOH:O  | 14:N:174:ARG:HG2  | 2.07                     | 0.55              |
| 16:P:59:VAL:HG23 | 16:P:111:VAL:HG23 | 1.87                     | 0.55              |
| 21:U:48:VAL:HG13 | 21:U:49:GLU:N     | 2.21                     | 0.55              |
| 1:A:317:A:H5''   | 21:U:52:ARG:HD2   | 1.89                     | 0.55              |
| 1:A:1102:C:H2'   | 1:A:1103:C:H6     | 1.72                     | 0.55              |
| 1:A:2291:A:C8    | 1:A:2309:C:H5'    | 2.42                     | 0.55              |
| 8:H:28:ALA:HB3   | 8:H:99:THR:HG23   | 1.89                     | 0.55              |
| 15:O:154:LEU:HG  | 15:O:155:GLU:H    | 1.71                     | 0.55              |
| 20:T:29:ASP:OD1  | 20:T:31:ARG:HG3   | 2.05                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 23:W:39:ALA:N     | 23:W:40:PRO:CD   | 2.69                     | 0.55              |
| 1:A:470:U:O2'     | 28:2:16:HIS:HD2  | 1.89                     | 0.55              |
| 1:A:538:C:OP2     | 26:Z:134:HIS:HE1 | 1.89                     | 0.55              |
| 1:A:814:G:H4'     | 37:A:9719:HOH:O  | 2.05                     | 0.55              |
| 6:F:135:VAL:HG22  | 6:F:136:ARG:N    | 2.21                     | 0.55              |
| 7:G:3:VAL:HG22    | 7:G:49:ILE:HB    | 1.89                     | 0.55              |
| 7:G:11:VAL:CG1    | 7:G:12:ASP:N     | 2.69                     | 0.55              |
| 13:M:77:ALA:HB3   | 37:M:8402:HOH:O  | 2.05                     | 0.55              |
| 15:O:154:LEU:HG   | 15:O:155:GLU:N   | 2.21                     | 0.55              |
| 21:U:48:VAL:HG23  | 21:U:98:VAL:HA   | 1.87                     | 0.55              |
| 24:X:26:ILE:HG13  | 24:X:26:ILE:O    | 2.05                     | 0.55              |
| 25:Y:9:VAL:HG13   | 25:Y:88:GLU:OE2  | 2.06                     | 0.55              |
| 30:4:11:CYS:HB2   | 30:4:20:HIS:CE1  | 2.42                     | 0.55              |
| 1:A:324:G:O2'     | 1:A:325:U:H5'    | 2.07                     | 0.55              |
| 1:A:344:C:H2'     | 1:A:345:G:O4'    | 2.07                     | 0.55              |
| 1:A:2777:G:O2'    | 1:A:2778:A:H5'   | 2.06                     | 0.55              |
| 1:A:2816:A:H5''   | 1:A:2817:G:H5'   | 1.89                     | 0.55              |
| 2:B:3047:A:C2     | 2:B:3048:C:C2    | 2.94                     | 0.55              |
| 4:D:214:PRO:HD2   | 37:D:8522:HOH:O  | 2.06                     | 0.55              |
| 10:J:109:ASP:HB2  | 37:J:8347:HOH:O  | 2.05                     | 0.55              |
| 15:O:184:ILE:HG22 | 15:O:185:GLU:HG3 | 1.88                     | 0.55              |
| 24:X:1:MET:HE3    | 24:X:101:LEU:HA  | 1.87                     | 0.55              |
| 24:X:21:LEU:HD21  | 24:X:48:VAL:HG11 | 1.87                     | 0.55              |
| 1:A:2247:C:H5''   | 37:A:6916:HOH:O  | 2.07                     | 0.55              |
| 1:A:2314:G:C2'    | 1:A:2315:C:H5'   | 2.37                     | 0.55              |
| 1:A:2795:C:O2'    | 1:A:2796:U:H5'   | 2.06                     | 0.55              |
| 3:C:217:ARG:HG2   | 3:C:229:ALA:HB2  | 1.88                     | 0.55              |
| 5:E:77:ALA:O      | 5:E:78:ARG:HG3   | 2.07                     | 0.55              |
| 7:G:93:MET:HE2    | 7:G:107:PHE:CD1  | 2.42                     | 0.55              |
| 23:W:39:ALA:O     | 23:W:41:GLU:N    | 2.40                     | 0.55              |
| 24:X:88:THR:CG2   | 24:X:89:ASP:H    | 2.15                     | 0.55              |
| 26:Z:186:ARG:HG2  | 26:Z:186:ARG:NH1 | 2.21                     | 0.55              |
| 1:A:88:G:H5'      | 1:A:88:G:H8      | 1.71                     | 0.55              |
| 1:A:245:C:H2'     | 1:A:246:G:H5'    | 1.89                     | 0.55              |
| 1:A:1166:A:H61    | 1:A:1180:U:H3    | 1.54                     | 0.55              |
| 1:A:1391:G:C5     | 1:A:1435:U:C4    | 2.95                     | 0.55              |
| 1:A:1909:A:N1     | 1:A:2128:G:H1'   | 2.22                     | 0.55              |
| 1:A:2453:G:H3'    | 37:A:5499:HOH:O  | 2.06                     | 0.55              |
| 2:B:3044:A:O4'    | 6:F:76:ARG:NE    | 2.40                     | 0.55              |
| 10:J:62:GLU:OE2   | 10:J:66:VAL:CG2  | 2.54                     | 0.55              |
| 13:M:73:VAL:HG23  | 13:M:74:THR:H    | 1.70                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:Z:154:ARG:O   | 26:Z:154:ARG:HG2  | 2.07                     | 0.55              |
| 1:A:56:G:H5''    | 23:W:50:ARG:NH1   | 2.22                     | 0.54              |
| 1:A:383:A:H4'    | 37:A:4903:HOH:O   | 2.07                     | 0.54              |
| 1:A:1189:A:H1'   | 1:A:1209:C:O4'    | 2.07                     | 0.54              |
| 1:A:2679:G:H2'   | 1:A:2681:A:OP2    | 2.06                     | 0.54              |
| 37:A:6994:HOH:O  | 21:U:9:LYS:HB2    | 2.06                     | 0.54              |
| 10:J:35:ASN:HD21 | 10:J:80:ASN:HA    | 1.72                     | 0.54              |
| 14:N:59:GLY:HA3  | 14:N:141:ILE:HD12 | 1.89                     | 0.54              |
| 15:O:48:VAL:HG12 | 37:O:8554:HOH:O   | 2.05                     | 0.54              |
| 1:A:602:A:O2'    | 1:A:605:C:H4'     | 2.07                     | 0.54              |
| 1:A:777:U:O2'    | 28:2:11:LYS:HG2   | 2.07                     | 0.54              |
| 1:A:2256:G:H2'   | 1:A:2257:G:C5'    | 2.37                     | 0.54              |
| 6:F:170:TYR:O    | 6:F:171:ASP:HB3   | 2.06                     | 0.54              |
| 10:J:39:GLY:O    | 10:J:41:THR:N     | 2.40                     | 0.54              |
| 10:J:75:SER:O    | 10:J:79:ALA:HB2   | 2.07                     | 0.54              |
| 15:O:155:GLU:O   | 15:O:156:GLU:HG3  | 2.08                     | 0.54              |
| 1:A:542:A:H2'    | 1:A:543:G:O4'     | 2.06                     | 0.54              |
| 1:A:1079:A:N1    | 1:A:2068:G:O2'    | 2.40                     | 0.54              |
| 1:A:1995:G:O2'   | 1:A:1997:A:N7     | 2.40                     | 0.54              |
| 3:C:36:ASP:O     | 3:C:38:ILE:N      | 2.41                     | 0.54              |
| 4:D:82:VAL:O     | 4:D:82:VAL:CG1    | 2.53                     | 0.54              |
| 4:D:238:ASN:ND2  | 4:D:240:GLY:H     | 2.05                     | 0.54              |
| 8:H:46:GLU:OE1   | 8:H:100:ASP:HA    | 2.08                     | 0.54              |
| 10:J:83:PHE:HZ   | 10:J:146:TRP:HE1  | 1.54                     | 0.54              |
| 22:V:14:GLU:OE1  | 22:V:15:PRO:CD    | 2.52                     | 0.54              |
| 1:A:138:U:H5''   | 1:A:139:C:OP2     | 2.08                     | 0.54              |
| 1:A:894:A:C2     | 5:E:87:ARG:NH2    | 2.75                     | 0.54              |
| 1:A:1787:C:OP1   | 17:Q:68:LYS:HE2   | 2.07                     | 0.54              |
| 1:A:2241:C:O2'   | 1:A:2242:U:H5'    | 2.06                     | 0.54              |
| 6:F:11:HIS:C     | 6:F:13:MET:H      | 2.15                     | 0.54              |
| 10:J:5:MET:HG3   | 37:J:8367:HOH:O   | 2.07                     | 0.54              |
| 10:J:85:ILE:HB   | 10:J:132:PHE:CE2  | 2.42                     | 0.54              |
| 19:S:18:LEU:HB2  | 19:S:143:VAL:CG1  | 2.37                     | 0.54              |
| 27:1:58:GLY:CA   | 37:1:8439:HOH:O   | 2.50                     | 0.54              |
| 1:A:396:U:OP2    | 30:4:38:ARG:NH1   | 2.39                     | 0.54              |
| 1:A:1015:C:C2    | 1:A:1016:U:C5     | 2.95                     | 0.54              |
| 1:A:2070:G:H5''  | 37:A:3359:HOH:O   | 2.06                     | 0.54              |
| 4:D:51:VAL:HG23  | 4:D:329:TYR:O     | 2.08                     | 0.54              |
| 6:F:54:ALA:CB    | 6:F:69:ILE:HD12   | 2.37                     | 0.54              |
| 10:J:69:ASN:O    | 10:J:72:VAL:HG12  | 2.07                     | 0.54              |
| 15:O:37:ARG:HD3  | 35:O:8507:CL:CL   | 2.45                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:16:VAL:HG12 | 17:Q:17:GLY:N    | 2.22                     | 0.54              |
| 18:R:25:PRO:HB2  | 37:R:4350:HOH:O  | 2.07                     | 0.54              |
| 1:A:877:G:H5'    | 1:A:878:G:OP1    | 2.07                     | 0.54              |
| 1:A:1299:G:H5'   | 37:A:3648:HOH:O  | 2.08                     | 0.54              |
| 1:A:1505:U:H6    | 1:A:1505:U:H5'   | 1.72                     | 0.54              |
| 1:A:2324:G:H4'   | 1:A:2418:G:O2'   | 2.07                     | 0.54              |
| 1:A:2548:C:OP2   | 4:D:5:ARG:NH2    | 2.39                     | 0.54              |
| 37:A:8936:HOH:O  | 29:3:3:LYS:HE3   | 2.07                     | 0.54              |
| 3:C:223:ARG:HG3  | 37:C:8604:HOH:O  | 2.06                     | 0.54              |
| 6:F:10:PHE:CE1   | 6:F:11:HIS:HB3   | 2.42                     | 0.54              |
| 7:G:15:GLN:NE2   | 7:G:40:VAL:O     | 2.41                     | 0.54              |
| 8:H:100:ASP:O    | 8:H:101:ALA:O    | 2.26                     | 0.54              |
| 15:O:49:THR:CG2  | 15:O:56:ASP:HB2  | 2.36                     | 0.54              |
| 30:4:56:PRO:N    | 37:4:8550:HOH:O  | 2.39                     | 0.54              |
| 1:A:319:A:H4'    | 1:A:338:C:C4     | 2.43                     | 0.54              |
| 1:A:902:G:N7     | 13:M:18:HIS:HD2  | 2.06                     | 0.54              |
| 1:A:1299:G:O6    | 13:M:6:ARG:HD3   | 2.08                     | 0.54              |
| 1:A:2761:A:C4    | 1:A:2763:G:C8    | 2.95                     | 0.54              |
| 1:A:2781:U:C2'   | 1:A:2782:G:H5'   | 2.37                     | 0.54              |
| 4:D:162:MET:CE   | 4:D:308:LEU:HD21 | 2.27                     | 0.54              |
| 17:Q:143:ALA:HA  | 37:Q:5521:HOH:O  | 2.05                     | 0.54              |
| 24:X:38:THR:O    | 24:X:42:ARG:HB2  | 2.08                     | 0.54              |
| 27:1:11:THR:CG2  | 27:1:23:ARG:HB2  | 2.38                     | 0.54              |
| 28:2:28:HIS:CD2  | 28:2:31:LYS:H    | 2.26                     | 0.54              |
| 1:A:669:G:O2'    | 1:A:670:G:H5'    | 2.07                     | 0.54              |
| 1:A:2359:G:N7    | 37:A:3279:HOH:O  | 2.34                     | 0.54              |
| 37:A:6203:HOH:O  | 10:J:150:LYS:HE2 | 2.08                     | 0.54              |
| 4:D:221:GLN:HE22 | 12:L:42:ASN:ND2  | 2.05                     | 0.54              |
| 12:L:132:VAL:C   | 37:L:3160:HOH:O  | 2.51                     | 0.54              |
| 15:O:139:TRP:HA  | 15:O:139:TRP:CE3 | 2.43                     | 0.54              |
| 17:Q:13:VAL:HG21 | 17:Q:41:ARG:HG2  | 1.88                     | 0.54              |
| 17:Q:71:LYS:HG3  | 17:Q:71:LYS:O    | 2.08                     | 0.54              |
| 19:S:106:GLY:HA2 | 19:S:109:MET:CE  | 2.38                     | 0.54              |
| 1:A:1523:G:H2'   | 1:A:1524:U:C6    | 2.43                     | 0.54              |
| 1:A:1641:A:H2'   | 1:A:1642:A:H5'   | 1.89                     | 0.54              |
| 1:A:2270:G:H4'   | 3:C:223:ARG:NH1  | 2.21                     | 0.54              |
| 37:A:9144:HOH:O  | 4:D:267:LYS:HD3  | 2.06                     | 0.54              |
| 3:C:36:ASP:HA    | 3:C:83:GLY:HA3   | 1.90                     | 0.54              |
| 7:G:86:VAL:CG1   | 7:G:129:GLU:HA   | 2.37                     | 0.54              |
| 1:A:714:U:H3'    | 37:A:6516:HOH:O  | 2.07                     | 0.54              |
| 1:A:812:A:H1'    | 37:A:3533:HOH:O  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:2837:U:H1'   | 4:D:307:ARG:HH12  | 1.73                     | 0.54              |
| 5:E:200:PRO:HB3  | 5:E:212:VAL:HG23  | 1.90                     | 0.54              |
| 5:E:236:THR:O    | 5:E:237:GLU:C     | 2.50                     | 0.54              |
| 10:J:26:LYS:HD3  | 10:J:89:PRO:HG3   | 1.90                     | 0.54              |
| 11:K:75:PRO:HG2  | 11:K:105:LEU:HD21 | 1.89                     | 0.54              |
| 26:Z:112:GLU:OE1 | 26:Z:112:GLU:HA   | 2.08                     | 0.54              |
| 28:2:8:GLN:HE22  | 28:2:11:LYS:NZ    | 2.06                     | 0.54              |
| 37:A:7253:HOH:O  | 14:N:154:ARG:HB2  | 2.07                     | 0.53              |
| 10:J:86:ARG:HD3  | 10:J:130:HIS:HD2  | 1.73                     | 0.53              |
| 21:U:32:ARG:NH1  | 21:U:38:ARG:HH12  | 2.06                     | 0.53              |
| 24:X:5:VAL:HG22  | 24:X:32:CYS:HB2   | 1.90                     | 0.53              |
| 29:3:48:ASP:O    | 29:3:49:GLU:HB2   | 2.08                     | 0.53              |
| 30:4:31:THR:HB   | 30:4:33:MET:HE3   | 1.90                     | 0.53              |
| 1:A:485:A:O2'    | 1:A:487:G:H5'     | 2.08                     | 0.53              |
| 1:A:1669:A:H2'   | 1:A:1670:G:C8     | 2.43                     | 0.53              |
| 1:A:2326:U:H4'   | 1:A:2412:G:H4'    | 1.91                     | 0.53              |
| 3:C:100:PRO:HG2  | 3:C:103:VAL:CG2   | 2.35                     | 0.53              |
| 3:C:171:LYS:NZ   | 37:C:8527:HOH:O   | 2.41                     | 0.53              |
| 3:C:191:GLY:HA2  | 3:C:194:MET:CE    | 2.36                     | 0.53              |
| 5:E:115:LEU:O    | 5:E:118:THR:HB    | 2.07                     | 0.53              |
| 7:G:31:ARG:HH12  | 7:G:68:HIS:CE1    | 2.27                     | 0.53              |
| 7:G:79:GLY:HA3   | 37:G:7046:HOH:O   | 2.08                     | 0.53              |
| 12:L:30:LYS:O    | 12:L:55:VAL:HG13  | 2.08                     | 0.53              |
| 16:P:21:SER:OG   | 16:P:106:PRO:HB2  | 2.08                     | 0.53              |
| 22:V:6:CYS:O     | 22:V:8:TYR:N      | 2.41                     | 0.53              |
| 24:X:21:LEU:HD21 | 24:X:48:VAL:CG1   | 2.39                     | 0.53              |
| 24:X:76:ASP:O    | 24:X:77:ALA:C     | 2.51                     | 0.53              |
| 27:1:57:CYS:SG   | 27:1:59:HIS:HB3   | 2.48                     | 0.53              |
| 1:A:779:U:H5'    | 1:A:1836:A:C2     | 2.42                     | 0.53              |
| 1:A:2001:G:O2'   | 1:A:2002:C:H5'    | 2.09                     | 0.53              |
| 1:A:2251:G:H2'   | 1:A:2252:A:C8     | 2.44                     | 0.53              |
| 1:A:2359:G:H3'   | 37:A:5266:HOH:O   | 2.08                     | 0.53              |
| 1:A:2755:G:H1'   | 37:A:4258:HOH:O   | 2.08                     | 0.53              |
| 1:A:2780:C:H2'   | 1:A:2781:U:C6     | 2.44                     | 0.53              |
| 7:G:22:VAL:O     | 7:G:28:SER:HA     | 2.08                     | 0.53              |
| 12:L:48:GLY:C    | 37:L:5632:HOH:O   | 2.50                     | 0.53              |
| 22:V:8:TYR:OH    | 37:V:3805:HOH:O   | 2.18                     | 0.53              |
| 24:X:4:LEU:O     | 24:X:32:CYS:HA    | 2.09                     | 0.53              |
| 1:A:316:A:N3     | 1:A:336:G:O2'     | 2.40                     | 0.53              |
| 1:A:1097:A:H5''  | 24:X:125:HIS:CE1  | 2.43                     | 0.53              |
| 1:A:2314:G:H2'   | 1:A:2315:C:H5'    | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:2656:G:O2'   | 1:A:2657:G:H5'    | 2.09                     | 0.53              |
| 5:E:47:GLY:HA2   | 5:E:92:PRO:HB2    | 1.89                     | 0.53              |
| 5:E:133:ARG:HD2  | 37:E:8406:HOH:O   | 2.08                     | 0.53              |
| 5:E:162:VAL:HG12 | 5:E:192:ILE:HD11  | 1.89                     | 0.53              |
| 5:E:162:VAL:HG13 | 5:E:232:LEU:HD21  | 1.90                     | 0.53              |
| 7:G:31:ARG:HH12  | 7:G:68:HIS:CG     | 2.26                     | 0.53              |
| 10:J:46:VAL:O    | 10:J:146:TRP:HH2  | 1.91                     | 0.53              |
| 15:O:90:LEU:HB2  | 15:O:186:LEU:HD22 | 1.90                     | 0.53              |
| 19:S:39:THR:HB   | 19:S:42:GLU:CD    | 2.33                     | 0.53              |
| 1:A:257:G:O2'    | 1:A:258:G:H5'     | 2.08                     | 0.53              |
| 1:A:1654:U:H2'   | 3:C:47:HIS:CD2    | 2.44                     | 0.53              |
| 3:C:109:GLU:HG2  | 3:C:116:GLY:N     | 2.23                     | 0.53              |
| 6:F:154:LYS:H    | 6:F:154:LYS:CD    | 2.15                     | 0.53              |
| 7:G:11:VAL:HG13  | 7:G:23:GLU:O      | 2.08                     | 0.53              |
| 27:1:13:ARG:NH1  | 27:1:14:PHE:CZ    | 2.77                     | 0.53              |
| 1:A:272:A:H5'    | 1:A:273:G:OP2     | 2.09                     | 0.53              |
| 1:A:315:G:C6     | 1:A:316:A:C6      | 2.96                     | 0.53              |
| 1:A:1873:G:H2'   | 1:A:1874:U:H5'    | 1.90                     | 0.53              |
| 6:F:38:GLU:HB3   | 6:F:49:PRO:HG2    | 1.91                     | 0.53              |
| 24:X:122:ARG:HG2 | 24:X:122:ARG:NH1  | 2.23                     | 0.53              |
| 24:X:129:LYS:HG2 | 37:X:1990:HOH:O   | 2.09                     | 0.53              |
| 25:Y:51:ASP:OD2  | 25:Y:52:PRO:HD2   | 2.08                     | 0.53              |
| 27:1:42:CYS:SG   | 27:1:44:PHE:HB2   | 2.48                     | 0.53              |
| 1:A:474:C:O3'    | 5:E:73:LEU:HD21   | 2.09                     | 0.53              |
| 1:A:660:A:H4'    | 1:A:661:G:O5'     | 2.09                     | 0.53              |
| 1:A:1495:C:H1'   | 1:A:1573:A:H1'    | 1.91                     | 0.53              |
| 1:A:1778:A:H2'   | 1:A:1779:A:H5'    | 1.91                     | 0.53              |
| 5:E:127:ARG:HG2  | 5:E:127:ARG:NH1   | 2.23                     | 0.53              |
| 37:E:8356:HOH:O  | 16:P:3:THR:HG21   | 2.08                     | 0.53              |
| 8:H:47:LEU:HB2   | 8:H:108:LEU:HD11  | 1.91                     | 0.53              |
| 10:J:130:HIS:CG  | 10:J:133:ILE:HD11 | 2.43                     | 0.53              |
| 16:P:25:VAL:HG23 | 16:P:26:TRP:H     | 1.74                     | 0.53              |
| 27:1:38:LYS:HE2  | 27:1:45:LYS:CE    | 2.34                     | 0.53              |
| 27:1:77:LYS:HA   | 27:1:80:MET:HE2   | 1.91                     | 0.53              |
| 30:4:55:VAL:HB   | 30:4:56:PRO:HD2   | 1.91                     | 0.53              |
| 1:A:407:A:H5'    | 37:A:5603:HOH:O   | 2.07                     | 0.53              |
| 1:A:1097:A:H5''  | 24:X:125:HIS:NE2  | 2.24                     | 0.53              |
| 1:A:1168:C:H2'   | 1:A:1169:U:O4'    | 2.08                     | 0.53              |
| 1:A:1477:C:H5'   | 1:A:1868:G:C5'    | 2.39                     | 0.53              |
| 1:A:1666:C:C2'   | 1:A:1667:A:C5'    | 2.87                     | 0.53              |
| 3:C:1:GLY:HA2    | 3:C:197:VAL:HG23  | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:N:67:ILE:CD1  | 14:N:104:ARG:HD2  | 2.39                     | 0.53              |
| 25:Y:43:VAL:CG1  | 25:Y:47:ALA:HB3   | 2.38                     | 0.53              |
| 1:A:289:G:N2     | 1:A:363:A:H2      | 2.04                     | 0.53              |
| 1:A:628:A:C8     | 1:A:2071:C:N4     | 2.77                     | 0.53              |
| 1:A:1164:U:C4'   | 1:A:1165:G:OP1    | 2.52                     | 0.53              |
| 1:A:2064:U:H5'   | 1:A:2652:U:H4'    | 1.90                     | 0.53              |
| 1:A:2613:G:O2'   | 1:A:2614:C:H5'    | 2.09                     | 0.53              |
| 37:A:3421:HOH:O  | 10:J:11:LYS:HE2   | 2.08                     | 0.53              |
| 37:A:8903:HOH:O  | 27:1:16:PRO:HG3   | 2.07                     | 0.53              |
| 4:D:320:GLN:HG3  | 4:D:321:PRO:HD2   | 1.90                     | 0.53              |
| 5:E:51:TYR:CE2   | 28:2:53:LYS:HB3   | 2.44                     | 0.53              |
| 7:G:7:ILE:HD11   | 7:G:11:VAL:O      | 2.07                     | 0.53              |
| 7:G:31:ARG:HH12  | 7:G:68:HIS:CD2    | 2.27                     | 0.53              |
| 8:H:22:VAL:HG21  | 8:H:104:ALA:HB2   | 1.90                     | 0.53              |
| 11:K:107:ASN:C   | 11:K:107:ASN:HD22 | 2.17                     | 0.53              |
| 15:O:182:GLY:N   | 37:O:8571:HOH:O   | 2.41                     | 0.53              |
| 23:W:57:LYS:HA   | 23:W:60:GLN:HE21  | 1.73                     | 0.53              |
| 28:2:25:LYS:HE2  | 37:3:7213:HOH:O   | 2.09                     | 0.53              |
| 1:A:1589:G:N2    | 1:A:1605:G:H1'    | 2.24                     | 0.53              |
| 1:A:2779:G:H1'   | 37:A:5684:HOH:O   | 2.09                     | 0.53              |
| 4:D:119:HIS:O    | 4:D:121:PRO:HD3   | 2.08                     | 0.53              |
| 10:J:139:ASP:N   | 10:J:140:PRO:CD   | 2.71                     | 0.53              |
| 21:U:6:LYS:NZ    | 37:U:644:HOH:O    | 2.42                     | 0.53              |
| 1:A:92:G:H4'     | 23:W:44:GLY:HA3   | 1.90                     | 0.52              |
| 1:A:830:G:O2'    | 1:A:831:U:H5'     | 2.09                     | 0.52              |
| 1:A:1500:U:P     | 17:Q:41:ARG:HH22  | 2.31                     | 0.52              |
| 1:A:1783:A:O2'   | 1:A:1784:U:H5'    | 2.09                     | 0.52              |
| 1:A:2271:G:H2'   | 1:A:2271:G:N3     | 2.24                     | 0.52              |
| 37:A:4405:HOH:O  | 11:K:47:THR:CB    | 2.55                     | 0.52              |
| 12:L:32:ILE:HD11 | 12:L:56:SER:HB3   | 1.90                     | 0.52              |
| 14:N:35:PRO:HD2  | 14:N:38:VAL:HG21  | 1.91                     | 0.52              |
| 14:N:149:TRP:O   | 14:N:152:ARG:HG2  | 2.09                     | 0.52              |
| 24:X:26:ILE:O    | 24:X:26:ILE:CG1   | 2.56                     | 0.52              |
| 25:Y:78:GLU:HG2  | 25:Y:79:GLU:N     | 2.17                     | 0.52              |
| 1:A:2435:U:H1'   | 37:A:5006:HOH:O   | 2.09                     | 0.52              |
| 4:D:24:PRO:CG    | 4:D:204:GLY:HA2   | 2.39                     | 0.52              |
| 4:D:274:GLU:HA   | 4:D:292:GLY:O     | 2.08                     | 0.52              |
| 4:D:304:PRO:HD2  | 4:D:307:ARG:HD2   | 1.92                     | 0.52              |
| 10:J:150:LYS:HA  | 10:J:153:VAL:HG22 | 1.91                     | 0.52              |
| 12:L:34:VAL:CG2  | 12:L:47:ALA:HB2   | 2.40                     | 0.52              |
| 12:L:125:ALA:C   | 12:L:127:ALA:H    | 2.17                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:S:39:THR:O    | 19:S:40:ALA:C     | 2.51                     | 0.52              |
| 27:1:30:GLU:HA   | 27:1:33:HIS:CB    | 2.40                     | 0.52              |
| 1:A:682:A:H3'    | 1:A:683:G:H8      | 1.74                     | 0.52              |
| 1:A:1527:A:H1'   | 1:A:1528:A:C8     | 2.44                     | 0.52              |
| 4:D:74:ILE:HD13  | 4:D:309:VAL:HG21  | 1.91                     | 0.52              |
| 5:E:234:VAL:HG22 | 5:E:234:VAL:O     | 2.08                     | 0.52              |
| 12:L:9:THR:O     | 12:L:10:GLN:C     | 2.50                     | 0.52              |
| 14:N:164:THR:HB  | 37:N:8519:HOH:O   | 2.10                     | 0.52              |
| 20:T:32:ALA:HA   | 20:T:36:GLU:OE1   | 2.09                     | 0.52              |
| 24:X:13:MET:HE2  | 24:X:18:GLN:CA    | 2.39                     | 0.52              |
| 24:X:38:THR:HG22 | 24:X:39:ASP:N     | 2.25                     | 0.52              |
| 1:A:259:G:H21    | 14:N:58:GLN:NE2   | 2.06                     | 0.52              |
| 1:A:1268:C:O2'   | 26:Z:169:ARG:HB2  | 2.08                     | 0.52              |
| 5:E:16:VAL:HG12  | 5:E:17:ASP:H      | 1.73                     | 0.52              |
| 5:E:129:HIS:HD2  | 5:E:165:ASP:OD2   | 1.91                     | 0.52              |
| 8:H:46:GLU:N     | 37:H:3461:HOH:O   | 2.43                     | 0.52              |
| 15:O:167:ASP:O   | 15:O:168:LEU:HD23 | 2.10                     | 0.52              |
| 15:O:180:LEU:O   | 15:O:181:ASP:HB3  | 2.08                     | 0.52              |
| 28:2:28:HIS:CD2  | 28:2:30:LYS:HB2   | 2.44                     | 0.52              |
| 1:A:1855:G:H8    | 3:C:144:GLU:OE2   | 1.93                     | 0.52              |
| 1:A:2082:G:O2'   | 1:A:2083:A:H5'    | 2.08                     | 0.52              |
| 24:X:141:HIS:HB2 | 24:X:146:ILE:HG12 | 1.90                     | 0.52              |
| 1:A:51:G:O2'     | 1:A:52:A:H5'      | 2.10                     | 0.52              |
| 1:A:119:A:H2'    | 1:A:120:A:H5''    | 1.91                     | 0.52              |
| 1:A:962:C:C1'    | 15:O:5:ARG:NH1    | 2.65                     | 0.52              |
| 1:A:1819:G:H5'   | 37:A:4285:HOH:O   | 2.10                     | 0.52              |
| 1:A:2769:C:O2'   | 1:A:2770:G:H5'    | 2.09                     | 0.52              |
| 37:E:8364:HOH:O  | 21:U:2:LYS:HE2    | 2.09                     | 0.52              |
| 6:F:10:PHE:CG    | 6:F:11:HIS:N      | 2.77                     | 0.52              |
| 10:J:71:TYR:C    | 10:J:73:GLN:N     | 2.66                     | 0.52              |
| 14:N:154:ARG:HD3 | 37:N:8640:HOH:O   | 2.10                     | 0.52              |
| 21:U:12:ARG:NH1  | 37:U:3035:HOH:O   | 2.42                     | 0.52              |
| 24:X:13:MET:CE   | 24:X:17:ILE:HG22  | 2.40                     | 0.52              |
| 24:X:125:HIS:HD2 | 24:X:127:GLY:H    | 1.57                     | 0.52              |
| 25:Y:18:ARG:NH1  | 37:Y:4132:HOH:O   | 2.41                     | 0.52              |
| 1:A:1127:C:C2'   | 1:A:1128:U:H5'    | 2.40                     | 0.52              |
| 1:A:1562:C:O2    | 1:A:1562:C:H2'    | 2.10                     | 0.52              |
| 1:A:1666:C:H2'   | 1:A:1667:A:C5'    | 2.40                     | 0.52              |
| 1:A:1934:A:C8    | 1:A:1935:C:C5     | 2.97                     | 0.52              |
| 1:A:1947:G:N2    | 1:A:1966:U:C2     | 2.78                     | 0.52              |
| 1:A:2604:A:H5'   | 37:A:5367:HOH:O   | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2718:C:H6     | 1:A:2718:C:H5'    | 1.75                     | 0.52              |
| 1:A:2781:U:H2'    | 1:A:2782:G:H5'    | 1.91                     | 0.52              |
| 6:F:84:LEU:C      | 6:F:86:THR:H      | 2.18                     | 0.52              |
| 7:G:84:MET:HE2    | 7:G:133:VAL:HG21  | 1.91                     | 0.52              |
| 11:K:142:ASN:O    | 11:K:144:THR:N    | 2.43                     | 0.52              |
| 14:N:37:VAL:CG1   | 14:N:63:VAL:HG11  | 2.40                     | 0.52              |
| 15:O:48:VAL:HG11  | 15:O:55:ASP:HB3   | 1.89                     | 0.52              |
| 20:T:29:ASP:CG    | 20:T:31:ARG:NH1   | 2.68                     | 0.52              |
| 24:X:122:ARG:HG2  | 24:X:152:ALA:O    | 2.09                     | 0.52              |
| 1:A:818:A:O2'     | 27:1:13:ARG:HD3   | 2.10                     | 0.52              |
| 1:A:1118:A:H8     | 1:A:1119:G:H5''   | 1.75                     | 0.52              |
| 1:A:1470:A:OP1    | 14:N:93:ARG:HD2   | 2.10                     | 0.52              |
| 1:A:1942:A:O2'    | 1:A:1943:C:H5'    | 2.10                     | 0.52              |
| 37:A:3640:HOH:O   | 4:D:27:ASN:HB2    | 2.10                     | 0.52              |
| 3:C:51:ARG:NH2    | 37:C:8609:HOH:O   | 2.42                     | 0.52              |
| 3:C:211:LYS:HB3   | 3:C:212:PRO:CD    | 2.33                     | 0.52              |
| 5:E:214:THR:HB    | 37:E:8325:HOH:O   | 2.10                     | 0.52              |
| 5:E:233:THR:CG2   | 5:E:234:VAL:N     | 2.73                     | 0.52              |
| 10:J:62:GLU:OE2   | 10:J:66:VAL:HG23  | 2.09                     | 0.52              |
| 15:O:11:ARG:HG3   | 15:O:14:ARG:NH1   | 2.24                     | 0.52              |
| 17:Q:18:LYS:O     | 17:Q:21:VAL:HG22  | 2.09                     | 0.52              |
| 26:Z:126:PRO:HG2  | 26:Z:128:PHE:CZ   | 2.44                     | 0.52              |
| 1:A:67:A:H5''     | 1:A:69:A:C8       | 2.45                     | 0.52              |
| 1:A:1333:U:H2'    | 1:A:1334:C:H6     | 1.75                     | 0.52              |
| 1:A:2862:G:H4'    | 4:D:336:GLN:O     | 2.10                     | 0.52              |
| 3:C:97:ALA:HB2    | 3:C:150:PRO:HB2   | 1.91                     | 0.52              |
| 4:D:27:ASN:HB3    | 37:D:8630:HOH:O   | 2.08                     | 0.52              |
| 6:F:58:VAL:HG12   | 6:F:59:GLY:N      | 2.25                     | 0.52              |
| 8:H:58:GLU:HA     | 8:H:61:MET:HG3    | 1.92                     | 0.52              |
| 10:J:28:ILE:HA    | 10:J:62:GLU:OE1   | 2.10                     | 0.52              |
| 10:J:129:ASN:HD22 | 10:J:129:ASN:N    | 2.08                     | 0.52              |
| 12:L:34:VAL:HG22  | 12:L:47:ALA:HB2   | 1.91                     | 0.52              |
| 21:U:38:ARG:HH11  | 21:U:38:ARG:HG3   | 1.74                     | 0.52              |
| 22:V:34:SER:O     | 22:V:38:ASN:ND2   | 2.42                     | 0.52              |
| 24:X:142:ASP:HB3  | 24:X:145:GLY:H    | 1.73                     | 0.52              |
| 25:Y:72:VAL:HG22  | 25:Y:85:VAL:CG1   | 2.38                     | 0.52              |
| 26:Z:185:VAL:HA   | 37:Z:8152:HOH:O   | 2.08                     | 0.52              |
| 1:A:183:A:H5'     | 14:N:157:LEU:HD12 | 1.92                     | 0.52              |
| 1:A:290:C:O2'     | 1:A:291:C:H5'     | 2.10                     | 0.52              |
| 1:A:1209:C:C2     | 1:A:1210:G:C8     | 2.97                     | 0.52              |
| 1:A:2044:G:OP1    | 25:Y:23:HIS:CE1   | 2.60                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2329:C:O2'    | 1:A:2330:U:H5'    | 2.10                     | 0.52              |
| 9:I:12:ILE:HG22   | 9:I:12:ILE:O      | 2.08                     | 0.52              |
| 10:J:46:VAL:HG12  | 10:J:146:TRP:CZ3  | 2.43                     | 0.52              |
| 37:L:7438:HOH:O   | 22:V:20:MET:HE1   | 2.10                     | 0.52              |
| 15:O:159:TYR:HE2  | 15:O:163:PHE:HE2  | 1.58                     | 0.52              |
| 19:S:132:ARG:CZ   | 37:S:8587:HOH:O   | 2.58                     | 0.52              |
| 1:A:245:C:C2'     | 1:A:246:G:H5'     | 2.40                     | 0.51              |
| 1:A:329:A:OP2     | 5:E:206:ASN:HB2   | 2.09                     | 0.51              |
| 1:A:431:G:P       | 14:N:48:ARG:HH12  | 2.34                     | 0.51              |
| 1:A:644:G:N3      | 1:A:644:G:H5'     | 2.24                     | 0.51              |
| 1:A:684:G:H2'     | 1:A:685:C:C6      | 2.45                     | 0.51              |
| 1:A:920:C:H5'     | 1:A:921:G:C4      | 2.45                     | 0.51              |
| 1:A:1120:U:H5''   | 1:A:1120:U:H6     | 1.75                     | 0.51              |
| 1:A:1973:A:H5'    | 1:A:1973:A:C8     | 2.43                     | 0.51              |
| 1:A:2779:G:O2'    | 1:A:2780:C:H5'    | 2.10                     | 0.51              |
| 6:F:99:ASP:CB     | 6:F:103:ASN:HB2   | 2.39                     | 0.51              |
| 10:J:56:ILE:HG22  | 10:J:61:LEU:HD22  | 1.91                     | 0.51              |
| 18:R:16:ASN:ND2   | 18:R:45:PRO:HG2   | 2.25                     | 0.51              |
| 23:W:27:LEU:O     | 23:W:30:ALA:N     | 2.43                     | 0.51              |
| 24:X:31:HIS:HB3   | 37:X:5420:HOH:O   | 2.10                     | 0.51              |
| 24:X:88:THR:CG2   | 24:X:89:ASP:N     | 2.72                     | 0.51              |
| 1:A:1123:A:C6     | 1:A:1238:C:H5'    | 2.45                     | 0.51              |
| 1:A:1654:U:H2'    | 3:C:47:HIS:HD2    | 1.74                     | 0.51              |
| 1:A:1717:A:H5''   | 17:Q:54:LYS:HB2   | 1.93                     | 0.51              |
| 1:A:2894:C:O2'    | 1:A:2895:C:H5'    | 2.09                     | 0.51              |
| 7:G:11:VAL:HG12   | 7:G:12:ASP:H      | 1.75                     | 0.51              |
| 14:N:186:SER:O    | 14:N:189:VAL:HG12 | 2.10                     | 0.51              |
| 22:V:52:THR:HG22  | 22:V:54:THR:HB    | 1.93                     | 0.51              |
| 24:X:42:ARG:O     | 24:X:45:VAL:HG22  | 2.10                     | 0.51              |
| 24:X:122:ARG:HH22 | 24:X:154:ARG:C    | 2.18                     | 0.51              |
| 26:Z:144:ARG:CZ   | 37:Z:8197:HOH:O   | 2.59                     | 0.51              |
| 1:A:92:G:H5'      | 37:W:7247:HOH:O   | 2.10                     | 0.51              |
| 1:A:319:A:H4'     | 1:A:338:C:C5      | 2.46                     | 0.51              |
| 1:A:331:A:C6      | 1:A:332:G:C4      | 2.97                     | 0.51              |
| 4:D:217:ARG:HG3   | 4:D:257:THR:HG22  | 1.91                     | 0.51              |
| 4:D:231:GLY:N     | 37:D:8524:HOH:O   | 2.35                     | 0.51              |
| 13:M:104:ASP:HB3  | 37:M:8437:HOH:O   | 2.09                     | 0.51              |
| 14:N:173:LEU:HD23 | 14:N:183:VAL:HG12 | 1.92                     | 0.51              |
| 26:Z:144:ARG:HH11 | 26:Z:144:ARG:HG3  | 1.75                     | 0.51              |
| 1:A:1189:A:H1'    | 1:A:1209:C:H1'    | 1.93                     | 0.51              |
| 1:A:1595:G:O2'    | 1:A:1596:U:H5'    | 2.11                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:3049:G:H2'    | 2:B:3050:G:O4'   | 2.10                     | 0.51              |
| 3:C:170:VAL:HG22  | 27:1:22:ILE:HG23 | 1.92                     | 0.51              |
| 6:F:23:VAL:O      | 6:F:23:VAL:CG2   | 2.58                     | 0.51              |
| 14:N:77:PHE:HD2   | 37:N:8527:HOH:O  | 1.94                     | 0.51              |
| 15:O:143:ARG:HH12 | 15:O:173:ASP:CG  | 2.18                     | 0.51              |
| 17:Q:94:TRP:CZ2   | 17:Q:98:ILE:HG13 | 2.46                     | 0.51              |
| 19:S:39:THR:HG22  | 19:S:42:GLU:H    | 1.74                     | 0.51              |
| 21:U:55:PHE:CD2   | 21:U:77:VAL:HG13 | 2.46                     | 0.51              |
| 1:A:2764:C:H2'    | 1:A:2765:C:H6    | 1.74                     | 0.51              |
| 8:H:16:ALA:HA     | 8:H:111:ILE:HD13 | 1.92                     | 0.51              |
| 10:J:14:TYR:N     | 10:J:91:HIS:CE1  | 2.79                     | 0.51              |
| 10:J:75:SER:HB3   | 10:J:79:ALA:HB1  | 1.92                     | 0.51              |
| 13:M:17:SER:C     | 13:M:19:LYS:H    | 2.18                     | 0.51              |
| 14:N:48:ARG:NH2   | 37:N:8562:HOH:O  | 2.42                     | 0.51              |
| 15:O:73:ALA:N     | 37:O:8567:HOH:O  | 2.44                     | 0.51              |
| 21:U:49:GLU:OE2   | 21:U:97:ARG:HD2  | 2.11                     | 0.51              |
| 23:W:64:GLY:O     | 23:W:65:ASP:CB   | 2.56                     | 0.51              |
| 28:2:28:HIS:CE1   | 28:2:31:LYS:HE2  | 2.45                     | 0.51              |
| 1:A:907:A:H2'     | 1:A:908:A:H8     | 1.76                     | 0.51              |
| 3:C:69:LEU:C      | 3:C:69:LEU:HD12  | 2.34                     | 0.51              |
| 3:C:129:LEU:CD1   | 3:C:145:MET:HE1  | 2.41                     | 0.51              |
| 4:D:76:THR:N      | 4:D:77:PRO:HD3   | 2.26                     | 0.51              |
| 4:D:215:VAL:HA    | 4:D:220:VAL:HG22 | 1.93                     | 0.51              |
| 6:F:10:PHE:CD1    | 6:F:11:HIS:N     | 2.78                     | 0.51              |
| 12:L:101:ASN:HB3  | 37:L:6456:HOH:O  | 2.11                     | 0.51              |
| 13:M:101:ASP:C    | 13:M:103:ALA:H   | 2.17                     | 0.51              |
| 14:N:43:PRO:HG3   | 14:N:62:VAL:HG21 | 1.93                     | 0.51              |
| 14:N:106:ASN:ND2  | 35:N:8518:CL:CL  | 2.81                     | 0.51              |
| 15:O:47:LEU:HD12  | 15:O:92:ALA:HB1  | 1.92                     | 0.51              |
| 1:A:113:A:OP2     | 1:A:114:A:H2'    | 2.11                     | 0.51              |
| 1:A:1132:A:N6     | 1:A:1229:C:H2'   | 2.26                     | 0.51              |
| 1:A:2044:G:C6     | 1:A:2045:G:C5    | 2.98                     | 0.51              |
| 1:A:2392:C:H4'    | 37:R:2875:HOH:O  | 2.10                     | 0.51              |
| 3:C:105:VAL:CG1   | 3:C:106:CYS:N    | 2.74                     | 0.51              |
| 8:H:107:VAL:O     | 8:H:111:ILE:HG13 | 2.10                     | 0.51              |
| 8:H:117:GLU:C     | 8:H:119:ARG:H    | 2.19                     | 0.51              |
| 14:N:45:ARG:CZ    | 14:N:48:ARG:HG3  | 2.41                     | 0.51              |
| 14:N:122:GLU:OE2  | 14:N:127:LYS:HE2 | 2.11                     | 0.51              |
| 19:S:33:ARG:NH1   | 37:S:8544:HOH:O  | 2.44                     | 0.51              |
| 26:Z:172:THR:HG22 | 26:Z:173:ALA:N   | 2.25                     | 0.51              |
| 1:A:558:C:C2'     | 1:A:559:U:C5'    | 2.89                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1192:A:H3'    | 1:A:1193:A:H5'   | 1.91                     | 0.51              |
| 1:A:1804:A:H2'    | 1:A:1805:G:C8    | 2.44                     | 0.51              |
| 37:A:3804:HOH:O   | 29:3:38:LYS:HE3  | 2.11                     | 0.51              |
| 37:A:5104:HOH:O   | 14:N:58:GLN:HG3  | 2.10                     | 0.51              |
| 2:B:3042:C:H2'    | 37:B:8500:HOH:O  | 2.10                     | 0.51              |
| 4:D:82:VAL:HG12   | 4:D:101:TRP:CE3  | 2.46                     | 0.51              |
| 4:D:243:ASN:HA    | 4:D:244:PRO:C    | 2.36                     | 0.51              |
| 18:R:66:LYS:HB2   | 18:R:70:ALA:O    | 2.11                     | 0.51              |
| 21:U:48:VAL:CG2   | 21:U:98:VAL:HA   | 2.40                     | 0.51              |
| 22:V:31:PHE:CE2   | 22:V:37:GLU:HA   | 2.46                     | 0.51              |
| 27:1:59:HIS:HA    | 37:1:8441:HOH:O  | 2.09                     | 0.51              |
| 1:A:154:C:H2'     | 1:A:155:C:H6     | 1.76                     | 0.51              |
| 1:A:1477:C:O2'    | 1:A:1478:U:H5'   | 2.11                     | 0.51              |
| 1:A:1940:C:H4'    | 37:A:6918:HOH:O  | 2.10                     | 0.51              |
| 1:A:2866:U:H4'    | 1:A:2867:G:H5'   | 1.92                     | 0.51              |
| 37:B:8519:HOH:O   | 15:O:107:ASN:HB3 | 2.10                     | 0.51              |
| 4:D:7:ARG:CD      | 4:D:9:GLY:O      | 2.59                     | 0.51              |
| 9:I:64:ASN:O      | 9:I:68:GLU:HG3   | 2.11                     | 0.51              |
| 10:J:65:ARG:HB3   | 37:J:8387:HOH:O  | 2.10                     | 0.51              |
| 10:J:65:ARG:NH1   | 37:J:8387:HOH:O  | 2.44                     | 0.51              |
| 11:K:130:VAL:HG12 | 11:K:131:THR:N   | 2.26                     | 0.51              |
| 21:U:24:ARG:HH21  | 21:U:39:ASN:ND2  | 2.08                     | 0.51              |
| 22:V:9:CYS:CA     | 22:V:52:THR:HG23 | 2.40                     | 0.51              |
| 24:X:125:HIS:CD2  | 24:X:127:GLY:H   | 2.29                     | 0.51              |
| 1:A:790:A:H1'     | 1:A:1710:A:H2'   | 1.93                     | 0.51              |
| 1:A:1847:A:OP1    | 3:C:175:LYS:NZ   | 2.42                     | 0.51              |
| 1:A:2712:G:OP1    | 12:L:43:ARG:NH1  | 2.43                     | 0.51              |
| 1:A:2832:C:H5     | 37:A:6784:HOH:O  | 1.94                     | 0.51              |
| 4:D:305:ASP:O     | 4:D:306:LYS:CB   | 2.58                     | 0.51              |
| 6:F:57:THR:HG23   | 6:F:63:ILE:CB    | 2.41                     | 0.51              |
| 6:F:102:GLY:O     | 6:F:134:LEU:HD12 | 2.11                     | 0.51              |
| 8:H:50:VAL:CG2    | 8:H:63:ILE:HG21  | 2.40                     | 0.51              |
| 19:S:47:LEU:O     | 19:S:51:ILE:HG13 | 2.09                     | 0.51              |
| 25:Y:26:ALA:HB1   | 25:Y:59:TRP:CE2  | 2.45                     | 0.51              |
| 27:1:46:LYS:O     | 27:1:57:CYS:HA   | 2.10                     | 0.51              |
| 1:A:256:C:H2'     | 1:A:257:G:O4'    | 2.11                     | 0.50              |
| 1:A:1174:A:C5     | 1:A:1201:C:H4'   | 2.46                     | 0.50              |
| 4:D:7:ARG:HD3     | 4:D:9:GLY:O      | 2.12                     | 0.50              |
| 4:D:238:ASN:HD22  | 4:D:240:GLY:N    | 2.06                     | 0.50              |
| 6:F:53:LYS:HA     | 6:F:67:ASP:O     | 2.11                     | 0.50              |
| 11:K:131:THR:HG22 | 11:K:133:GLY:N   | 2.26                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:143:THR:CG2 | 13:M:144:ASP:H    | 2.23                     | 0.50              |
| 17:Q:98:ILE:HD12 | 17:Q:102:ARG:NE   | 2.26                     | 0.50              |
| 1:A:338:C:H4'    | 5:E:174:ILE:CD1   | 2.41                     | 0.50              |
| 1:A:1060:C:H6    | 1:A:1060:C:H5'    | 1.76                     | 0.50              |
| 1:A:2781:U:H1'   | 7:G:139:GLU:OE2   | 2.11                     | 0.50              |
| 37:A:5771:HOH:O  | 29:3:44:ARG:HG2   | 2.10                     | 0.50              |
| 2:B:3055:U:H4'   | 2:B:3056:A:C8     | 2.46                     | 0.50              |
| 3:C:88:ILE:HD13  | 3:C:100:PRO:CD    | 2.36                     | 0.50              |
| 7:G:21:THR:HG23  | 7:G:30:THR:OG1    | 2.11                     | 0.50              |
| 7:G:93:MET:HE1   | 7:G:165:GLY:H     | 1.76                     | 0.50              |
| 13:M:73:VAL:HG23 | 13:M:74:THR:N     | 2.25                     | 0.50              |
| 15:O:163:PHE:HA  | 37:O:8519:HOH:O   | 2.10                     | 0.50              |
| 20:T:57:THR:C    | 20:T:59:ASP:H     | 2.19                     | 0.50              |
| 24:X:106:THR:OG1 | 24:X:109:GLU:HG3  | 2.11                     | 0.50              |
| 24:X:122:ARG:CG  | 24:X:152:ALA:O    | 2.59                     | 0.50              |
| 1:A:639:A:H2'    | 1:A:640:G:C8      | 2.45                     | 0.50              |
| 1:A:920:C:H4'    | 1:A:921:G:C2      | 2.46                     | 0.50              |
| 1:A:1116:U:H3    | 1:A:1246:A:N6     | 2.01                     | 0.50              |
| 1:A:1139:U:H2'   | 1:A:1140:C:C6     | 2.46                     | 0.50              |
| 1:A:1162:G:H2'   | 37:A:6156:HOH:O   | 2.11                     | 0.50              |
| 1:A:2365:G:H4'   | 18:R:45:PRO:O     | 2.11                     | 0.50              |
| 5:E:107:ARG:HH11 | 5:E:107:ARG:CB    | 2.24                     | 0.50              |
| 8:H:107:VAL:HG23 | 37:H:6617:HOH:O   | 2.11                     | 0.50              |
| 1:A:125:U:H2'    | 37:A:3346:HOH:O   | 2.11                     | 0.50              |
| 1:A:710:G:OP1    | 16:P:24:ALA:HB3   | 2.12                     | 0.50              |
| 4:D:54:VAL:HB    | 37:D:8614:HOH:O   | 2.11                     | 0.50              |
| 4:D:275:GLY:O    | 4:D:291:ASP:HA    | 2.11                     | 0.50              |
| 6:F:27:ILE:O     | 6:F:69:ILE:HG22   | 2.11                     | 0.50              |
| 13:M:134:GLU:HA  | 13:M:138:GLY:O    | 2.12                     | 0.50              |
| 15:O:61:ALA:CB   | 15:O:88:ALA:HB2   | 2.41                     | 0.50              |
| 15:O:163:PHE:HE1 | 15:O:171:HIS:HD1  | 1.59                     | 0.50              |
| 16:P:14:LEU:CD2  | 16:P:102:ILE:HD11 | 2.40                     | 0.50              |
| 24:X:41:TYR:HA   | 24:X:44:MET:HE3   | 1.93                     | 0.50              |
| 1:A:1102:C:H2'   | 1:A:1103:C:C6     | 2.46                     | 0.50              |
| 6:F:140:ARG:O    | 6:F:144:ARG:HG2   | 2.11                     | 0.50              |
| 10:J:85:ILE:HG23 | 10:J:85:ILE:O     | 2.12                     | 0.50              |
| 14:N:186:SER:OG  | 14:N:189:VAL:CG1  | 2.59                     | 0.50              |
| 15:O:171:HIS:CE1 | 37:O:8567:HOH:O   | 2.64                     | 0.50              |
| 15:O:182:GLY:O   | 15:O:183:ASP:O    | 2.29                     | 0.50              |
| 24:X:108:ARG:HE  | 24:X:114:PRO:HG3  | 1.76                     | 0.50              |
| 1:A:951:A:C2'    | 1:A:952:G:H5'     | 2.42                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1161:A:H8    | 1:A:1161:A:O5'    | 1.95                     | 0.50              |
| 1:A:2113:G:C6    | 1:A:2114:C:C4     | 3.00                     | 0.50              |
| 3:C:93:THR:C     | 3:C:94:LEU:HD23   | 2.36                     | 0.50              |
| 5:E:33:LYS:HE2   | 37:E:8358:HOH:O   | 2.12                     | 0.50              |
| 7:G:81:GLU:HG2   | 7:G:134:SER:CB    | 2.39                     | 0.50              |
| 16:P:38:ARG:NH1  | 37:P:7674:HOH:O   | 2.45                     | 0.50              |
| 16:P:88:LYS:O    | 37:P:4826:HOH:O   | 2.20                     | 0.50              |
| 23:W:12:THR:HG23 | 23:W:14:ALA:H     | 1.76                     | 0.50              |
| 1:A:553:G:P      | 26:Z:204:ARG:HH22 | 2.34                     | 0.50              |
| 1:A:825:U:H5''   | 1:A:826:U:OP1     | 2.12                     | 0.50              |
| 1:A:1462:C:H2'   | 1:A:1463:A:C8     | 2.47                     | 0.50              |
| 1:A:1594:C:C2    | 1:A:1601:G:C2     | 3.00                     | 0.50              |
| 1:A:2004:U:O2    | 1:A:2004:U:H2'    | 2.11                     | 0.50              |
| 1:A:2506:A:O2'   | 1:A:2507:G:O5'    | 2.30                     | 0.50              |
| 2:B:3031:C:O2'   | 2:B:3032:G:H5'    | 2.11                     | 0.50              |
| 11:K:52:GLN:HG3  | 11:K:53:ILE:H     | 1.74                     | 0.50              |
| 13:M:112:GLY:O   | 13:M:132:LYS:NZ   | 2.33                     | 0.50              |
| 1:A:625:U:H5''   | 1:A:1044:C:N4     | 2.26                     | 0.50              |
| 1:A:1846:U:O2'   | 3:C:172:ALA:HB2   | 2.11                     | 0.50              |
| 4:D:103:ASP:HB2  | 37:D:8595:HOH:O   | 2.11                     | 0.50              |
| 6:F:27:ILE:HD11  | 6:F:37:ALA:CB     | 2.42                     | 0.50              |
| 10:J:26:LYS:HD2  | 10:J:28:ILE:CG1   | 2.42                     | 0.50              |
| 14:N:52:LEU:HD13 | 14:N:116:ASN:HB3  | 1.94                     | 0.50              |
| 14:N:63:VAL:HG21 | 14:N:109:PHE:CE1  | 2.47                     | 0.50              |
| 19:S:15:LYS:HE3  | 37:S:8581:HOH:O   | 2.12                     | 0.50              |
| 1:A:113:A:OP2    | 1:A:114:A:H5''    | 2.12                     | 0.50              |
| 1:A:399:C:H5'    | 14:N:179:GLY:O    | 2.12                     | 0.50              |
| 1:A:514:G:OP1    | 1:A:514:G:H2'     | 2.12                     | 0.50              |
| 1:A:1525:G:H5'   | 1:A:1526:A:OP2    | 2.12                     | 0.50              |
| 1:A:2274:A:H1'   | 14:N:86:MET:SD    | 2.52                     | 0.50              |
| 2:B:3030:C:OP1   | 6:F:137:PRO:O     | 2.29                     | 0.50              |
| 2:B:3059:C:H2'   | 2:B:3060:C:C6     | 2.47                     | 0.50              |
| 2:B:3076:G:C3'   | 2:B:3077:A:H5''   | 2.23                     | 0.50              |
| 4:D:248:ARG:O    | 4:D:251:VAL:HG13  | 2.11                     | 0.50              |
| 5:E:111:VAL:HB   | 37:E:8322:HOH:O   | 2.11                     | 0.50              |
| 6:F:94:ALA:HB3   | 6:F:174:VAL:HA    | 1.94                     | 0.50              |
| 7:G:97:VAL:C     | 37:G:4191:HOH:O   | 2.54                     | 0.50              |
| 9:I:12:ILE:HD12  | 37:I:692:HOH:O    | 2.11                     | 0.50              |
| 19:S:39:THR:HG22 | 19:S:41:GLY:N     | 2.26                     | 0.50              |
| 27:1:11:THR:HG23 | 27:1:23:ARG:HD2   | 1.94                     | 0.50              |
| 1:A:275:G:C2     | 1:A:376:C:N3      | 2.80                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:306:A:P       | 21:U:38:ARG:HH21  | 2.35                     | 0.49              |
| 1:A:638:C:H2'     | 1:A:639:A:C8      | 2.47                     | 0.49              |
| 1:A:1840:A:H4'    | 1:A:1841:C:O5'    | 2.12                     | 0.49              |
| 1:A:2506:A:C1'    | 37:A:5633:HOH:O   | 2.60                     | 0.49              |
| 2:B:3036:C:C5     | 2:B:3037:C:C5     | 3.00                     | 0.49              |
| 4:D:79:MET:HE1    | 37:D:8627:HOH:O   | 2.12                     | 0.49              |
| 7:G:145:ALA:HB1   | 7:G:168:ILE:CD1   | 2.42                     | 0.49              |
| 14:N:35:PRO:HD2   | 14:N:38:VAL:CG2   | 2.42                     | 0.49              |
| 14:N:114:VAL:HB   | 14:N:159:THR:HG23 | 1.94                     | 0.49              |
| 14:N:165:SER:HB3  | 37:N:8533:HOH:O   | 2.12                     | 0.49              |
| 27:1:51:GLY:HA3   | 37:1:8417:HOH:O   | 2.11                     | 0.49              |
| 1:A:182:G:O3'     | 14:N:157:LEU:CD1  | 2.61                     | 0.49              |
| 1:A:731:U:O2'     | 1:A:732:C:H5'     | 2.12                     | 0.49              |
| 1:A:816:G:H5'     | 1:A:1598:A:H4'    | 1.93                     | 0.49              |
| 1:A:820:G:C5      | 3:C:171:LYS:HB2   | 2.48                     | 0.49              |
| 6:F:146:LYS:HZ1   | 15:O:107:ASN:HD21 | 1.54                     | 0.49              |
| 17:Q:41:ARG:O     | 17:Q:44:VAL:HB    | 2.12                     | 0.49              |
| 29:3:22:PRO:HB2   | 29:3:24:TRP:CD1   | 2.47                     | 0.49              |
| 1:A:275:G:N2      | 1:A:376:C:C2      | 2.80                     | 0.49              |
| 1:A:703:G:O2'     | 1:A:704:C:H5'     | 2.12                     | 0.49              |
| 1:A:1120:U:H5'    | 1:A:1121:G:OP2    | 2.12                     | 0.49              |
| 1:A:1422:U:H2'    | 1:A:1423:C:C6     | 2.48                     | 0.49              |
| 1:A:2300:A:H4'    | 1:A:2301:A:O5'    | 2.13                     | 0.49              |
| 4:D:205:VAL:O     | 4:D:307:ARG:NE    | 2.45                     | 0.49              |
| 6:F:95:THR:C      | 6:F:97:GLN:N      | 2.60                     | 0.49              |
| 7:G:43:ASP:HA     | 37:G:5864:HOH:O   | 2.12                     | 0.49              |
| 8:H:105:ALA:HB2   | 37:H:5522:HOH:O   | 2.12                     | 0.49              |
| 11:K:45:VAL:HG22  | 11:K:46:ILE:N     | 2.25                     | 0.49              |
| 24:X:139:GLY:O    | 24:X:141:HIS:CD2  | 2.64                     | 0.49              |
| 1:A:152:A:O2'     | 1:A:153:C:H5'     | 2.12                     | 0.49              |
| 3:C:170:VAL:HG13  | 27:1:22:ILE:HG21  | 1.95                     | 0.49              |
| 5:E:142:ASP:OD2   | 5:E:238:SER:OG    | 2.21                     | 0.49              |
| 8:H:101:ALA:HB2   | 8:H:108:LEU:HD22  | 1.94                     | 0.49              |
| 10:J:48:LEU:HD13  | 10:J:146:TRP:HB3  | 1.93                     | 0.49              |
| 14:N:47:ASP:CG    | 14:N:48:ARG:N     | 2.71                     | 0.49              |
| 16:P:105:ASN:HD21 | 16:P:109:SER:H    | 1.61                     | 0.49              |
| 30:4:3:MET:O      | 30:4:90:PHE:HA    | 2.11                     | 0.49              |
| 1:A:665:A:H2'     | 1:A:666:A:C8      | 2.47                     | 0.49              |
| 1:A:2729:C:H2'    | 1:A:2730:G:H8     | 1.78                     | 0.49              |
| 2:B:3020:G:P      | 37:B:8435:HOH:O   | 2.71                     | 0.49              |
| 6:F:27:ILE:HG22   | 6:F:28:GLY:N      | 2.22                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:154:THR:HB   | 10:J:155:PRO:HD3  | 1.95                     | 0.49              |
| 16:P:99:GLU:HA    | 37:P:7481:HOH:O   | 2.12                     | 0.49              |
| 16:P:113:VAL:O    | 16:P:114:ILE:HD13 | 2.13                     | 0.49              |
| 25:Y:25:ARG:HD3   | 25:Y:64:ALA:O     | 2.13                     | 0.49              |
| 30:4:74:CYS:N     | 37:4:8561:HOH:O   | 2.46                     | 0.49              |
| 1:A:390:G:C5      | 1:A:391:U:C5      | 3.00                     | 0.49              |
| 1:A:1151:G:P      | 9:I:16:LYS:HZ1    | 2.32                     | 0.49              |
| 1:A:1684:A:O2'    | 1:A:1685:A:H5''   | 2.13                     | 0.49              |
| 4:D:314:ALA:CB    | 4:D:317:PRO:HG3   | 2.42                     | 0.49              |
| 5:E:35:VAL:HG21   | 5:E:227:GLY:HA2   | 1.93                     | 0.49              |
| 15:O:141:ARG:HB3  | 37:O:8570:HOH:O   | 2.13                     | 0.49              |
| 17:Q:10:ALA:O     | 17:Q:13:VAL:HG12  | 2.13                     | 0.49              |
| 17:Q:131:PHE:CD1  | 17:Q:137:LEU:HD13 | 2.46                     | 0.49              |
| 22:V:20:MET:CG    | 22:V:28:THR:HG23  | 2.43                     | 0.49              |
| 24:X:51:PHE:N     | 24:X:51:PHE:CD1   | 2.79                     | 0.49              |
| 26:Z:200:THR:HG22 | 26:Z:201:GLU:HG2  | 1.94                     | 0.49              |
| 1:A:1189:A:O2'    | 1:A:1208:C:H2'    | 2.12                     | 0.49              |
| 1:A:1682:A:H5''   | 37:A:9036:HOH:O   | 2.12                     | 0.49              |
| 2:B:3064:C:H2'    | 2:B:3065:A:H5'    | 1.95                     | 0.49              |
| 3:C:149:ASP:OD1   | 3:C:151:GLN:HB2   | 2.12                     | 0.49              |
| 4:D:140:LEU:HD23  | 37:D:8583:HOH:O   | 2.13                     | 0.49              |
| 6:F:57:THR:HG23   | 6:F:63:ILE:CG2    | 2.41                     | 0.49              |
| 6:F:99:ASP:O      | 6:F:159:PRO:HG3   | 2.13                     | 0.49              |
| 10:J:26:LYS:HD3   | 10:J:89:PRO:CG    | 2.43                     | 0.49              |
| 14:N:9:ARG:HG3    | 37:N:8544:HOH:O   | 2.12                     | 0.49              |
| 15:O:37:ARG:NH2   | 37:O:8534:HOH:O   | 2.45                     | 0.49              |
| 1:A:1370:G:C4     | 37:A:9727:HOH:O   | 2.65                     | 0.49              |
| 2:B:3095:C:O2'    | 2:B:3096:C:H5'    | 2.13                     | 0.49              |
| 5:E:133:ARG:NH2   | 37:E:8421:HOH:O   | 2.46                     | 0.49              |
| 6:F:19:GLU:O      | 6:F:133:ASN:HB3   | 2.12                     | 0.49              |
| 14:N:113:ARG:NH1  | 14:N:152:ARG:O    | 2.42                     | 0.49              |
| 21:U:38:ARG:HG3   | 21:U:38:ARG:NH1   | 2.27                     | 0.49              |
| 1:A:169:A:H4'     | 37:N:8534:HOH:O   | 2.12                     | 0.49              |
| 1:A:440:C:H2'     | 1:A:441:A:C8      | 2.48                     | 0.49              |
| 1:A:797:A:H4'     | 27:1:10:ARG:N     | 2.27                     | 0.49              |
| 1:A:1235:G:C1'    | 11:K:63:ILE:HG23  | 2.42                     | 0.49              |
| 1:A:2420:G:H4'    | 37:A:3671:HOH:O   | 2.13                     | 0.49              |
| 1:A:2837:U:H2'    | 37:A:6412:HOH:O   | 2.13                     | 0.49              |
| 5:E:84:VAL:O      | 5:E:85:LYS:CB     | 2.60                     | 0.49              |
| 6:F:23:VAL:HG21   | 6:F:45:THR:CG2    | 2.42                     | 0.49              |
| 12:L:45:PRO:HB2   | 37:L:7169:HOH:O   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:449:A:C8     | 5:E:43:LYS:HG2    | 2.47                     | 0.49              |
| 1:A:812:A:H2'    | 1:A:813:C:C6      | 2.48                     | 0.49              |
| 1:A:1119:G:C8    | 11:K:52:GLN:NE2   | 2.81                     | 0.49              |
| 1:A:1205:U:C2'   | 1:A:1206:U:C5'    | 2.90                     | 0.49              |
| 1:A:2896:A:H2'   | 1:A:2896:A:N3     | 2.28                     | 0.49              |
| 37:A:8974:HOH:O  | 27:1:34:LYS:HD3   | 2.13                     | 0.49              |
| 3:C:200:PRO:HG2  | 3:C:225:VAL:HG21  | 1.95                     | 0.49              |
| 6:F:51:ARG:HD3   | 37:F:7636:HOH:O   | 2.13                     | 0.49              |
| 6:F:64:ARG:HG2   | 6:F:66:GLY:O      | 2.13                     | 0.49              |
| 13:M:72:ASN:HB2  | 37:M:8453:HOH:O   | 2.12                     | 0.49              |
| 14:N:108:LYS:HD3 | 14:N:108:LYS:N    | 2.28                     | 0.49              |
| 15:O:132:ASN:O   | 15:O:135:VAL:HG12 | 2.12                     | 0.49              |
| 15:O:161:GLY:O   | 15:O:162:ASP:C    | 2.55                     | 0.49              |
| 19:S:96:VAL:HG13 | 19:S:106:GLY:HA3  | 1.94                     | 0.49              |
| 22:V:36:CYS:O    | 22:V:37:GLU:C     | 2.56                     | 0.49              |
| 1:A:907:A:H2'    | 1:A:908:A:C8      | 2.47                     | 0.48              |
| 1:A:1166:A:H1'   | 1:A:1192:A:N1     | 2.26                     | 0.48              |
| 1:A:1236:A:H2'   | 1:A:1237:U:O4'    | 2.13                     | 0.48              |
| 1:A:2505:G:H8    | 37:A:5216:HOH:O   | 1.96                     | 0.48              |
| 2:B:3055:U:H4'   | 2:B:3056:A:H8     | 1.78                     | 0.48              |
| 4:D:84:LEU:O     | 4:D:84:LEU:HD13   | 2.13                     | 0.48              |
| 10:J:31:PHE:CD2  | 10:J:85:ILE:HG23  | 2.48                     | 0.48              |
| 15:O:139:TRP:HA  | 15:O:139:TRP:HE3  | 1.78                     | 0.48              |
| 19:S:76:ASP:OD1  | 19:S:77:ALA:N     | 2.45                     | 0.48              |
| 21:U:28:SER:O    | 21:U:32:ARG:HG3   | 2.12                     | 0.48              |
| 25:Y:85:VAL:HG12 | 25:Y:86:GLU:N     | 2.27                     | 0.48              |
| 30:4:40:ARG:HD2  | 37:4:8549:HOH:O   | 2.13                     | 0.48              |
| 1:A:289:G:O2'    | 1:A:290:C:H5'     | 2.12                     | 0.48              |
| 1:A:1118:A:C8    | 1:A:1118:A:C3'    | 2.85                     | 0.48              |
| 1:A:1334:C:H2'   | 1:A:1335:C:H6     | 1.77                     | 0.48              |
| 1:A:2428:G:C4    | 1:A:2461:U:C5     | 3.01                     | 0.48              |
| 1:A:2597:U:OP2   | 37:A:3404:HOH:O   | 2.20                     | 0.48              |
| 37:A:5846:HOH:O  | 17:Q:59:ARG:HD3   | 2.13                     | 0.48              |
| 37:A:9381:HOH:O  | 12:L:39:GLY:HA3   | 2.12                     | 0.48              |
| 2:B:3029:C:C2'   | 2:B:3030:C:H5'    | 2.43                     | 0.48              |
| 8:H:101:ALA:HB2  | 8:H:108:LEU:CD2   | 2.43                     | 0.48              |
| 10:J:44:ALA:HB3  | 10:J:136:VAL:O    | 2.13                     | 0.48              |
| 12:L:101:ASN:O   | 12:L:102:GLU:HB2  | 2.13                     | 0.48              |
| 21:U:26:THR:HA   | 21:U:39:ASN:HB3   | 1.95                     | 0.48              |
| 25:Y:43:VAL:HG12 | 25:Y:44:ASP:N     | 2.27                     | 0.48              |
| 1:A:1972:U:H2'   | 1:A:1973:A:C5'    | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2356:A:H2'    | 1:A:2357:G:O4'    | 2.13                     | 0.48              |
| 1:A:2421:G:H3'    | 1:A:2422:U:H5''   | 1.95                     | 0.48              |
| 1:A:2547:C:H2'    | 1:A:2548:C:H6     | 1.78                     | 0.48              |
| 1:A:2727:A:H2'    | 1:A:2728:C:H5'    | 1.94                     | 0.48              |
| 1:A:2791:U:H1'    | 1:A:2792:A:H5''   | 1.96                     | 0.48              |
| 3:C:199:HIS:HD2   | 3:C:201:PHE:HB2   | 1.78                     | 0.48              |
| 11:K:107:ASN:HD22 | 11:K:109:TYR:H    | 1.59                     | 0.48              |
| 12:L:55:VAL:CG1   | 12:L:56:SER:N     | 2.77                     | 0.48              |
| 14:N:79:LYS:NZ    | 37:N:8566:HOH:O   | 2.46                     | 0.48              |
| 25:Y:76:ARG:HG3   | 25:Y:76:ARG:NH1   | 2.26                     | 0.48              |
| 26:Z:187:VAL:O    | 26:Z:187:VAL:HG13 | 2.13                     | 0.48              |
| 28:2:28:HIS:CD2   | 28:2:31:LYS:HG3   | 2.48                     | 0.48              |
| 1:A:837:U:H4'     | 37:A:9979:HOH:O   | 2.12                     | 0.48              |
| 1:A:1299:G:N2     | 37:A:4259:HOH:O   | 2.46                     | 0.48              |
| 1:A:1425:G:O2'    | 1:A:1426:C:H5'    | 2.13                     | 0.48              |
| 1:A:1701:A:H4'    | 1:A:1702:U:C5'    | 2.42                     | 0.48              |
| 1:A:1930:A:H2'    | 1:A:1931:A:C8     | 2.48                     | 0.48              |
| 5:E:107:ARG:NH2   | 37:E:8454:HOH:O   | 2.44                     | 0.48              |
| 7:G:31:ARG:NH1    | 37:G:5919:HOH:O   | 2.45                     | 0.48              |
| 7:G:77:THR:OG1    | 7:G:78:GLU:N      | 2.44                     | 0.48              |
| 8:H:26:THR:HB     | 8:H:102:GLY:HA3   | 1.95                     | 0.48              |
| 9:I:73:ASP:O      | 37:I:2218:HOH:O   | 2.20                     | 0.48              |
| 15:O:157:PRO:HA   | 37:O:8526:HOH:O   | 2.12                     | 0.48              |
| 19:S:132:ARG:HG2  | 19:S:133:ALA:N    | 2.27                     | 0.48              |
| 24:X:48:VAL:CG1   | 24:X:48:VAL:O     | 2.59                     | 0.48              |
| 1:A:390:G:C4      | 1:A:391:U:C6      | 3.02                     | 0.48              |
| 1:A:1486:A:C5     | 29:3:2:LYS:HG3    | 2.48                     | 0.48              |
| 1:A:2445:U:H2'    | 1:A:2446:G:C8     | 2.48                     | 0.48              |
| 1:A:2727:A:C5     | 1:A:2756:U:C4     | 3.01                     | 0.48              |
| 1:A:2834:G:C4     | 1:A:2847:G:N2     | 2.81                     | 0.48              |
| 1:A:2904:U:H4'    | 25:Y:8:ARG:NH1    | 2.28                     | 0.48              |
| 3:C:123:GLY:HA2   | 3:C:159:VAL:O     | 2.14                     | 0.48              |
| 5:E:185:LYS:NZ    | 37:E:8416:HOH:O   | 2.44                     | 0.48              |
| 6:F:35:ALA:HB1    | 37:F:3279:HOH:O   | 2.11                     | 0.48              |
| 13:M:17:SER:C     | 13:M:19:LYS:N     | 2.71                     | 0.48              |
| 24:X:110:GLN:HE21 | 24:X:110:GLN:HA   | 1.78                     | 0.48              |
| 1:A:130:C:H5'     | 37:A:4789:HOH:O   | 2.13                     | 0.48              |
| 1:A:1057:A:C6     | 1:A:1058:A:C6     | 3.02                     | 0.48              |
| 1:A:1117:A:C2     | 1:A:1244:U:C2     | 3.01                     | 0.48              |
| 1:A:1162:G:H2'    | 1:A:1162:G:N3     | 2.28                     | 0.48              |
| 1:A:1768:C:H2'    | 1:A:1769:C:O4'    | 2.14                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:2401:A:H5'   | 37:A:9075:HOH:O   | 2.12                     | 0.48              |
| 1:A:2821:C:H4'   | 4:D:116:PRO:CB    | 2.41                     | 0.48              |
| 5:E:65:ARG:HG3   | 5:E:67:GLN:HB2    | 1.95                     | 0.48              |
| 5:E:237:GLU:N    | 37:E:8445:HOH:O   | 2.46                     | 0.48              |
| 6:F:23:VAL:HG12  | 6:F:130:VAL:HG22  | 1.96                     | 0.48              |
| 10:J:45:GLN:HE21 | 10:J:135:TRP:NE1  | 2.12                     | 0.48              |
| 10:J:112:ARG:O   | 10:J:113:ALA:C    | 2.56                     | 0.48              |
| 10:J:165:GLY:C   | 10:J:166:ASN:HD22 | 2.22                     | 0.48              |
| 11:K:75:PRO:HG2  | 11:K:105:LEU:CD2  | 2.44                     | 0.48              |
| 13:M:61:ALA:HA   | 37:M:8437:HOH:O   | 2.14                     | 0.48              |
| 16:P:54:GLU:HG2  | 16:P:73:ASP:O     | 2.14                     | 0.48              |
| 19:S:34:GLU:HG2  | 19:S:46:TYR:OH    | 2.14                     | 0.48              |
| 19:S:35:ILE:O    | 19:S:38:LYS:HB2   | 2.13                     | 0.48              |
| 30:4:18:GLN:OE1  | 30:4:73:GLU:HB3   | 2.13                     | 0.48              |
| 1:A:29:C:OP2     | 37:A:9723:HOH:O   | 2.20                     | 0.48              |
| 1:A:154:C:N3     | 1:A:155:C:C5      | 2.81                     | 0.48              |
| 1:A:1114:A:H2'   | 1:A:1115:U:H6     | 1.77                     | 0.48              |
| 1:A:2559:C:H4'   | 37:A:6828:HOH:O   | 2.13                     | 0.48              |
| 3:C:199:HIS:CD2  | 3:C:201:PHE:HB2   | 2.48                     | 0.48              |
| 7:G:84:MET:HE2   | 7:G:133:VAL:HG23  | 1.95                     | 0.48              |
| 10:J:31:PHE:HA   | 10:J:85:ILE:CG2   | 2.44                     | 0.48              |
| 18:R:77:ASP:N    | 18:R:80:LYS:O     | 2.44                     | 0.48              |
| 18:R:93:ARG:HH11 | 18:R:93:ARG:HG3   | 1.78                     | 0.48              |
| 19:S:14:ALA:HB3  | 19:S:147:LEU:HB2  | 1.96                     | 0.48              |
| 20:T:6:LYS:HB2   | 20:T:27:ALA:O     | 2.13                     | 0.48              |
| 27:1:11:THR:OG1  | 27:1:23:ARG:HB2   | 2.14                     | 0.48              |
| 1:A:23:G:C6      | 1:A:24:G:N1       | 2.81                     | 0.48              |
| 1:A:371:U:H2'    | 1:A:372:A:C8      | 2.47                     | 0.48              |
| 1:A:1507:C:H4'   | 37:A:3185:HOH:O   | 2.13                     | 0.48              |
| 1:A:2385:G:H2'   | 1:A:2386:U:H6     | 1.78                     | 0.48              |
| 37:A:3555:HOH:O  | 30:4:57:GLY:HA2   | 2.14                     | 0.48              |
| 3:C:76:VAL:CG2   | 27:1:63:LYS:HB3   | 2.43                     | 0.48              |
| 3:C:192:VAL:HG12 | 3:C:207:GLN:HB3   | 1.95                     | 0.48              |
| 4:D:55:ASN:HB3   | 4:D:64:GLY:H      | 1.78                     | 0.48              |
| 6:F:41:LEU:HA    | 6:F:44:ILE:CG2    | 2.44                     | 0.48              |
| 8:H:34:ASN:HA    | 14:N:4:ALA:HB2    | 1.96                     | 0.48              |
| 8:H:37:THR:O     | 8:H:41:GLU:HG3    | 2.13                     | 0.48              |
| 8:H:59:ILE:O     | 8:H:59:ILE:HG22   | 2.14                     | 0.48              |
| 15:O:139:TRP:HH2 | 15:O:176:ARG:HH11 | 1.62                     | 0.48              |
| 17:Q:83:LYS:O    | 17:Q:86:ALA:HB3   | 2.14                     | 0.48              |
| 26:Z:99:ALA:HB2  | 26:Z:233:TYR:CE2  | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:40:C:H6       | 1:A:40:C:O5'      | 1.97                     | 0.48              |
| 1:A:51:G:N2       | 1:A:111:C:C2      | 2.81                     | 0.48              |
| 1:A:484:A:N1      | 1:A:506:G:H4'     | 2.29                     | 0.48              |
| 1:A:559:U:H2'     | 1:A:560:C:O4'     | 2.14                     | 0.48              |
| 1:A:612:U:H2'     | 1:A:613:C:C6      | 2.49                     | 0.48              |
| 1:A:920:C:H5''    | 1:A:921:G:O5'     | 2.14                     | 0.48              |
| 1:A:1180:U:H2'    | 1:A:1181:A:O4'    | 2.14                     | 0.48              |
| 1:A:2780:C:H2'    | 1:A:2781:U:H6     | 1.78                     | 0.48              |
| 1:A:2906:A:H5'    | 1:A:2907:C:O4'    | 2.14                     | 0.48              |
| 5:E:246:ARG:HH11  | 5:E:246:ARG:CB    | 2.19                     | 0.48              |
| 7:G:84:MET:HB2    | 7:G:131:LEU:HB2   | 1.94                     | 0.48              |
| 13:M:1:THR:HA     | 37:M:8393:HOH:O   | 2.13                     | 0.48              |
| 14:N:123:ASP:C    | 14:N:123:ASP:OD1  | 2.54                     | 0.48              |
| 25:Y:12:ILE:HG23  | 25:Y:36:HIS:CG    | 2.48                     | 0.48              |
| 1:A:349:U:O2'     | 1:A:350:C:H5'     | 2.14                     | 0.48              |
| 1:A:675:U:O2'     | 5:E:42:ARG:NH1    | 2.47                     | 0.48              |
| 1:A:682:A:H2'     | 1:A:683:G:O4'     | 2.14                     | 0.48              |
| 1:A:2326:U:H4'    | 1:A:2412:G:C4'    | 2.44                     | 0.48              |
| 5:E:118:THR:HG22  | 5:E:137:PRO:HB3   | 1.96                     | 0.48              |
| 10:J:117:LYS:O    | 10:J:119:VAL:HG13 | 2.13                     | 0.48              |
| 13:M:128:GLY:O    | 13:M:132:LYS:HG3  | 2.13                     | 0.48              |
| 20:T:57:THR:CG2   | 20:T:58:MET:N     | 2.77                     | 0.48              |
| 23:W:16:ARG:NH2   | 23:W:63:GLU:HG3   | 2.29                     | 0.48              |
| 30:4:65:THR:HB    | 30:4:83:TRP:H     | 1.78                     | 0.48              |
| 1:A:795:G:N3      | 1:A:817:G:C2      | 2.82                     | 0.47              |
| 1:A:797:A:O4'     | 27:1:10:ARG:N     | 2.47                     | 0.47              |
| 1:A:1462:C:O2'    | 1:A:1463:A:H5'    | 2.14                     | 0.47              |
| 1:A:1593:C:OP1    | 17:Q:117:SER:HB3  | 2.14                     | 0.47              |
| 1:A:1741:U:O2'    | 1:A:2723:G:H4'    | 2.13                     | 0.47              |
| 1:A:2507:G:H2'    | 1:A:2510:C:H42    | 1.79                     | 0.47              |
| 2:B:3026:C:OP2    | 37:B:8441:HOH:O   | 2.19                     | 0.47              |
| 4:D:1:PRO:O       | 4:D:2:GLN:HB2     | 2.14                     | 0.47              |
| 4:D:141:ARG:HD2   | 4:D:163:GLU:OE2   | 2.13                     | 0.47              |
| 11:K:131:THR:HB   | 11:K:134:GLU:HG3  | 1.95                     | 0.47              |
| 16:P:77:ALA:HB1   | 16:P:98:LEU:HD12  | 1.96                     | 0.47              |
| 17:Q:143:ALA:CA   | 37:Q:5521:HOH:O   | 2.61                     | 0.47              |
| 19:S:111:ILE:HG23 | 19:S:145:LEU:HD11 | 1.96                     | 0.47              |
| 24:X:22:GLU:HG2   | 24:X:27:HIS:CD2   | 2.48                     | 0.47              |
| 24:X:137:GLN:HG3  | 24:X:137:GLN:O    | 2.14                     | 0.47              |
| 1:A:56:G:H5''     | 23:W:50:ARG:HH12  | 1.78                     | 0.47              |
| 1:A:128:A:H3'     | 1:A:128:A:C8      | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:736:A:H2'     | 1:A:737:A:O4'     | 2.13                     | 0.47              |
| 1:A:1167:G:O2'    | 1:A:1168:C:H5'    | 2.14                     | 0.47              |
| 1:A:1634:G:H3'    | 37:A:3471:HOH:O   | 2.13                     | 0.47              |
| 1:A:1947:G:P      | 37:A:3246:HOH:O   | 2.69                     | 0.47              |
| 37:A:6716:HOH:O   | 29:3:24:TRP:CD1   | 2.67                     | 0.47              |
| 2:B:3056:A:H1'    | 6:F:14:ARG:HG2    | 1.97                     | 0.47              |
| 4:D:52:VAL:O      | 4:D:53:LEU:HD12   | 2.14                     | 0.47              |
| 4:D:280:VAL:HG13  | 4:D:334:SER:HA    | 1.96                     | 0.47              |
| 7:G:9:GLU:HA      | 37:G:5240:HOH:O   | 2.13                     | 0.47              |
| 14:N:85:ARG:HA    | 14:N:87:MET:HE2   | 1.96                     | 0.47              |
| 17:Q:61:ARG:HG3   | 17:Q:61:ARG:NH1   | 2.28                     | 0.47              |
| 19:S:65:GLY:C     | 37:S:8517:HOH:O   | 2.57                     | 0.47              |
| 19:S:72:VAL:CG1   | 19:S:75:TRP:HB3   | 2.44                     | 0.47              |
| 21:U:73:HIS:CD2   | 21:U:88:PRO:HG3   | 2.48                     | 0.47              |
| 1:A:401:C:P       | 37:A:5369:HOH:O   | 2.72                     | 0.47              |
| 1:A:447:A:O2'     | 1:A:448:G:H5'     | 2.15                     | 0.47              |
| 1:A:514:G:H8      | 1:A:514:G:O5'     | 1.97                     | 0.47              |
| 1:A:603:A:H4'     | 1:A:604:G:O5'     | 2.14                     | 0.47              |
| 1:A:737:A:H2'     | 1:A:738:G:O4'     | 2.14                     | 0.47              |
| 1:A:1019:C:O2     | 18:R:94:GLN:NE2   | 2.47                     | 0.47              |
| 1:A:1440:U:P      | 37:A:4043:HOH:O   | 2.72                     | 0.47              |
| 1:A:1878:G:C1'    | 37:A:5700:HOH:O   | 2.60                     | 0.47              |
| 1:A:2361:A:H2'    | 1:A:2362:A:C8     | 2.48                     | 0.47              |
| 1:A:2385:G:H2'    | 1:A:2386:U:C6     | 2.49                     | 0.47              |
| 2:B:3049:G:O2'    | 2:B:3050:G:H5'    | 2.14                     | 0.47              |
| 3:C:153:ARG:HB2   | 3:C:153:ARG:NH1   | 2.23                     | 0.47              |
| 4:D:177:HIS:O     | 4:D:181:ILE:HG13  | 2.14                     | 0.47              |
| 6:F:99:ASP:HB2    | 6:F:103:ASN:H     | 1.79                     | 0.47              |
| 12:L:20:CYS:HB3   | 12:L:26:ALA:O     | 2.15                     | 0.47              |
| 13:M:120:LEU:HD12 | 13:M:133:VAL:HG21 | 1.95                     | 0.47              |
| 14:N:57:LYS:HB3   | 14:N:60:ILE:HD12  | 1.96                     | 0.47              |
| 14:N:154:ARG:HG3  | 37:N:8612:HOH:O   | 2.15                     | 0.47              |
| 24:X:63:GLU:HG2   | 24:X:93:ILE:HG22  | 1.96                     | 0.47              |
| 24:X:90:TYR:N     | 24:X:90:TYR:CD1   | 2.81                     | 0.47              |
| 1:A:1114:A:H2'    | 1:A:1115:U:C6     | 2.49                     | 0.47              |
| 1:A:2274:A:C4'    | 14:N:77:PHE:HE1   | 2.27                     | 0.47              |
| 1:A:2377:U:O5'    | 1:A:2377:U:H6     | 1.97                     | 0.47              |
| 4:D:189:ALA:HB1   | 37:D:8567:HOH:O   | 2.14                     | 0.47              |
| 5:E:1:MET:HG2     | 5:E:2:GLN:NE2     | 2.30                     | 0.47              |
| 6:F:169:THR:O     | 6:F:170:TYR:HB2   | 2.15                     | 0.47              |
| 11:K:93:ARG:HB3   | 11:K:93:ARG:NH1   | 2.27                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:109:LEU:HD13 | 12:L:113:ILE:HD11 | 1.95                     | 0.47              |
| 14:N:27:ARG:O     | 14:N:30:GLU:N     | 2.45                     | 0.47              |
| 16:P:35:LYS:HD3   | 37:P:3360:HOH:O   | 2.15                     | 0.47              |
| 17:Q:80:ARG:HG2   | 17:Q:87:ARG:CZ    | 2.44                     | 0.47              |
| 17:Q:131:PHE:CE1  | 17:Q:137:LEU:HD13 | 2.49                     | 0.47              |
| 22:V:52:THR:HG21  | 22:V:54:THR:HB    | 1.96                     | 0.47              |
| 23:W:11:MET:HB3   | 23:W:15:GLU:HB2   | 1.95                     | 0.47              |
| 25:Y:76:ARG:O     | 25:Y:77:PHE:HB3   | 2.14                     | 0.47              |
| 1:A:95:A:H5''     | 1:A:97:G:O4'      | 2.14                     | 0.47              |
| 1:A:107:U:H2'     | 1:A:108:U:H5'     | 1.96                     | 0.47              |
| 1:A:516:A:OP2     | 37:A:5223:HOH:O   | 2.20                     | 0.47              |
| 1:A:542:A:C8      | 1:A:542:A:C5'     | 2.91                     | 0.47              |
| 1:A:2389:U:H4'    | 18:R:53:HIS:HD2   | 1.80                     | 0.47              |
| 1:A:2415:A:O2'    | 15:O:29:SER:HB3   | 2.13                     | 0.47              |
| 1:A:2769:C:H2'    | 1:A:2770:G:H5'    | 1.97                     | 0.47              |
| 4:D:315:VAL:HG23  | 4:D:316:ARG:HG2   | 1.96                     | 0.47              |
| 5:E:54:LEU:HD23   | 5:E:79:ARG:HG3    | 1.96                     | 0.47              |
| 6:F:173:GLU:O     | 6:F:174:VAL:C     | 2.58                     | 0.47              |
| 7:G:34:TRP:HA     | 37:G:4572:HOH:O   | 2.14                     | 0.47              |
| 7:G:69:ILE:HA     | 7:G:72:MET:HE3    | 1.95                     | 0.47              |
| 9:I:71:LEU:C      | 9:I:73:ASP:H      | 2.21                     | 0.47              |
| 1:A:319:A:H2'     | 1:A:320:G:C8      | 2.49                     | 0.47              |
| 1:A:536:A:H3'     | 37:A:4623:HOH:O   | 2.13                     | 0.47              |
| 1:A:1370:G:N3     | 37:A:9727:HOH:O   | 2.35                     | 0.47              |
| 1:A:2524:G:H21    | 1:A:2526:C:N4     | 2.12                     | 0.47              |
| 4:D:36:PRO:HA     | 4:D:168:GLY:HA2   | 1.93                     | 0.47              |
| 8:H:47:LEU:HD22   | 8:H:108:LEU:CD1   | 2.45                     | 0.47              |
| 11:K:103:VAL:HG12 | 37:K:5907:HOH:O   | 2.14                     | 0.47              |
| 12:L:22:ASP:C     | 12:L:22:ASP:OD1   | 2.57                     | 0.47              |
| 15:O:141:ARG:N    | 37:O:8570:HOH:O   | 2.47                     | 0.47              |
| 19:S:29:LYS:HD3   | 37:S:8533:HOH:O   | 2.15                     | 0.47              |
| 21:U:24:ARG:O     | 21:U:93:THR:OG1   | 2.23                     | 0.47              |
| 22:V:33:SER:O     | 22:V:37:GLU:HG3   | 2.14                     | 0.47              |
| 30:4:60:LYS:CG    | 30:4:61:PRO:HD2   | 2.40                     | 0.47              |
| 1:A:584:U:H3'     | 37:A:5674:HOH:O   | 2.13                     | 0.47              |
| 1:A:844:A:C6      | 1:A:882:A:C5      | 3.02                     | 0.47              |
| 1:A:960:G:N3      | 1:A:960:G:C2'     | 2.77                     | 0.47              |
| 1:A:1209:C:H2'    | 1:A:1210:G:C8     | 2.46                     | 0.47              |
| 1:A:1218:U:H2'    | 1:A:1219:U:C6     | 2.50                     | 0.47              |
| 1:A:1385:G:O3'    | 25:Y:49:ARG:NH1   | 2.48                     | 0.47              |
| 1:A:1543:G:N1     | 1:A:1641:A:OP2    | 2.34                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:2389:U:H4'    | 18:R:53:HIS:CD2  | 2.50                     | 0.47              |
| 1:A:2456:A:H2'    | 1:A:2457:U:C6    | 2.50                     | 0.47              |
| 1:A:2769:C:H2'    | 1:A:2770:G:C5'   | 2.44                     | 0.47              |
| 1:A:2775:A:C6     | 1:A:2799:A:C8    | 3.02                     | 0.47              |
| 37:A:9350:HOH:O   | 13:M:41:HIS:CE1  | 2.62                     | 0.47              |
| 2:B:3008:G:O6     | 15:O:11:ARG:NH1  | 2.47                     | 0.47              |
| 3:C:211:LYS:NZ    | 37:C:8625:HOH:O  | 2.46                     | 0.47              |
| 6:F:29:HIS:C      | 37:F:5858:HOH:O  | 2.57                     | 0.47              |
| 10:J:26:LYS:HD2   | 10:J:28:ILE:HB   | 1.96                     | 0.47              |
| 10:J:26:LYS:CG    | 10:J:28:ILE:H    | 2.17                     | 0.47              |
| 10:J:157:ILE:HG22 | 10:J:158:ASN:N   | 2.30                     | 0.47              |
| 14:N:69:LYS:HD3   | 14:N:125:ARG:HA  | 1.96                     | 0.47              |
| 16:P:60:VAL:C     | 16:P:62:GLY:H    | 2.23                     | 0.47              |
| 17:Q:58:SER:HB3   | 37:Q:4744:HOH:O  | 2.13                     | 0.47              |
| 19:S:132:ARG:NH1  | 37:S:8587:HOH:O  | 2.48                     | 0.47              |
| 24:X:13:MET:HE2   | 24:X:18:GLN:HA   | 1.97                     | 0.47              |
| 24:X:66:LEU:HD23  | 24:X:66:LEU:HA   | 1.79                     | 0.47              |
| 26:Z:106:THR:CG2  | 26:Z:107:PRO:HD2 | 2.45                     | 0.47              |
| 28:2:21:ARG:HD2   | 28:2:39:PHE:HB2  | 1.96                     | 0.47              |
| 1:A:694:A:C2'     | 1:A:695:C:H5'    | 2.45                     | 0.47              |
| 1:A:889:C:H2'     | 1:A:890:C:C6     | 2.50                     | 0.47              |
| 1:A:1377:C:H1'    | 37:A:6844:HOH:O  | 2.14                     | 0.47              |
| 1:A:1453:G:N2     | 1:A:1675:C:C2    | 2.83                     | 0.47              |
| 1:A:1878:G:O2'    | 1:A:1879:U:C6    | 2.67                     | 0.47              |
| 2:B:3076:G:C8     | 2:B:3077:A:H2'   | 2.50                     | 0.47              |
| 7:G:162:PHE:CD1   | 7:G:162:PHE:N    | 2.82                     | 0.47              |
| 8:H:26:THR:HB     | 8:H:102:GLY:C    | 2.39                     | 0.47              |
| 10:J:84:ARG:CZ    | 10:J:135:TRP:HH2 | 2.26                     | 0.47              |
| 19:S:25:PHE:CE2   | 19:S:29:LYS:CE   | 2.98                     | 0.47              |
| 19:S:33:ARG:NH2   | 37:S:8533:HOH:O  | 2.39                     | 0.47              |
| 24:X:6:GLN:HA     | 24:X:52:VAL:HG23 | 1.96                     | 0.47              |
| 1:A:10:U:H5'      | 37:A:5616:HOH:O  | 2.13                     | 0.47              |
| 1:A:142:G:O2'     | 1:A:143:C:H5'    | 2.14                     | 0.47              |
| 1:A:677:C:H4'     | 5:E:246:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:739:G:N7      | 37:A:7119:HOH:O  | 2.46                     | 0.47              |
| 1:A:926:A:O2'     | 13:M:41:HIS:CD2  | 2.68                     | 0.47              |
| 1:A:1161:A:O5'    | 1:A:1161:A:C8    | 2.68                     | 0.47              |
| 1:A:1304:U:H2'    | 1:A:1305:C:C6    | 2.50                     | 0.47              |
| 1:A:2474:A:N3     | 37:A:4234:HOH:O  | 2.36                     | 0.47              |
| 9:I:67:LEU:O      | 9:I:71:LEU:HG    | 2.15                     | 0.47              |
| 18:R:40:HIS:CE1   | 18:R:94:GLN:HA   | 2.50                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 24:X:76:ASP:O     | 24:X:77:ALA:O    | 2.33                     | 0.47              |
| 1:A:308:U:H5'     | 21:U:97:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:1477:C:H5'    | 1:A:1868:G:H5''  | 1.96                     | 0.47              |
| 1:A:2531:U:O2'    | 1:A:2532:A:H5'   | 2.14                     | 0.47              |
| 1:A:2785:C:H4'    | 1:A:2786:G:OP2   | 2.15                     | 0.47              |
| 3:C:11:ARG:HD3    | 37:C:8519:HOH:O  | 2.15                     | 0.47              |
| 3:C:169:PHE:O     | 3:C:170:VAL:HB   | 2.15                     | 0.47              |
| 5:E:196:THR:HG23  | 37:E:8395:HOH:O  | 2.14                     | 0.47              |
| 6:F:64:ARG:O      | 6:F:67:ASP:OD2   | 2.32                     | 0.47              |
| 9:I:16:LYS:O      | 9:I:20:VAL:HG23  | 2.15                     | 0.47              |
| 13:M:130:ARG:O    | 13:M:131:GLU:C   | 2.57                     | 0.47              |
| 15:O:67:ALA:C     | 15:O:69:TYR:N    | 2.73                     | 0.47              |
| 22:V:6:CYS:C      | 22:V:8:TYR:N     | 2.70                     | 0.47              |
| 1:A:329:A:H5'     | 1:A:347:A:C1'    | 2.45                     | 0.46              |
| 1:A:474:C:O3'     | 5:E:73:LEU:CD2   | 2.63                     | 0.46              |
| 1:A:564:G:H1'     | 37:A:5885:HOH:O  | 2.15                     | 0.46              |
| 1:A:1151:G:P      | 9:I:16:LYS:NZ    | 2.87                     | 0.46              |
| 1:A:1616:A:H5''   | 1:A:1617:C:OP1   | 2.14                     | 0.46              |
| 3:C:100:PRO:O     | 3:C:103:VAL:HG23 | 2.14                     | 0.46              |
| 3:C:175:LYS:HE2   | 37:C:8577:HOH:O  | 2.15                     | 0.46              |
| 10:J:166:ASN:N    | 10:J:166:ASN:ND2 | 2.60                     | 0.46              |
| 12:L:101:ASN:O    | 12:L:102:GLU:CB  | 2.63                     | 0.46              |
| 13:M:59:GLU:HG2   | 13:M:104:ASP:OD2 | 2.14                     | 0.46              |
| 21:U:106:GLU:HG3  | 37:U:4913:HOH:O  | 2.14                     | 0.46              |
| 24:X:65:VAL:CA    | 24:X:68:THR:HG22 | 2.45                     | 0.46              |
| 1:A:622:G:H5'     | 1:A:1357:A:H61   | 1.79                     | 0.46              |
| 1:A:962:C:H5''    | 37:A:4487:HOH:O  | 2.14                     | 0.46              |
| 1:A:2445:U:H2'    | 1:A:2446:G:H8    | 1.80                     | 0.46              |
| 1:A:2737:C:H2'    | 37:A:5721:HOH:O  | 2.14                     | 0.46              |
| 1:A:2783:A:O2'    | 1:A:2784:A:H5'   | 2.15                     | 0.46              |
| 1:A:2897:C:H2'    | 1:A:2898:G:H8    | 1.78                     | 0.46              |
| 1:A:2900:G:H2'    | 1:A:2901:C:O4'   | 2.15                     | 0.46              |
| 5:E:246:ARG:NE    | 37:E:8419:HOH:O  | 2.48                     | 0.46              |
| 13:M:73:VAL:HG21  | 13:M:116:HIS:CD2 | 2.50                     | 0.46              |
| 15:O:175:LEU:HD11 | 37:O:8539:HOH:O  | 2.15                     | 0.46              |
| 17:Q:10:ALA:HA    | 17:Q:13:VAL:HG12 | 1.96                     | 0.46              |
| 20:T:11:THR:H     | 20:T:14:ALA:HB3  | 1.80                     | 0.46              |
| 21:U:41:ARG:NH1   | 21:U:42:VAL:O    | 2.49                     | 0.46              |
| 24:X:80:ASP:O     | 24:X:84:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:21:G:H5''     | 19:S:1:GLY:O     | 2.16                     | 0.46              |
| 1:A:2415:A:N3     | 15:O:26:LEU:HD13 | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2656:G:C2'    | 1:A:2657:G:H5'    | 2.45                     | 0.46              |
| 4:D:60:SER:C      | 4:D:62:ARG:H      | 2.23                     | 0.46              |
| 5:E:150:THR:HA    | 5:E:203:ALA:O     | 2.16                     | 0.46              |
| 10:J:57:ARG:HG3   | 10:J:57:ARG:HH11  | 1.81                     | 0.46              |
| 16:P:26:TRP:HB2   | 37:P:3062:HOH:O   | 2.14                     | 0.46              |
| 19:S:25:PHE:CE2   | 19:S:29:LYS:HE2   | 2.50                     | 0.46              |
| 20:T:73:ASP:OD1   | 20:T:75:GLN:HB2   | 2.15                     | 0.46              |
| 24:X:1:MET:HB2    | 24:X:103:GLU:HG2  | 1.97                     | 0.46              |
| 28:2:5:THR:N      | 28:2:6:PRO:HD2    | 2.29                     | 0.46              |
| 1:A:182:G:O3'     | 14:N:157:LEU:HD13 | 2.16                     | 0.46              |
| 1:A:380:A:OP2     | 14:N:9:ARG:HD2    | 2.16                     | 0.46              |
| 1:A:506:G:N2      | 1:A:509:A:H5''    | 2.22                     | 0.46              |
| 1:A:841:A:OP2     | 19:S:128:ARG:HD2  | 2.15                     | 0.46              |
| 1:A:1250:C:O2'    | 1:A:1251:C:H5'    | 2.16                     | 0.46              |
| 1:A:1594:C:C2     | 1:A:1601:G:N2     | 2.83                     | 0.46              |
| 9:I:12:ILE:HB     | 37:I:4714:HOH:O   | 2.15                     | 0.46              |
| 10:J:157:ILE:CG2  | 10:J:158:ASN:N    | 2.79                     | 0.46              |
| 12:L:99:ASP:OD1   | 12:L:101:ASN:N    | 2.47                     | 0.46              |
| 14:N:39:ARG:HA    | 14:N:63:VAL:HG22  | 1.98                     | 0.46              |
| 14:N:87:MET:H     | 14:N:87:MET:HG3   | 1.29                     | 0.46              |
| 15:O:50:LEU:HD12  | 15:O:50:LEU:HA    | 1.71                     | 0.46              |
| 19:S:111:ILE:HG23 | 19:S:145:LEU:CD1  | 2.45                     | 0.46              |
| 22:V:44:ARG:CB    | 37:V:3805:HOH:O   | 2.63                     | 0.46              |
| 24:X:13:MET:HA    | 37:X:4944:HOH:O   | 2.16                     | 0.46              |
| 24:X:21:LEU:HB3   | 24:X:26:ILE:HG12  | 1.97                     | 0.46              |
| 24:X:65:VAL:HA    | 24:X:68:THR:CG2   | 2.45                     | 0.46              |
| 24:X:122:ARG:NH1  | 24:X:122:ARG:CG   | 2.79                     | 0.46              |
| 26:Z:178:HIS:CG   | 26:Z:179:PRO:HD2  | 2.51                     | 0.46              |
| 27:1:50:ALA:HB3   | 27:1:54:ILE:HG22  | 1.97                     | 0.46              |
| 1:A:275:G:C2      | 1:A:376:C:C2      | 3.04                     | 0.46              |
| 1:A:283:U:H5''    | 1:A:284:C:OP2     | 2.16                     | 0.46              |
| 1:A:382:U:O2'     | 1:A:430:A:H1'     | 2.15                     | 0.46              |
| 1:A:426:G:H2'     | 1:A:427:C:O4'     | 2.15                     | 0.46              |
| 1:A:1384:C:H5'    | 25:Y:30:MET:HG2   | 1.96                     | 0.46              |
| 1:A:1902:G:N2     | 1:A:1936:C:C2     | 2.83                     | 0.46              |
| 1:A:2443:C:H3'    | 37:A:3056:HOH:O   | 2.15                     | 0.46              |
| 37:B:8465:HOH:O   | 15:O:147:ILE:HB   | 2.15                     | 0.46              |
| 3:C:70:ALA:HA     | 3:C:71:PRO:HD3    | 1.74                     | 0.46              |
| 3:C:232:ARG:NH2   | 3:C:236:GLY:O     | 2.40                     | 0.46              |
| 4:D:54:VAL:O      | 4:D:55:ASN:C      | 2.58                     | 0.46              |
| 4:D:313:PRO:O     | 4:D:314:ALA:C     | 2.59                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:59:GLY:C      | 6:F:61:PHE:H      | 2.20                     | 0.46              |
| 6:F:94:ALA:O      | 6:F:95:THR:O      | 2.33                     | 0.46              |
| 11:K:39:VAL:HG12  | 11:K:40:ASN:ND2   | 2.31                     | 0.46              |
| 14:N:155:HIS:CE1  | 14:N:158:ARG:HE   | 2.33                     | 0.46              |
| 1:A:51:G:C2       | 1:A:111:C:C2      | 3.04                     | 0.46              |
| 1:A:121:U:OP2     | 29:3:10:ARG:NH2   | 2.36                     | 0.46              |
| 1:A:417:G:P       | 37:A:6989:HOH:O   | 2.72                     | 0.46              |
| 1:A:816:G:C6      | 1:A:817:G:N1      | 2.83                     | 0.46              |
| 1:A:1335:C:H2'    | 1:A:1336:U:C6     | 2.51                     | 0.46              |
| 1:A:2673:U:C2     | 1:A:2817:G:N2     | 2.84                     | 0.46              |
| 1:A:2909:G:O2'    | 1:A:2910:A:H5'    | 2.16                     | 0.46              |
| 5:E:118:THR:CG2   | 5:E:137:PRO:HB3   | 2.45                     | 0.46              |
| 6:F:23:VAL:CG2    | 6:F:73:VAL:HB     | 2.45                     | 0.46              |
| 7:G:5:LEU:HD21    | 7:G:66:GLN:HG3    | 1.98                     | 0.46              |
| 8:H:110:GLU:HA    | 8:H:113:ASP:OD2   | 2.15                     | 0.46              |
| 10:J:1:LYS:HA     | 10:J:2:PRO:HD3    | 1.67                     | 0.46              |
| 12:L:13:GLU:O     | 12:L:14:LYS:C     | 2.59                     | 0.46              |
| 14:N:164:THR:HG23 | 14:N:165:SER:OG   | 2.15                     | 0.46              |
| 15:O:32:PRO:HD2   | 15:O:99:GLU:O     | 2.16                     | 0.46              |
| 15:O:71:TRP:N     | 37:O:8539:HOH:O   | 2.48                     | 0.46              |
| 16:P:47:ARG:NH1   | 37:P:4564:HOH:O   | 2.48                     | 0.46              |
| 17:Q:64:GLU:HG2   | 37:Q:2495:HOH:O   | 2.14                     | 0.46              |
| 27:1:34:LYS:HE2   | 37:1:8426:HOH:O   | 2.15                     | 0.46              |
| 1:A:425:U:O2'     | 1:A:426:G:H5'     | 2.16                     | 0.46              |
| 1:A:1185:U:H5'    | 37:A:7039:HOH:O   | 2.16                     | 0.46              |
| 1:A:2266:A:H2'    | 1:A:2267:G:C8     | 2.51                     | 0.46              |
| 1:A:2500:C:O2'    | 1:A:2501:G:H5'    | 2.16                     | 0.46              |
| 1:A:2533:C:H5'    | 1:A:2533:C:C6     | 2.41                     | 0.46              |
| 5:E:218:VAL:HG12  | 37:E:8419:HOH:O   | 2.15                     | 0.46              |
| 6:F:58:VAL:CG1    | 6:F:59:GLY:N      | 2.78                     | 0.46              |
| 14:N:164:THR:HG23 | 14:N:165:SER:H    | 1.76                     | 0.46              |
| 15:O:91:ARG:HG3   | 15:O:186:LEU:HD23 | 1.98                     | 0.46              |
| 1:A:80:A:H5''     | 21:U:41:ARG:CZ    | 2.46                     | 0.46              |
| 1:A:177:A:H2'     | 1:A:178:U:O4'     | 2.16                     | 0.46              |
| 1:A:1377:C:H5'    | 1:A:1377:C:C6     | 2.47                     | 0.46              |
| 1:A:2443:C:O3'    | 13:M:56:LYS:HE3   | 2.15                     | 0.46              |
| 2:B:3041:C:H4'    | 6:F:48:MET:HB2    | 1.98                     | 0.46              |
| 3:C:85:ASP:HA     | 37:C:8620:HOH:O   | 2.14                     | 0.46              |
| 4:D:211:THR:HA    | 4:D:255:GLY:O     | 2.16                     | 0.46              |
| 6:F:41:LEU:CA     | 6:F:44:ILE:HG22   | 2.45                     | 0.46              |
| 6:F:91:ALA:HB1    | 37:F:5198:HOH:O   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 7:G:69:ILE:HA    | 7:G:72:MET:HE2     | 1.97                     | 0.46              |
| 12:L:82:ARG:NH2  | 12:L:115:ARG:HG2   | 2.31                     | 0.46              |
| 13:M:146:GLY:C   | 13:M:148:GLU:H     | 2.24                     | 0.46              |
| 14:N:184:ARG:HG3 | 14:N:185:PRO:HA    | 1.98                     | 0.46              |
| 18:R:28:ARG:HG2  | 37:R:4350:HOH:O    | 2.16                     | 0.46              |
| 19:S:8:ALA:CB    | 19:S:13:THR:HG21   | 2.37                     | 0.46              |
| 1:A:396:U:O2'    | 1:A:418:C:H4'      | 2.16                     | 0.46              |
| 1:A:429:A:C6     | 1:A:430:A:C6       | 3.04                     | 0.46              |
| 1:A:559:U:H5'    | 1:A:559:U:C6       | 2.42                     | 0.46              |
| 1:A:1301:C:O2'   | 1:A:1331:A:H4'     | 2.16                     | 0.46              |
| 1:A:1419:U:O2    | 1:A:1419:U:H3'     | 2.16                     | 0.46              |
| 1:A:1461:U:H2'   | 1:A:1462:C:C6      | 2.51                     | 0.46              |
| 1:A:2502:C:C4'   | 10:J:151:MET:HG2   | 2.46                     | 0.46              |
| 1:A:2712:G:O2'   | 1:A:2713:G:H5'     | 2.16                     | 0.46              |
| 4:D:43:GLY:O     | 4:D:308:LEU:HD12   | 2.15                     | 0.46              |
| 5:E:27:ARG:O     | 5:E:31:ILE:HG13    | 2.16                     | 0.46              |
| 6:F:21:VAL:HG13  | 6:F:131:THR:O      | 2.16                     | 0.46              |
| 7:G:68:HIS:O     | 7:G:72:MET:HG3     | 2.16                     | 0.46              |
| 8:H:60:VAL:O     | 8:H:60:VAL:HG12    | 2.16                     | 0.46              |
| 15:O:73:ALA:HB2  | 15:O:163:PHE:CZ    | 2.51                     | 0.46              |
| 1:A:716:G:C2'    | 1:A:717:C:O5'      | 2.64                     | 0.46              |
| 1:A:1134:G:C5'   | 10:J:151:MET:HE1   | 2.46                     | 0.46              |
| 1:A:2072:G:C6    | 1:A:2533:C:H1'     | 2.51                     | 0.46              |
| 1:A:2251:G:H4'   | 37:A:6980:HOH:O    | 2.16                     | 0.46              |
| 3:C:36:ASP:HB2   | 3:C:84:VAL:N       | 2.31                     | 0.46              |
| 3:C:66:ARG:HB2   | 3:C:66:ARG:HH11    | 1.80                     | 0.46              |
| 4:D:132:HIS:HB2  | 4:D:137:LEU:HD22   | 1.97                     | 0.46              |
| 10:J:35:ASN:ND2  | 10:J:79:ALA:O      | 2.49                     | 0.46              |
| 10:J:114:PRO:O   | 10:J:115:PHE:C     | 2.58                     | 0.46              |
| 10:J:132:PHE:O   | 10:J:133:ILE:HD13  | 2.16                     | 0.46              |
| 14:N:35:PRO:CG   | 14:N:38:VAL:CG2    | 2.87                     | 0.46              |
| 19:S:75:TRP:CG   | 19:S:76:ASP:H      | 2.34                     | 0.46              |
| 1:A:702:G:O2'    | 1:A:703:G:H5'      | 2.16                     | 0.45              |
| 1:A:861:A:H2'    | 1:A:862:U:C6       | 2.51                     | 0.45              |
| 1:A:941:G:O2'    | 1:A:942:U:H5'      | 2.16                     | 0.45              |
| 1:A:1368:U:O5'   | 1:A:1368:U:H6      | 1.99                     | 0.45              |
| 1:A:2346:C:O3'   | 6:F:52:THR:HG23    | 2.16                     | 0.45              |
| 1:A:2361:A:H5'   | 1:A:2361:A:H8      | 1.81                     | 0.45              |
| 1:A:2645:U:H4'   | 31:A:8600:ZIT:H172 | 1.98                     | 0.45              |
| 10:J:26:LYS:CD   | 10:J:28:ILE:HB     | 2.46                     | 0.45              |
| 23:W:38:GLY:C    | 23:W:40:PRO:HD2    | 2.41                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:380:A:H5''    | 14:N:48:ARG:NH2  | 2.31                     | 0.45              |
| 1:A:790:A:H2'     | 1:A:791:A:O4'    | 2.16                     | 0.45              |
| 1:A:2413:A:N7     | 15:O:109:PRO:HB3 | 2.32                     | 0.45              |
| 4:D:144:THR:HG22  | 4:D:145:HIS:N    | 2.31                     | 0.45              |
| 5:E:126:ASP:C     | 5:E:128:GLY:N    | 2.72                     | 0.45              |
| 7:G:11:VAL:CG1    | 7:G:12:ASP:H     | 2.29                     | 0.45              |
| 7:G:95:VAL:O      | 7:G:126:ILE:HD13 | 2.16                     | 0.45              |
| 8:H:50:VAL:CG1    | 8:H:60:VAL:HG11  | 2.43                     | 0.45              |
| 11:K:45:VAL:HG21  | 11:K:129:PHE:CD1 | 2.52                     | 0.45              |
| 13:M:54:PRO:HG2   | 13:M:57:VAL:CG2  | 2.47                     | 0.45              |
| 14:N:62:VAL:C     | 14:N:63:VAL:HG23 | 2.41                     | 0.45              |
| 15:O:154:LEU:CG   | 15:O:155:GLU:H   | 2.27                     | 0.45              |
| 17:Q:103:THR:O    | 17:Q:107:GLU:HG3 | 2.16                     | 0.45              |
| 21:U:96:VAL:HG13  | 21:U:97:ARG:N    | 2.31                     | 0.45              |
| 1:A:57:C:H5''     | 37:A:6335:HOH:O  | 2.16                     | 0.45              |
| 1:A:314:G:N2      | 1:A:316:A:H3'    | 2.31                     | 0.45              |
| 1:A:492:C:C2'     | 1:A:493:U:H5'    | 2.46                     | 0.45              |
| 1:A:913:A:N3      | 1:A:1042:U:O2'   | 2.48                     | 0.45              |
| 1:A:1060:C:O2'    | 1:A:1061:C:H5'   | 2.16                     | 0.45              |
| 1:A:1129:C:H5''   | 1:A:1130:U:OP2   | 2.16                     | 0.45              |
| 1:A:1450:C:C4'    | 1:A:1451:C:OP2   | 2.59                     | 0.45              |
| 1:A:1617:C:C4     | 1:A:1643:C:H4'   | 2.51                     | 0.45              |
| 1:A:1669:A:H2'    | 1:A:1670:G:H8    | 1.81                     | 0.45              |
| 3:C:200:PRO:HD3   | 37:C:8523:HOH:O  | 2.15                     | 0.45              |
| 4:D:88:GLU:O      | 4:D:88:GLU:HG3   | 2.15                     | 0.45              |
| 6:F:94:ALA:HB3    | 6:F:174:VAL:CA   | 2.46                     | 0.45              |
| 7:G:133:VAL:HG12  | 7:G:141:VAL:HG13 | 1.98                     | 0.45              |
| 15:O:184:ILE:HG22 | 15:O:185:GLU:N   | 2.30                     | 0.45              |
| 30:4:87:ARG:HG3   | 37:4:8572:HOH:O  | 2.16                     | 0.45              |
| 1:A:45:A:N6       | 1:A:147:G:C4     | 2.84                     | 0.45              |
| 1:A:278:A:H2'     | 1:A:279:C:O4'    | 2.17                     | 0.45              |
| 1:A:1972:U:H2'    | 1:A:1973:A:H5'   | 1.99                     | 0.45              |
| 1:A:2661:U:H3     | 1:A:2812:A:H62   | 1.64                     | 0.45              |
| 1:A:2814:A:OP2    | 37:A:4646:HOH:O  | 2.21                     | 0.45              |
| 1:A:2852:A:H5''   | 37:A:4808:HOH:O  | 2.16                     | 0.45              |
| 3:C:153:ARG:HD3   | 37:C:8533:HOH:O  | 2.15                     | 0.45              |
| 4:D:248:ARG:HG2   | 37:K:3517:HOH:O  | 2.15                     | 0.45              |
| 5:E:211:ASP:HB2   | 5:E:231:ARG:HH12 | 1.81                     | 0.45              |
| 6:F:84:LEU:HA     | 6:F:87:ALA:HB3   | 1.98                     | 0.45              |
| 6:F:92:GLU:O      | 6:F:93:LEU:O     | 2.33                     | 0.45              |
| 10:J:84:ARG:CZ    | 10:J:135:TRP:CH2 | 3.00                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:99:ASP:OD1   | 12:L:99:ASP:C     | 2.58                     | 0.45              |
| 13:M:20:ASN:O     | 13:M:22:ARG:N     | 2.50                     | 0.45              |
| 14:N:114:VAL:HG21 | 14:N:159:THR:HG21 | 1.99                     | 0.45              |
| 15:O:37:ARG:HD3   | 15:O:37:ARG:HA    | 1.82                     | 0.45              |
| 15:O:37:ARG:HA    | 35:O:8507:CL:CL   | 2.53                     | 0.45              |
| 16:P:77:ALA:HA    | 16:P:96:VAL:O     | 2.16                     | 0.45              |
| 1:A:236:A:H4'     | 1:A:237:G:OP1     | 2.16                     | 0.45              |
| 1:A:303:C:H2'     | 1:A:304:G:O4'     | 2.16                     | 0.45              |
| 1:A:1815:A:H4'    | 1:A:2751:C:O4'    | 2.16                     | 0.45              |
| 3:C:192:VAL:HG12  | 3:C:192:VAL:O     | 2.16                     | 0.45              |
| 4:D:36:PRO:CA     | 4:D:168:GLY:HA3   | 2.43                     | 0.45              |
| 4:D:320:GLN:HG3   | 4:D:321:PRO:CD    | 2.46                     | 0.45              |
| 5:E:246:ARG:NH2   | 37:E:8419:HOH:O   | 2.50                     | 0.45              |
| 6:F:59:GLY:O      | 6:F:61:PHE:N      | 2.38                     | 0.45              |
| 7:G:132:THR:O     | 7:G:132:THR:HG23  | 2.16                     | 0.45              |
| 10:J:13:ALA:HA    | 10:J:91:HIS:CE1   | 2.52                     | 0.45              |
| 12:L:72:VAL:HG11  | 12:L:121:PHE:CD1  | 2.52                     | 0.45              |
| 12:L:87:ARG:CZ    | 37:L:4854:HOH:O   | 2.63                     | 0.45              |
| 17:Q:16:VAL:CG1   | 17:Q:17:GLY:N     | 2.80                     | 0.45              |
| 23:W:39:ALA:C     | 23:W:41:GLU:N     | 2.74                     | 0.45              |
| 24:X:90:TYR:CE2   | 24:X:99:ALA:HB2   | 2.51                     | 0.45              |
| 28:2:37:CYS:SG    | 28:2:39:PHE:HB2   | 2.56                     | 0.45              |
| 1:A:236:A:C4'     | 1:A:237:G:H5'     | 2.40                     | 0.45              |
| 1:A:240:C:O2      | 1:A:240:C:H2'     | 2.17                     | 0.45              |
| 1:A:1750:C:N4     | 1:A:1751:G:C6     | 2.85                     | 0.45              |
| 1:A:2316:G:H4'    | 37:A:5671:HOH:O   | 2.16                     | 0.45              |
| 1:A:2860:G:H1'    | 37:A:6376:HOH:O   | 2.16                     | 0.45              |
| 37:A:3563:HOH:O   | 21:U:82:THR:HA    | 2.17                     | 0.45              |
| 3:C:39:ALA:HB3    | 3:C:61:GLU:OE2    | 2.16                     | 0.45              |
| 3:C:132:ASP:OD1   | 3:C:133:ARG:N     | 2.48                     | 0.45              |
| 8:H:48:VAL:CG2    | 8:H:74:PHE:HB3    | 2.46                     | 0.45              |
| 12:L:40:THR:O     | 12:L:41:LYS:C     | 2.60                     | 0.45              |
| 14:N:37:VAL:HG22  | 14:N:65:VAL:HG22  | 1.99                     | 0.45              |
| 16:P:73:ASP:HA    | 16:P:92:VAL:O     | 2.17                     | 0.45              |
| 18:R:22:GLY:O     | 18:R:23:THR:C     | 2.59                     | 0.45              |
| 20:T:15:MET:HE1   | 20:T:18:MET:HE1   | 1.98                     | 0.45              |
| 24:X:67:ALA:HB2   | 24:X:93:ILE:HD13  | 1.98                     | 0.45              |
| 26:Z:187:VAL:HG12 | 26:Z:205:ILE:HA   | 1.97                     | 0.45              |
| 1:A:123:U:H2'     | 1:A:124:C:C6      | 2.52                     | 0.45              |
| 1:A:625:U:H5'     | 37:A:9771:HOH:O   | 2.15                     | 0.45              |
| 1:A:885:G:H5''    | 1:A:886:A:H5'     | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1118:A:C8    | 1:A:1119:G:H5''  | 2.52                     | 0.45              |
| 1:A:1197:G:N2    | 37:A:5811:HOH:O  | 2.49                     | 0.45              |
| 1:A:1209:C:O2    | 1:A:1210:G:C8    | 2.69                     | 0.45              |
| 1:A:1335:C:OP2   | 26:Z:207:SER:CB  | 2.65                     | 0.45              |
| 1:A:1730:G:H5'   | 1:A:1731:C:C6    | 2.52                     | 0.45              |
| 1:A:2353:A:H4'   | 1:A:2354:A:O5'   | 2.17                     | 0.45              |
| 1:A:2781:U:H2'   | 1:A:2782:G:C5'   | 2.46                     | 0.45              |
| 3:C:164:ARG:HB2  | 27:1:68:CYS:SG   | 2.56                     | 0.45              |
| 6:F:159:PRO:O    | 6:F:162:ALA:HB3  | 2.16                     | 0.45              |
| 8:H:48:VAL:HG23  | 8:H:74:PHE:CB    | 2.47                     | 0.45              |
| 15:O:37:ARG:CZ   | 37:O:8534:HOH:O  | 2.64                     | 0.45              |
| 15:O:38:LYS:HE3  | 15:O:38:LYS:HB2  | 1.64                     | 0.45              |
| 22:V:17:THR:HG22 | 22:V:18:GLY:N    | 2.31                     | 0.45              |
| 25:Y:43:VAL:HG22 | 25:Y:76:ARG:NH1  | 2.32                     | 0.45              |
| 28:2:44:LYS:NZ   | 37:2:8458:HOH:O  | 2.46                     | 0.45              |
| 29:3:18:ASN:HD22 | 29:3:18:ASN:HA   | 1.58                     | 0.45              |
| 1:A:716:G:H2'    | 1:A:717:C:O5'    | 2.17                     | 0.45              |
| 1:A:1205:U:C2'   | 1:A:1206:U:H5'   | 2.41                     | 0.45              |
| 1:A:2106:C:H2'   | 1:A:2107:U:C6    | 2.51                     | 0.45              |
| 1:A:2670:G:O2'   | 1:A:2671:U:H5'   | 2.16                     | 0.45              |
| 1:A:2851:G:C2'   | 1:A:2852:A:H5'   | 2.47                     | 0.45              |
| 2:B:3042:C:O2    | 6:F:76:ARG:NH1   | 2.50                     | 0.45              |
| 2:B:3064:C:C2'   | 2:B:3065:A:H5'   | 2.47                     | 0.45              |
| 2:B:3096:C:H2'   | 2:B:3097:U:C6    | 2.52                     | 0.45              |
| 3:C:94:LEU:HG    | 3:C:99:ILE:CD1   | 2.46                     | 0.45              |
| 7:G:107:PHE:CZ   | 7:G:108:LEU:HD13 | 2.52                     | 0.45              |
| 13:M:97:VAL:HG12 | 13:M:98:GLU:O    | 2.17                     | 0.45              |
| 13:M:130:ARG:NH2 | 37:M:8418:HOH:O  | 2.50                     | 0.45              |
| 18:R:72:LYS:HG2  | 18:R:85:ILE:HD13 | 1.99                     | 0.45              |
| 26:Z:187:VAL:HB  | 37:Z:8158:HOH:O  | 2.17                     | 0.45              |
| 30:4:91:GLN:O    | 30:4:92:GLU:HB2  | 2.17                     | 0.45              |
| 1:A:949:U:O2'    | 18:R:40:HIS:HE1  | 2.00                     | 0.45              |
| 1:A:1252:A:H2'   | 1:A:1253:C:O4'   | 2.17                     | 0.45              |
| 1:A:1574:C:H6    | 1:A:1574:C:O5'   | 1.99                     | 0.45              |
| 1:A:1593:C:OP1   | 17:Q:117:SER:CB  | 2.65                     | 0.45              |
| 1:A:1635:U:O2'   | 1:A:1636:G:H5'   | 2.17                     | 0.45              |
| 1:A:2050:G:H5''  | 19:S:80:TYR:O    | 2.17                     | 0.45              |
| 1:A:2729:C:O2'   | 1:A:2730:G:H5'   | 2.17                     | 0.45              |
| 2:B:3004:G:O2'   | 15:O:44:ARG:NH2  | 2.50                     | 0.45              |
| 6:F:35:ALA:C     | 6:F:37:ALA:N     | 2.74                     | 0.45              |
| 6:F:65:GLU:HA    | 37:F:6752:HOH:O  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:169:THR:C    | 6:F:170:TYR:HD1  | 2.24                     | 0.45              |
| 12:L:30:LYS:C    | 12:L:55:VAL:HG13 | 2.42                     | 0.45              |
| 14:N:55:LYS:HB2  | 14:N:60:ILE:CD1  | 2.46                     | 0.45              |
| 15:O:67:ALA:HA   | 15:O:71:TRP:H    | 1.82                     | 0.45              |
| 18:R:64:GLU:HG3  | 18:R:74:ASP:OD2  | 2.17                     | 0.45              |
| 19:S:82:GLU:HG3  | 19:S:83:LYS:H    | 1.81                     | 0.45              |
| 19:S:119:VAL:O   | 19:S:119:VAL:CG1 | 2.63                     | 0.45              |
| 22:V:49:LEU:HD11 | 37:V:3805:HOH:O  | 2.16                     | 0.45              |
| 27:1:56:MET:HA   | 27:1:62:TYR:O    | 2.17                     | 0.45              |
| 30:4:70:ARG:HG2  | 30:4:70:ARG:NH1  | 2.32                     | 0.45              |
| 1:A:830:G:H2'    | 1:A:831:U:C6     | 2.51                     | 0.45              |
| 1:A:1535:G:H2'   | 1:A:1536:C:C6    | 2.52                     | 0.45              |
| 1:A:1634:G:H2'   | 1:A:1635:U:C6    | 2.51                     | 0.45              |
| 1:A:1810:C:OP1   | 22:V:44:ARG:NE   | 2.28                     | 0.45              |
| 1:A:2039:A:H4'   | 1:A:2760:C:O2'   | 2.17                     | 0.45              |
| 1:A:2273:C:OP1   | 37:A:9184:HOH:O  | 2.21                     | 0.45              |
| 37:A:8939:HOH:O  | 28:2:1:THR:HA    | 2.17                     | 0.45              |
| 5:E:214:THR:CG2  | 37:E:8433:HOH:O  | 2.55                     | 0.45              |
| 6:F:15:GLU:HA    | 6:F:16:PRO:HD3   | 1.89                     | 0.45              |
| 6:F:60:GLU:C     | 6:F:62:ASP:N     | 2.73                     | 0.45              |
| 10:J:71:TYR:O    | 10:J:73:GLN:N    | 2.50                     | 0.45              |
| 14:N:20:ILE:O    | 14:N:24:MET:HG2  | 2.17                     | 0.45              |
| 15:O:38:LYS:HE2  | 15:O:107:ASN:ND2 | 2.32                     | 0.45              |
| 15:O:58:LEU:HD12 | 15:O:58:LEU:N    | 2.32                     | 0.45              |
| 15:O:67:ALA:C    | 15:O:69:TYR:H    | 2.25                     | 0.45              |
| 15:O:163:PHE:O   | 15:O:164:ASP:O   | 2.35                     | 0.45              |
| 16:P:96:VAL:HG13 | 16:P:100:GLN:HB2 | 1.99                     | 0.45              |
| 16:P:107:GLU:O   | 16:P:108:GLY:C   | 2.60                     | 0.45              |
| 23:W:12:THR:HG23 | 23:W:14:ALA:N    | 2.32                     | 0.45              |
| 24:X:3:ALA:O     | 24:X:54:PHE:HA   | 2.17                     | 0.45              |
| 24:X:13:MET:HE3  | 24:X:17:ILE:CG2  | 2.46                     | 0.45              |
| 27:1:10:ARG:HG3  | 27:1:11:THR:N    | 2.32                     | 0.45              |
| 28:2:22:CYS:SG   | 28:2:24:GLU:HB2  | 2.57                     | 0.45              |
| 1:A:251:C:H1'    | 14:N:58:GLN:HE22 | 1.81                     | 0.44              |
| 1:A:542:A:H1'    | 37:A:4253:HOH:O  | 2.17                     | 0.44              |
| 1:A:869:G:OP1    | 14:N:79:LYS:HE2  | 2.16                     | 0.44              |
| 1:A:1008:C:OP1   | 10:J:16:ARG:NH2  | 2.49                     | 0.44              |
| 1:A:1164:U:O4'   | 1:A:1165:G:OP1   | 2.34                     | 0.44              |
| 1:A:1549:C:N3    | 1:A:1637:A:C2    | 2.84                     | 0.44              |
| 1:A:1666:C:O2'   | 1:A:1667:A:C5'   | 2.60                     | 0.44              |
| 1:A:2387:U:H2'   | 1:A:2388:C:C6    | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2898:G:H4'    | 4:D:288:GLY:HA2   | 1.98                     | 0.44              |
| 1:A:2911:C:H2'    | 1:A:2912:C:C6     | 2.53                     | 0.44              |
| 37:A:9534:HOH:O   | 25:Y:23:HIS:HD2   | 1.99                     | 0.44              |
| 2:B:3078:G:O2'    | 2:B:3079:U:P      | 2.75                     | 0.44              |
| 4:D:307:ARG:CG    | 4:D:307:ARG:NH1   | 2.80                     | 0.44              |
| 6:F:167:GLU:OE2   | 6:F:173:GLU:HG2   | 2.17                     | 0.44              |
| 10:J:82:LYS:NZ    | 10:J:82:LYS:CB    | 2.80                     | 0.44              |
| 17:Q:16:VAL:CG1   | 17:Q:20:ARG:HB2   | 2.48                     | 0.44              |
| 1:A:88:G:N7       | 29:3:28:LYS:HD2   | 2.31                     | 0.44              |
| 1:A:764:C:C2'     | 1:A:765:G:H5'     | 2.46                     | 0.44              |
| 1:A:1095:U:O2     | 24:X:120:PRO:HG2  | 2.17                     | 0.44              |
| 1:A:1532:G:C6     | 1:A:1533:A:C6     | 3.05                     | 0.44              |
| 3:C:101:GLU:HG2   | 3:C:131:HIS:ND1   | 2.32                     | 0.44              |
| 4:D:23:THR:HG23   | 4:D:162:MET:HE3   | 1.99                     | 0.44              |
| 10:J:58:HIS:CE1   | 10:J:59:ASN:ND2   | 2.85                     | 0.44              |
| 19:S:119:VAL:HG21 | 19:S:142:ASP:CG   | 2.42                     | 0.44              |
| 29:3:36:ASN:HB3   | 29:3:39:ARG:NE    | 2.32                     | 0.44              |
| 30:4:56:PRO:HA    | 37:4:8550:HOH:O   | 2.17                     | 0.44              |
| 1:A:120:A:H2'     | 1:A:120:A:N3      | 2.32                     | 0.44              |
| 1:A:764:C:H2'     | 1:A:765:G:O4'     | 2.17                     | 0.44              |
| 1:A:963:C:H2'     | 1:A:964:G:C8      | 2.52                     | 0.44              |
| 1:A:1746:A:N3     | 1:A:1748:U:C4     | 2.85                     | 0.44              |
| 1:A:2274:A:H4'    | 14:N:77:PHE:HE1   | 1.82                     | 0.44              |
| 2:B:3039:U:H3'    | 2:B:3040:C:H5'    | 1.98                     | 0.44              |
| 3:C:51:ARG:HB2    | 37:C:8609:HOH:O   | 2.16                     | 0.44              |
| 3:C:220:PRO:HD2   | 3:C:223:ARG:HD3   | 1.99                     | 0.44              |
| 7:G:36:PRO:HD3    | 11:K:127:ILE:HD12 | 1.98                     | 0.44              |
| 7:G:118:ILE:HG23  | 7:G:144:THR:HG21  | 1.99                     | 0.44              |
| 7:G:139:GLU:CD    | 37:G:5919:HOH:O   | 2.60                     | 0.44              |
| 9:I:63:ARG:HB2    | 9:I:66:LEU:HG     | 1.99                     | 0.44              |
| 10:J:137:ASN:O    | 10:J:138:PRO:C    | 2.58                     | 0.44              |
| 14:N:47:ASP:CG    | 14:N:48:ARG:H     | 2.25                     | 0.44              |
| 15:O:48:VAL:HG13  | 15:O:55:ASP:HB3   | 1.95                     | 0.44              |
| 17:Q:13:VAL:HG11  | 17:Q:40:VAL:CG1   | 2.48                     | 0.44              |
| 18:R:41:LEU:HB3   | 18:R:52:PHE:CZ    | 2.52                     | 0.44              |
| 26:Z:144:ARG:HH11 | 26:Z:144:ARG:CG   | 2.29                     | 0.44              |
| 1:A:201:G:N2      | 1:A:202:U:C2      | 2.86                     | 0.44              |
| 1:A:244:C:OP2     | 8:H:38:LYS:HE3    | 2.18                     | 0.44              |
| 1:A:492:C:O2'     | 1:A:493:U:H5'     | 2.18                     | 0.44              |
| 1:A:853:C:H2'     | 1:A:854:G:O4'     | 2.17                     | 0.44              |
| 1:A:1157:C:C2     | 1:A:1158:G:C8     | 3.05                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1926:G:H2'    | 1:A:1927:A:C8    | 2.53                     | 0.44              |
| 1:A:2791:U:H4'    | 1:A:2792:A:OP1   | 2.17                     | 0.44              |
| 2:B:3027:C:OP1    | 15:O:39:SER:OG   | 2.33                     | 0.44              |
| 2:B:3031:C:H2'    | 2:B:3032:G:O4'   | 2.17                     | 0.44              |
| 6:F:81:GLU:C      | 6:F:83:PHE:N     | 2.76                     | 0.44              |
| 13:M:72:ASN:O     | 13:M:76:LEU:HG   | 2.18                     | 0.44              |
| 13:M:143:THR:HG21 | 37:M:8412:HOH:O  | 2.16                     | 0.44              |
| 14:N:74:ARG:HD3   | 14:N:91:ILE:HD12 | 2.00                     | 0.44              |
| 15:O:139:TRP:CH2  | 15:O:176:ARG:NH1 | 2.85                     | 0.44              |
| 16:P:32:ARG:HD3   | 16:P:32:ARG:C    | 2.41                     | 0.44              |
| 30:4:70:ARG:HG2   | 30:4:70:ARG:HH11 | 1.81                     | 0.44              |
| 1:A:61:G:C2       | 1:A:62:C:C2      | 3.05                     | 0.44              |
| 1:A:266:G:C2      | 1:A:267:G:C8     | 3.06                     | 0.44              |
| 1:A:1299:G:N7     | 13:M:6:ARG:NH1   | 2.65                     | 0.44              |
| 1:A:1747:A:O3'    | 1:A:2584:G:H5'   | 2.17                     | 0.44              |
| 1:A:2719:A:N1     | 4:D:70:PRO:HG3   | 2.32                     | 0.44              |
| 1:A:2781:U:O2'    | 1:A:2782:G:H5'   | 2.18                     | 0.44              |
| 37:A:4797:HOH:O   | 12:L:37:TYR:CE1  | 2.70                     | 0.44              |
| 2:B:3104:A:O2'    | 2:B:3105:A:H5'   | 2.18                     | 0.44              |
| 4:D:248:ARG:O     | 4:D:251:VAL:CG1  | 2.66                     | 0.44              |
| 5:E:27:ARG:HD2    | 16:P:5:PRO:HD2   | 2.00                     | 0.44              |
| 5:E:246:ARG:CZ    | 37:E:8419:HOH:O  | 2.65                     | 0.44              |
| 10:J:149:ALA:C    | 10:J:151:MET:H   | 2.24                     | 0.44              |
| 15:O:154:LEU:O    | 15:O:155:GLU:CB  | 2.63                     | 0.44              |
| 19:S:39:THR:HG22  | 19:S:41:GLY:H    | 1.82                     | 0.44              |
| 21:U:49:GLU:OE2   | 21:U:97:ARG:NH1  | 2.43                     | 0.44              |
| 26:Z:133:HIS:CD2  | 37:Z:8169:HOH:O  | 2.57                     | 0.44              |
| 1:A:686:A:O2'     | 1:A:747:G:H4'    | 2.18                     | 0.44              |
| 1:A:777:U:HO2'    | 28:2:11:LYS:HG2  | 1.81                     | 0.44              |
| 1:A:1072:G:OP2    | 26:Z:154:ARG:NH2 | 2.51                     | 0.44              |
| 1:A:1730:G:H4'    | 1:A:1731:C:O5'   | 2.17                     | 0.44              |
| 1:A:2505:G:C2'    | 1:A:2506:A:H5'   | 2.47                     | 0.44              |
| 1:A:2723:G:H1'    | 37:A:4410:HOH:O  | 2.16                     | 0.44              |
| 37:A:5139:HOH:O   | 12:L:41:LYS:HE3  | 2.17                     | 0.44              |
| 37:A:9281:HOH:O   | 4:D:254:GLN:HG3  | 2.16                     | 0.44              |
| 3:C:48:ASP:HB3    | 37:C:8609:HOH:O  | 2.17                     | 0.44              |
| 3:C:192:VAL:CG1   | 3:C:207:GLN:HB3  | 2.48                     | 0.44              |
| 3:C:195:ASN:O     | 3:C:196:ALA:C    | 2.60                     | 0.44              |
| 4:D:27:ASN:HD22   | 4:D:27:ASN:H     | 1.66                     | 0.44              |
| 4:D:60:SER:C      | 4:D:62:ARG:N     | 2.74                     | 0.44              |
| 7:G:11:VAL:HG11   | 7:G:22:VAL:HG13  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:99:THR:O     | 8:H:100:ASP:HB2  | 2.18                     | 0.44              |
| 10:J:141:ASN:CA  | 37:J:8369:HOH:O  | 2.56                     | 0.44              |
| 13:M:41:HIS:O    | 13:M:42:ASN:HB2  | 2.18                     | 0.44              |
| 23:W:1:THR:HG23  | 23:W:2:VAL:N     | 2.23                     | 0.44              |
| 27:1:30:GLU:O    | 27:1:33:HIS:HB3  | 2.17                     | 0.44              |
| 1:A:1380:U:O4    | 1:A:2043:U:H4'   | 2.17                     | 0.44              |
| 1:A:2659:U:C4'   | 19:S:76:ASP:HB3  | 2.48                     | 0.44              |
| 1:A:2727:A:N6    | 1:A:2756:U:C6    | 2.86                     | 0.44              |
| 2:B:3020:G:H3'   | 37:B:8435:HOH:O  | 2.17                     | 0.44              |
| 2:B:3054:A:O2'   | 2:B:3055:U:H5'   | 2.18                     | 0.44              |
| 14:N:46:LEU:HB2  | 37:N:8606:HOH:O  | 2.17                     | 0.44              |
| 15:O:108:SER:HA  | 15:O:109:PRO:HD3 | 1.84                     | 0.44              |
| 15:O:143:ARG:NH1 | 15:O:173:ASP:OD1 | 2.51                     | 0.44              |
| 24:X:40:ALA:O    | 24:X:44:MET:HG3  | 2.18                     | 0.44              |
| 28:2:45:ARG:NH1  | 37:2:8435:HOH:O  | 2.50                     | 0.44              |
| 1:A:10:U:HO2'    | 1:A:11:A:P       | 2.41                     | 0.44              |
| 1:A:134:U:C2     | 1:A:145:A:C2     | 3.06                     | 0.44              |
| 1:A:382:U:C5     | 1:A:406:G:N2     | 2.86                     | 0.44              |
| 1:A:820:G:OP2    | 3:C:171:LYS:NZ   | 2.44                     | 0.44              |
| 1:A:941:G:C5     | 1:A:942:U:C4     | 3.06                     | 0.44              |
| 1:A:2673:U:C2    | 1:A:2817:G:C2    | 3.06                     | 0.44              |
| 37:A:4159:HOH:O  | 14:N:87:MET:HE1  | 2.18                     | 0.44              |
| 37:A:5709:HOH:O  | 29:3:20:ARG:HB3  | 2.17                     | 0.44              |
| 4:D:129:ARG:O    | 4:D:133:GLU:HG3  | 2.18                     | 0.44              |
| 6:F:59:GLY:C     | 6:F:61:PHE:N     | 2.75                     | 0.44              |
| 11:K:6:PHE:HB3   | 11:K:109:TYR:OH  | 2.18                     | 0.44              |
| 15:O:154:LEU:C   | 15:O:156:GLU:H   | 2.24                     | 0.44              |
| 17:Q:134:VAL:O   | 17:Q:137:LEU:HB3 | 2.17                     | 0.44              |
| 1:A:241:A:N1     | 1:A:378:A:H4'    | 2.33                     | 0.44              |
| 1:A:316:A:H1'    | 1:A:336:G:N3     | 2.32                     | 0.44              |
| 1:A:394:G:H1     | 14:N:181:GLU:CD  | 2.26                     | 0.44              |
| 1:A:511:A:H1'    | 37:A:7229:HOH:O  | 2.18                     | 0.44              |
| 1:A:945:U:H2'    | 1:A:946:C:C6     | 2.53                     | 0.44              |
| 1:A:1021:G:O2'   | 1:A:1022:A:H5'   | 2.18                     | 0.44              |
| 1:A:1085:C:H2'   | 1:A:1086:A:O4'   | 2.18                     | 0.44              |
| 1:A:2467:A:H2'   | 37:A:5033:HOH:O  | 2.18                     | 0.44              |
| 1:A:2563:U:H2'   | 1:A:2565:C:O5'   | 2.17                     | 0.44              |
| 1:A:2831:C:H2'   | 1:A:2832:C:H5'   | 2.00                     | 0.44              |
| 3:C:57:ALA:HA    | 3:C:67:LEU:HD23  | 2.00                     | 0.44              |
| 6:F:99:ASP:HB2   | 6:F:103:ASN:CB   | 2.47                     | 0.44              |
| 8:H:79:GLN:HG3   | 8:H:82:ASP:OD2   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:140:PRO:HA  | 10:J:142:VAL:HG12 | 1.99                     | 0.44              |
| 14:N:18:GLY:O    | 14:N:21:ALA:HB3   | 2.18                     | 0.44              |
| 14:N:67:ILE:HD11 | 14:N:104:ARG:HD2  | 1.98                     | 0.44              |
| 15:O:73:ALA:HB1  | 15:O:74:PRO:CD    | 2.47                     | 0.44              |
| 15:O:73:ALA:HB1  | 15:O:74:PRO:HD2   | 1.99                     | 0.44              |
| 21:U:43:ASN:C    | 21:U:45:GLY:H     | 2.26                     | 0.44              |
| 23:W:12:THR:CG2  | 23:W:15:GLU:HG3   | 2.24                     | 0.44              |
| 28:2:8:GLN:HE22  | 28:2:11:LYS:HZ1   | 1.65                     | 0.44              |
| 1:A:159:G:H5''   | 14:N:74:ARG:HH22  | 1.82                     | 0.43              |
| 1:A:204:A:H2'    | 1:A:205:U:C5'     | 2.46                     | 0.43              |
| 1:A:213:G:O2'    | 1:A:214:U:OP2     | 2.36                     | 0.43              |
| 1:A:469:G:C6     | 1:A:473:A:N6      | 2.86                     | 0.43              |
| 1:A:926:A:O2'    | 13:M:41:HIS:HD2   | 2.00                     | 0.43              |
| 1:A:1434:A:H2'   | 1:A:1436:C:C5     | 2.53                     | 0.43              |
| 1:A:1656:A:H2'   | 1:A:1657:A:O4'    | 2.18                     | 0.43              |
| 1:A:1878:G:HO2'  | 1:A:1879:U:H6     | 1.61                     | 0.43              |
| 1:A:2251:G:H2'   | 1:A:2252:A:H8     | 1.83                     | 0.43              |
| 1:A:2421:G:H3'   | 1:A:2422:U:C5'    | 2.48                     | 0.43              |
| 1:A:2649:A:H5'   | 1:A:2649:A:H8     | 1.82                     | 0.43              |
| 2:B:3041:C:C6    | 6:F:50:VAL:HG21   | 2.52                     | 0.43              |
| 2:B:3056:A:C3'   | 2:B:3057:A:H5''   | 2.48                     | 0.43              |
| 4:D:16:ARG:NH1   | 37:D:8618:HOH:O   | 2.51                     | 0.43              |
| 11:K:6:PHE:O     | 11:K:8:ALA:N      | 2.51                     | 0.43              |
| 13:M:3:LYS:O     | 13:M:4:LYS:C      | 2.61                     | 0.43              |
| 17:Q:109:ARG:NH1 | 17:Q:119:TYR:CE2  | 2.86                     | 0.43              |
| 24:X:126:ASP:HB3 | 24:X:135:GLY:O    | 2.18                     | 0.43              |
| 25:Y:85:VAL:HG12 | 25:Y:86:GLU:H     | 1.83                     | 0.43              |
| 28:2:5:THR:HB    | 28:2:6:PRO:CD     | 2.48                     | 0.43              |
| 29:3:35:ARG:HB2  | 37:3:2691:HOH:O   | 2.17                     | 0.43              |
| 1:A:259:G:O2'    | 1:A:260:C:H5'     | 2.18                     | 0.43              |
| 1:A:416:G:OP1    | 1:A:417:G:H5'     | 2.18                     | 0.43              |
| 1:A:426:G:C2     | 1:A:427:C:C2      | 3.06                     | 0.43              |
| 1:A:821:U:H2'    | 1:A:822:C:H6      | 1.82                     | 0.43              |
| 1:A:1311:G:C2    | 1:A:1312:G:C8     | 3.06                     | 0.43              |
| 1:A:1555:G:O2'   | 1:A:1556:G:H5'    | 2.18                     | 0.43              |
| 1:A:1667:A:H2'   | 1:A:1668:U:C6     | 2.53                     | 0.43              |
| 1:A:1902:G:H2'   | 1:A:1903:U:O4'    | 2.19                     | 0.43              |
| 1:A:2289:G:H21   | 1:A:2291:A:H2     | 1.60                     | 0.43              |
| 1:A:2697:A:H2'   | 1:A:2698:G:O4'    | 2.18                     | 0.43              |
| 4:D:279:THR:OG1  | 4:D:290:VAL:HB    | 2.18                     | 0.43              |
| 4:D:316:ARG:N    | 4:D:317:PRO:HD3   | 2.34                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:123:LEU:HD23  | 5:E:123:LEU:HA   | 1.88                     | 0.43              |
| 7:G:80:TRP:O      | 7:G:134:SER:HA   | 2.17                     | 0.43              |
| 8:H:79:GLN:HB2    | 8:H:82:ASP:OD2   | 2.18                     | 0.43              |
| 10:J:72:VAL:HG11  | 10:J:81:TYR:CZ   | 2.53                     | 0.43              |
| 14:N:138:HIS:C    | 14:N:139:PRO:O   | 2.54                     | 0.43              |
| 14:N:157:LEU:HA   | 35:N:8518:CL:CL  | 2.55                     | 0.43              |
| 24:X:146:ILE:HG22 | 24:X:147:ASP:N   | 2.33                     | 0.43              |
| 26:Z:125:LYS:NZ   | 37:Z:8114:HOH:O  | 2.51                     | 0.43              |
| 1:A:135:G:H1'     | 14:N:135:ASP:OD2 | 2.18                     | 0.43              |
| 1:A:283:U:H5      | 1:A:284:C:H42    | 1.66                     | 0.43              |
| 1:A:812:A:C6      | 1:A:813:C:C4     | 3.06                     | 0.43              |
| 1:A:843:A:C2      | 1:A:846:A:C8     | 3.06                     | 0.43              |
| 1:A:1056:U:H2'    | 1:A:1057:A:O4'   | 2.18                     | 0.43              |
| 1:A:1313:A:H5''   | 26:Z:210:GLY:N   | 2.32                     | 0.43              |
| 1:A:1352:A:N1     | 5:E:48:SER:HB3   | 2.33                     | 0.43              |
| 1:A:1420:C:C2     | 1:A:1445:G:N2    | 2.86                     | 0.43              |
| 4:D:132:HIS:CE1   | 4:D:171:VAL:HG21 | 2.53                     | 0.43              |
| 7:G:7:ILE:HG22    | 7:G:45:ASP:O     | 2.19                     | 0.43              |
| 7:G:9:GLU:HG3     | 7:G:10:ASP:N     | 2.33                     | 0.43              |
| 9:I:20:VAL:O      | 9:I:24:VAL:HG23  | 2.18                     | 0.43              |
| 21:U:25:ALA:O     | 21:U:39:ASN:CB   | 2.67                     | 0.43              |
| 1:A:470:U:O2'     | 28:2:16:HIS:CD2  | 2.69                     | 0.43              |
| 1:A:920:C:H4'     | 1:A:921:G:N2     | 2.33                     | 0.43              |
| 1:A:1047:U:H2'    | 1:A:1048:G:H8    | 1.84                     | 0.43              |
| 1:A:1076:G:C2     | 1:A:1084:C:C2    | 3.06                     | 0.43              |
| 1:A:1098:A:H2'    | 1:A:1099:G:O4'   | 2.18                     | 0.43              |
| 1:A:2379:G:N7     | 1:A:2408:A:N1    | 2.65                     | 0.43              |
| 1:A:2497:A:H2'    | 1:A:2498:C:C6    | 2.52                     | 0.43              |
| 1:A:2776:A:H2'    | 1:A:2777:G:O4'   | 2.17                     | 0.43              |
| 1:A:2840:A:OP1    | 4:D:211:THR:HG23 | 2.18                     | 0.43              |
| 1:A:2909:G:H2'    | 1:A:2910:A:H8    | 1.83                     | 0.43              |
| 3:C:192:VAL:O     | 3:C:192:VAL:CG1  | 2.66                     | 0.43              |
| 5:E:25:PRO:HD2    | 37:E:8424:HOH:O  | 2.17                     | 0.43              |
| 5:E:46:TYR:CE2    | 5:E:98:ARG:NH1   | 2.86                     | 0.43              |
| 11:K:74:ARG:C     | 11:K:76:ASP:N    | 2.76                     | 0.43              |
| 23:W:5:VAL:CG1    | 23:W:9:ARG:NH1   | 2.81                     | 0.43              |
| 27:1:41:VAL:HG12  | 27:1:42:CYS:N    | 2.32                     | 0.43              |
| 1:A:68:U:O2'      | 1:A:69:A:H5''    | 2.18                     | 0.43              |
| 1:A:396:U:H4'     | 37:4:8531:HOH:O  | 2.18                     | 0.43              |
| 1:A:794:U:H5      | 37:A:3763:HOH:O  | 2.01                     | 0.43              |
| 1:A:814:G:H2'     | 1:A:815:U:O4'    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1309:U:C2'    | 1:A:1310:U:H5'   | 2.49                     | 0.43              |
| 1:A:1323:G:C2     | 1:A:1324:G:C8    | 3.07                     | 0.43              |
| 1:A:1407:A:O2'    | 1:A:1408:U:H3'   | 2.19                     | 0.43              |
| 1:A:1562:C:H42    | 1:A:2738:G:H1    | 1.65                     | 0.43              |
| 1:A:1815:A:H3'    | 1:A:1816:C:C6    | 2.53                     | 0.43              |
| 1:A:1878:G:O2'    | 1:A:1879:U:P     | 2.76                     | 0.43              |
| 1:A:2868:C:H2'    | 1:A:2869:G:O4'   | 2.19                     | 0.43              |
| 3:C:51:ARG:CZ     | 37:C:8609:HOH:O  | 2.66                     | 0.43              |
| 3:C:150:PRO:HG3   | 37:C:8598:HOH:O  | 2.18                     | 0.43              |
| 4:D:63:GLU:O      | 4:D:63:GLU:HG3   | 2.18                     | 0.43              |
| 4:D:139:ASP:HB2   | 4:D:165:ARG:HE   | 1.84                     | 0.43              |
| 14:N:137:ASP:HA   | 14:N:142:LYS:HE3 | 2.01                     | 0.43              |
| 15:O:86:LEU:HD12  | 15:O:125:ALA:CB  | 2.43                     | 0.43              |
| 23:W:42:ASN:O     | 23:W:44:GLY:N    | 2.51                     | 0.43              |
| 24:X:73:LEU:HA    | 24:X:73:LEU:HD12 | 1.81                     | 0.43              |
| 1:A:604:G:H2'     | 37:A:7331:HOH:O  | 2.18                     | 0.43              |
| 1:A:783:C:OP1     | 3:C:180:LYS:HE3  | 2.19                     | 0.43              |
| 1:A:876:A:N3      | 1:A:876:A:H2'    | 2.34                     | 0.43              |
| 1:A:1603:A:H5''   | 1:A:1604:G:H3'   | 1.99                     | 0.43              |
| 1:A:2502:C:C4'    | 10:J:151:MET:SD  | 3.06                     | 0.43              |
| 1:A:2833:C:O2     | 1:A:2906:A:O2'   | 2.36                     | 0.43              |
| 4:D:11:LEU:HA     | 37:D:8618:HOH:O  | 2.19                     | 0.43              |
| 7:G:54:ASP:OD1    | 7:G:54:ASP:N     | 2.52                     | 0.43              |
| 8:H:22:VAL:CG2    | 8:H:104:ALA:HB2  | 2.49                     | 0.43              |
| 8:H:91:VAL:CG1    | 8:H:92:GLY:H     | 2.28                     | 0.43              |
| 10:J:55:GLN:HE22  | 10:J:91:HIS:CD2  | 2.37                     | 0.43              |
| 14:N:115:LEU:HD13 | 14:N:116:ASN:HB2 | 2.01                     | 0.43              |
| 15:O:5:ARG:HG3    | 18:R:18:PRO:CB   | 2.49                     | 0.43              |
| 18:R:25:PRO:HA    | 18:R:26:PRO:HD3  | 1.85                     | 0.43              |
| 21:U:50:VAL:HG12  | 21:U:56:ALA:HA   | 2.00                     | 0.43              |
| 27:1:56:MET:HE2   | 27:1:63:LYS:CD   | 2.48                     | 0.43              |
| 1:A:392:U:C5'     | 14:N:193:LYS:HB3 | 2.49                     | 0.43              |
| 1:A:661:G:C4      | 1:A:686:A:C2     | 3.07                     | 0.43              |
| 1:A:1164:U:C1'    | 1:A:1165:G:OP1   | 2.66                     | 0.43              |
| 1:A:1301:C:O4'    | 1:A:1330:A:C2    | 2.71                     | 0.43              |
| 1:A:1314:U:H5''   | 1:A:1316:G:O4'   | 2.19                     | 0.43              |
| 1:A:1327:G:C6     | 1:A:1331:A:C6    | 3.07                     | 0.43              |
| 1:A:1375:A:C2'    | 1:A:1376:G:H5'   | 2.49                     | 0.43              |
| 1:A:2255:A:C6     | 1:A:2256:G:C5    | 3.06                     | 0.43              |
| 1:A:2506:A:H1'    | 37:A:3327:HOH:O  | 2.19                     | 0.43              |
| 3:C:214:SER:HA    | 3:C:227:ASP:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:156:LYS:HE3  | 37:D:8635:HOH:O   | 2.18                     | 0.43              |
| 7:G:11:VAL:HG11  | 7:G:22:VAL:CG1    | 2.49                     | 0.43              |
| 7:G:23:GLU:HG2   | 7:G:28:SER:HB2    | 2.01                     | 0.43              |
| 9:I:12:ILE:O     | 9:I:13:PRO:C      | 2.61                     | 0.43              |
| 9:I:66:LEU:O     | 9:I:69:ARG:HB3    | 2.18                     | 0.43              |
| 10:J:45:GLN:HG3  | 10:J:135:TRP:NE1  | 2.34                     | 0.43              |
| 11:K:22:VAL:O    | 11:K:26:VAL:HG23  | 2.19                     | 0.43              |
| 11:K:26:VAL:HG13 | 11:K:36:VAL:HG11  | 1.99                     | 0.43              |
| 11:K:38:VAL:HB   | 11:K:103:VAL:HG13 | 2.00                     | 0.43              |
| 14:N:39:ARG:NH2  | 37:N:8622:HOH:O   | 2.52                     | 0.43              |
| 15:O:175:LEU:O   | 15:O:176:ARG:C    | 2.62                     | 0.43              |
| 16:P:56:GLU:HB2  | 37:P:6111:HOH:O   | 2.17                     | 0.43              |
| 18:R:93:ARG:HG3  | 18:R:93:ARG:NH1   | 2.34                     | 0.43              |
| 1:A:13:G:H2'     | 1:A:14:C:C6       | 2.54                     | 0.43              |
| 1:A:137:U:OP1    | 1:A:259:G:O2'     | 2.36                     | 0.43              |
| 1:A:958:G:O2'    | 1:A:959:C:H5'     | 2.19                     | 0.43              |
| 1:A:1269:G:H5''  | 35:A:8520:CL:CL   | 2.55                     | 0.43              |
| 1:A:1659:A:H2'   | 1:A:1660:G:O4'    | 2.19                     | 0.43              |
| 1:A:1783:A:C2'   | 1:A:1784:U:H5'    | 2.49                     | 0.43              |
| 1:A:1787:C:H4'   | 1:A:2883:A:O4'    | 2.18                     | 0.43              |
| 1:A:2269:C:C2'   | 1:A:2270:G:H5'    | 2.48                     | 0.43              |
| 37:A:7470:HOH:O  | 15:O:1:ALA:CB     | 2.67                     | 0.43              |
| 3:C:135:VAL:N    | 37:C:8598:HOH:O   | 2.50                     | 0.43              |
| 4:D:168:GLY:H    | 4:D:174:ARG:HD3   | 1.82                     | 0.43              |
| 6:F:11:HIS:O     | 6:F:12:GLU:CB     | 2.66                     | 0.43              |
| 6:F:24:HIS:HB2   | 6:F:72:LYS:CB     | 2.49                     | 0.43              |
| 6:F:35:ALA:O     | 6:F:37:ALA:N      | 2.52                     | 0.43              |
| 6:F:63:ILE:C     | 37:F:5728:HOH:O   | 2.60                     | 0.43              |
| 10:J:31:PHE:HD2  | 10:J:85:ILE:O     | 2.01                     | 0.43              |
| 15:O:100:ALA:O   | 15:O:129:ILE:HG12 | 2.17                     | 0.43              |
| 18:R:33:PHE:N    | 18:R:71:TYR:OH    | 2.46                     | 0.43              |
| 26:Z:109:LEU:HA  | 37:Z:8159:HOH:O   | 2.18                     | 0.43              |
| 27:1:81:LYS:O    | 27:1:82:ALA:C     | 2.62                     | 0.43              |
| 28:2:28:HIS:O    | 28:2:32:LYS:N     | 2.43                     | 0.43              |
| 1:A:892:G:H5''   | 28:2:54:ALA:HB2   | 2.01                     | 0.43              |
| 1:A:1861:C:H4'   | 3:C:6:GLY:O       | 2.19                     | 0.43              |
| 2:B:3050:G:C6    | 2:B:3051:A:C6     | 3.06                     | 0.43              |
| 5:E:178:GLN:C    | 5:E:180:SER:N     | 2.74                     | 0.43              |
| 5:E:233:THR:HG22 | 5:E:234:VAL:H     | 1.82                     | 0.43              |
| 6:F:77:ASP:HB3   | 6:F:78:GLU:H      | 1.56                     | 0.43              |
| 8:H:101:ALA:HA   | 37:H:5413:HOH:O   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:42:ARG:HA    | 14:N:43:PRO:HD3   | 1.79                     | 0.43              |
| 14:N:59:GLY:C     | 14:N:141:ILE:HD11 | 2.44                     | 0.43              |
| 14:N:59:GLY:CA    | 14:N:141:ILE:HD11 | 2.48                     | 0.43              |
| 15:O:77:ASN:OD1   | 15:O:80:SER:HB2   | 2.19                     | 0.43              |
| 17:Q:143:ALA:HB2  | 37:Q:5521:HOH:O   | 2.18                     | 0.43              |
| 19:S:17:MET:HE1   | 19:S:19:ARG:CZ    | 2.46                     | 0.43              |
| 20:T:29:ASP:OD2   | 20:T:31:ARG:NH1   | 2.51                     | 0.43              |
| 24:X:64:THR:O     | 24:X:68:THR:HG22  | 2.18                     | 0.43              |
| 1:A:392:U:H4'     | 14:N:193:LYS:HB3  | 2.01                     | 0.43              |
| 1:A:829:A:C6      | 1:A:830:G:N7      | 2.87                     | 0.43              |
| 1:A:1450:C:O2'    | 1:A:1494:A:H5'    | 2.19                     | 0.43              |
| 1:A:1828:G:H2'    | 1:A:1829:A:H5'    | 2.00                     | 0.43              |
| 1:A:2010:A:H2'    | 37:A:5537:HOH:O   | 2.19                     | 0.43              |
| 2:B:3065:A:O2'    | 2:B:3066:G:P      | 2.76                     | 0.43              |
| 3:C:22:ARG:NH1    | 37:C:8567:HOH:O   | 2.52                     | 0.43              |
| 3:C:135:VAL:HG21  | 3:C:147:ARG:NH1   | 2.33                     | 0.43              |
| 3:C:194:MET:CE    | 3:C:199:HIS:HB2   | 2.45                     | 0.43              |
| 5:E:223:LEU:HD12  | 5:E:223:LEU:HA    | 1.78                     | 0.43              |
| 6:F:49:PRO:CG     | 37:F:5828:HOH:O   | 2.57                     | 0.43              |
| 6:F:49:PRO:HA     | 6:F:73:VAL:HG22   | 2.01                     | 0.43              |
| 8:H:104:ALA:HA    | 37:H:6617:HOH:O   | 2.19                     | 0.43              |
| 8:H:117:GLU:C     | 8:H:119:ARG:N     | 2.77                     | 0.43              |
| 9:I:18:GLU:O      | 9:I:21:ASP:HB2    | 2.18                     | 0.43              |
| 11:K:71:TYR:CG    | 11:K:72:PRO:HD2   | 2.54                     | 0.43              |
| 18:R:88:ALA:O     | 18:R:89:ALA:C     | 2.61                     | 0.43              |
| 21:U:71:VAL:CG1   | 21:U:90:PRO:HB3   | 2.24                     | 0.43              |
| 24:X:19:ASP:O     | 24:X:23:MET:HG3   | 2.18                     | 0.43              |
| 26:Z:187:VAL:HG23 | 26:Z:192:ASP:HB3  | 2.00                     | 0.43              |
| 29:3:19:SER:O     | 29:3:36:ASN:ND2   | 2.52                     | 0.43              |
| 1:A:539:G:H2'     | 1:A:540:A:C8      | 2.54                     | 0.42              |
| 1:A:820:G:H5'     | 1:A:821:U:H5'     | 2.00                     | 0.42              |
| 1:A:1269:G:H2'    | 1:A:1270:U:C6     | 2.54                     | 0.42              |
| 1:A:2269:C:H2'    | 1:A:2270:G:H5'    | 1.99                     | 0.42              |
| 1:A:2281:C:C2'    | 1:A:2282:U:H5'    | 2.48                     | 0.42              |
| 1:A:2820:A:H2'    | 1:A:2821:C:O4'    | 2.19                     | 0.42              |
| 4:D:217:ARG:HG3   | 4:D:257:THR:CG2   | 2.49                     | 0.42              |
| 4:D:248:ARG:NH2   | 37:D:8526:HOH:O   | 2.51                     | 0.42              |
| 6:F:60:GLU:O      | 6:F:62:ASP:N      | 2.52                     | 0.42              |
| 14:N:38:VAL:O     | 14:N:63:VAL:CG1   | 2.62                     | 0.42              |
| 15:O:22:GLN:HG2   | 15:O:26:LEU:HD22  | 2.00                     | 0.42              |
| 15:O:64:SER:C     | 15:O:66:LEU:N     | 2.75                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 21:U:49:GLU:HB3  | 21:U:59:GLU:CG   | 2.49                     | 0.42              |
| 1:A:42:C:H1'     | 37:A:4252:HOH:O  | 2.18                     | 0.42              |
| 1:A:290:C:H2'    | 1:A:291:C:O4'    | 2.19                     | 0.42              |
| 1:A:420:U:H2'    | 1:A:421:C:C6     | 2.54                     | 0.42              |
| 1:A:1114:A:O2'   | 1:A:1115:U:H5'   | 2.19                     | 0.42              |
| 1:A:1166:A:N3    | 1:A:1166:A:H2'   | 2.34                     | 0.42              |
| 1:A:1335:C:H2'   | 1:A:1336:U:H6    | 1.83                     | 0.42              |
| 1:A:1375:A:H2'   | 1:A:1376:G:H5'   | 2.01                     | 0.42              |
| 1:A:1657:A:H2'   | 1:A:1658:A:C8    | 2.54                     | 0.42              |
| 1:A:1947:G:H2'   | 1:A:1948:G:C8    | 2.53                     | 0.42              |
| 1:A:2760:C:H5''  | 37:A:4902:HOH:O  | 2.19                     | 0.42              |
| 2:B:3051:A:H5'   | 15:O:160:SER:HB3 | 2.01                     | 0.42              |
| 2:B:3060:C:O2'   | 2:B:3061:C:H5'   | 2.19                     | 0.42              |
| 11:K:129:PHE:CD1 | 11:K:129:PHE:C   | 2.96                     | 0.42              |
| 13:M:130:ARG:HA  | 37:M:8431:HOH:O  | 2.19                     | 0.42              |
| 15:O:80:SER:CB   | 37:O:8536:HOH:O  | 2.62                     | 0.42              |
| 24:X:38:THR:HG22 | 37:X:3580:HOH:O  | 2.18                     | 0.42              |
| 24:X:48:VAL:O    | 24:X:48:VAL:HG12 | 2.18                     | 0.42              |
| 24:X:108:ARG:O   | 24:X:111:GLY:N   | 2.49                     | 0.42              |
| 25:Y:70:ILE:O    | 25:Y:70:ILE:HG23 | 2.19                     | 0.42              |
| 1:A:111:C:H2'    | 1:A:112:G:O4'    | 2.19                     | 0.42              |
| 1:A:472:A:N1     | 1:A:888:U:O2'    | 2.51                     | 0.42              |
| 1:A:1014:A:H5''  | 2:B:3101:G:O2'   | 2.19                     | 0.42              |
| 1:A:1044:C:H5    | 37:A:6177:HOH:O  | 2.01                     | 0.42              |
| 1:A:1127:C:C5    | 1:A:1128:U:C4    | 3.07                     | 0.42              |
| 1:A:2092:G:H2'   | 1:A:2613:G:OP1   | 2.20                     | 0.42              |
| 3:C:88:ILE:CD1   | 3:C:100:PRO:HD3  | 2.40                     | 0.42              |
| 3:C:211:LYS:HB2  | 37:C:8624:HOH:O  | 2.17                     | 0.42              |
| 3:C:211:LYS:CB   | 3:C:212:PRO:HD2  | 2.35                     | 0.42              |
| 4:D:329:TYR:HE2  | 22:V:15:PRO:HG2  | 1.80                     | 0.42              |
| 5:E:76:ARG:HD2   | 37:E:8429:HOH:O  | 2.19                     | 0.42              |
| 6:F:48:MET:HA    | 6:F:49:PRO:HD3   | 1.84                     | 0.42              |
| 8:H:56:PRO:CG    | 14:N:44:THR:HA   | 2.49                     | 0.42              |
| 10:J:147:ARG:HA  | 10:J:150:LYS:NZ  | 2.34                     | 0.42              |
| 11:K:34:GLU:OE1  | 11:K:34:GLU:HA   | 2.19                     | 0.42              |
| 13:M:148:GLU:HG2 | 37:M:8425:HOH:O  | 2.20                     | 0.42              |
| 14:N:80:GLY:O    | 14:N:81:ARG:CD   | 2.61                     | 0.42              |
| 18:R:30:VAL:O    | 18:R:31:GLU:C    | 2.62                     | 0.42              |
| 21:U:55:PHE:CG   | 21:U:77:VAL:HG13 | 2.54                     | 0.42              |
| 1:A:128:A:O2'    | 1:A:129:A:H5'    | 2.19                     | 0.42              |
| 1:A:1014:A:H2'   | 1:A:1015:C:H5'   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1029:U:O2'   | 1:A:1273:C:OP1    | 2.34                     | 0.42              |
| 1:A:1380:U:H5'   | 37:A:8803:HOH:O   | 2.19                     | 0.42              |
| 1:A:1869:A:H2'   | 1:A:1870:C:O4'    | 2.20                     | 0.42              |
| 1:A:1940:C:H5''  | 3:C:234:GLY:HA3   | 2.02                     | 0.42              |
| 5:E:21:VAL:C     | 5:E:23:GLU:H      | 2.27                     | 0.42              |
| 6:F:52:THR:HB    | 6:F:70:GLY:O      | 2.19                     | 0.42              |
| 20:T:8:PRO:HD2   | 23:W:32:ALA:HA    | 2.02                     | 0.42              |
| 22:V:44:ARG:HB2  | 37:V:3805:HOH:O   | 2.19                     | 0.42              |
| 1:A:775:G:H3'    | 37:A:4010:HOH:O   | 2.20                     | 0.42              |
| 1:A:844:A:C6     | 1:A:882:A:C6      | 3.08                     | 0.42              |
| 1:A:1559:A:C1'   | 37:A:5443:HOH:O   | 2.66                     | 0.42              |
| 1:A:1857:A:N6    | 1:A:2247:C:H1'    | 2.34                     | 0.42              |
| 1:A:1920:C:O2'   | 1:A:1921:A:H5'    | 2.19                     | 0.42              |
| 1:A:2079:G:H2'   | 1:A:2080:G:O4'    | 2.20                     | 0.42              |
| 1:A:2436:U:H5'   | 30:4:68:LYS:HE2   | 1.99                     | 0.42              |
| 1:A:2756:U:N3    | 1:A:2896:A:H2     | 2.14                     | 0.42              |
| 3:C:51:ARG:O     | 3:C:52:SER:C      | 2.61                     | 0.42              |
| 4:D:154:VAL:CG1  | 4:D:156:LYS:HG2   | 2.49                     | 0.42              |
| 4:D:279:THR:CG2  | 4:D:280:VAL:N     | 2.82                     | 0.42              |
| 6:F:87:ALA:O     | 6:F:88:LEU:C      | 2.62                     | 0.42              |
| 11:K:39:VAL:HG13 | 11:K:106:GLY:O    | 2.19                     | 0.42              |
| 13:M:42:ASN:HB2  | 37:M:8421:HOH:O   | 2.18                     | 0.42              |
| 13:M:91:VAL:HG13 | 13:M:91:VAL:O     | 2.19                     | 0.42              |
| 14:N:133:LEU:O   | 14:N:134:ILE:HD13 | 2.19                     | 0.42              |
| 14:N:169:ARG:HD2 | 37:N:8590:HOH:O   | 2.20                     | 0.42              |
| 15:O:113:SER:CB  | 37:O:8559:HOH:O   | 2.55                     | 0.42              |
| 23:W:5:VAL:HG11  | 23:W:9:ARG:NH1    | 2.34                     | 0.42              |
| 23:W:19:GLU:OE1  | 23:W:19:GLU:HA    | 2.19                     | 0.42              |
| 25:Y:20:GLU:CD   | 25:Y:21:PRO:HD2   | 2.44                     | 0.42              |
| 27:1:11:THR:HG21 | 27:1:23:ARG:HB2   | 2.01                     | 0.42              |
| 1:A:500:G:H21    | 19:S:98:ASN:HD21  | 1.66                     | 0.42              |
| 1:A:682:A:H3'    | 1:A:683:G:C8      | 2.55                     | 0.42              |
| 1:A:1052:G:C5    | 1:A:1063:G:C6     | 3.08                     | 0.42              |
| 1:A:1183:C:N4    | 37:A:3977:HOH:O   | 2.46                     | 0.42              |
| 1:A:1389:G:N2    | 1:A:1391:G:H3'    | 2.35                     | 0.42              |
| 1:A:1785:G:OP1   | 17:Q:76:GLY:HA3   | 2.20                     | 0.42              |
| 1:A:1820:G:C6    | 1:A:2030:A:C2     | 3.08                     | 0.42              |
| 1:A:2040:C:H2'   | 1:A:2041:G:O4'    | 2.20                     | 0.42              |
| 1:A:2408:A:H2    | 37:4:8516:HOH:O   | 2.01                     | 0.42              |
| 3:C:47:HIS:O     | 3:C:49:PRO:HD3    | 2.19                     | 0.42              |
| 6:F:160:ALA:C    | 6:F:162:ALA:N     | 2.77                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:15:THR:HG22 | 10:J:91:HIS:HA   | 2.01                     | 0.42              |
| 10:J:31:PHE:HE2  | 10:J:87:LYS:O    | 2.03                     | 0.42              |
| 11:K:63:ILE:HG22 | 11:K:64:GLY:N    | 2.33                     | 0.42              |
| 14:N:82:ARG:O    | 14:N:83:SER:C    | 2.63                     | 0.42              |
| 15:O:93:GLN:HG2  | 37:O:8557:HOH:O  | 2.19                     | 0.42              |
| 21:U:51:LEU:HD11 | 21:U:97:ARG:HB2  | 2.02                     | 0.42              |
| 1:A:553:G:O4'    | 1:A:1325:G:H5'   | 2.19                     | 0.42              |
| 1:A:1007:A:H2'   | 10:J:19:TYR:CZ   | 2.55                     | 0.42              |
| 1:A:1094:G:H21   | 24:X:119:HIS:CE1 | 2.38                     | 0.42              |
| 1:A:1206:U:H2'   | 1:A:1207:A:O4'   | 2.19                     | 0.42              |
| 1:A:1555:G:H4'   | 1:A:1630:A:H2    | 1.85                     | 0.42              |
| 1:A:2892:G:C6    | 1:A:2893:C:C4    | 3.08                     | 0.42              |
| 37:A:9118:HOH:O  | 17:Q:81:LYS:HG2  | 2.20                     | 0.42              |
| 3:C:199:HIS:HD2  | 3:C:201:PHE:N    | 2.07                     | 0.42              |
| 4:D:115:VAL:HA   | 4:D:116:PRO:HD3  | 1.88                     | 0.42              |
| 4:D:138:GLY:O    | 4:D:139:ASP:C    | 2.61                     | 0.42              |
| 6:F:93:LEU:HG    | 37:F:3862:HOH:O  | 2.19                     | 0.42              |
| 14:N:61:ILE:HD12 | 14:N:61:ILE:N    | 2.34                     | 0.42              |
| 15:O:62:HIS:HB3  | 15:O:65:ASP:OD1  | 2.19                     | 0.42              |
| 19:S:50:VAL:HG22 | 19:S:55:GLN:O    | 2.20                     | 0.42              |
| 26:Z:155:ARG:NH1 | 37:Z:8147:HOH:O  | 2.52                     | 0.42              |
| 26:Z:205:ILE:O   | 26:Z:206:ALA:C   | 2.63                     | 0.42              |
| 1:A:65:C:O2'     | 1:A:66:G:H5'     | 2.19                     | 0.42              |
| 1:A:187:A:H3'    | 1:A:188:C:H6     | 1.83                     | 0.42              |
| 1:A:524:A:H5''   | 19:S:29:LYS:HE2  | 2.01                     | 0.42              |
| 1:A:772:G:N2     | 1:A:890:C:O2     | 2.53                     | 0.42              |
| 1:A:834:G:H4'    | 1:A:835:U:OP2    | 2.19                     | 0.42              |
| 1:A:1165:G:O2'   | 1:A:1166:A:OP1   | 2.25                     | 0.42              |
| 1:A:1189:A:N3    | 37:A:7254:HOH:O  | 2.52                     | 0.42              |
| 1:A:1270:U:H2'   | 1:A:1271:A:C8    | 2.55                     | 0.42              |
| 1:A:1331:A:OP2   | 26:Z:142:SER:OG  | 2.37                     | 0.42              |
| 1:A:2015:A:H2'   | 1:A:2016:U:O4'   | 2.19                     | 0.42              |
| 1:A:2575:C:H2'   | 1:A:2576:A:O4'   | 2.19                     | 0.42              |
| 1:A:2687:G:O2'   | 1:A:2688:U:H5'   | 2.19                     | 0.42              |
| 1:A:2764:C:H2'   | 1:A:2765:C:C6    | 2.54                     | 0.42              |
| 2:B:3078:G:O2'   | 2:B:3079:U:OP2   | 2.37                     | 0.42              |
| 3:C:3:ARG:HB2    | 3:C:8:ARG:NE     | 2.35                     | 0.42              |
| 3:C:179:MET:HA   | 3:C:179:MET:HE3  | 2.00                     | 0.42              |
| 4:D:127:GLN:HG3  | 37:D:8646:HOH:O  | 2.19                     | 0.42              |
| 4:D:182:VAL:O    | 4:D:183:GLU:C    | 2.62                     | 0.42              |
| 5:E:4:THR:HB     | 5:E:135:GLU:OE1  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:200:PRO:HB3  | 5:E:212:VAL:CG2   | 2.50                     | 0.42              |
| 6:F:104:PHE:CE2  | 6:F:166:ILE:CD1   | 3.02                     | 0.42              |
| 7:G:7:ILE:HA     | 7:G:8:PRO:HD3     | 1.88                     | 0.42              |
| 7:G:15:GLN:HG2   | 7:G:19:ASP:O      | 2.20                     | 0.42              |
| 14:N:72:SER:HB2  | 14:N:93:ARG:HG2   | 2.01                     | 0.42              |
| 14:N:147:LEU:O   | 14:N:148:SER:C    | 2.63                     | 0.42              |
| 16:P:59:VAL:CG2  | 16:P:111:VAL:HG23 | 2.49                     | 0.42              |
| 17:Q:98:ILE:O    | 17:Q:98:ILE:HD13  | 2.19                     | 0.42              |
| 18:R:41:LEU:N    | 18:R:41:LEU:HD12  | 2.34                     | 0.42              |
| 1:A:287:C:O5'    | 1:A:287:C:H6      | 2.02                     | 0.42              |
| 1:A:578:C:O2     | 1:A:1112:G:H4'    | 2.20                     | 0.42              |
| 1:A:622:G:H5'    | 1:A:1357:A:N6     | 2.34                     | 0.42              |
| 1:A:1523:G:C6    | 1:A:1524:U:O4     | 2.73                     | 0.42              |
| 1:A:1979:G:O2'   | 1:A:1980:U:OP1    | 2.38                     | 0.42              |
| 2:B:3114:G:O6    | 15:O:11:ARG:HD3   | 2.20                     | 0.42              |
| 4:D:277:GLU:N    | 4:D:278:PRO:HD2   | 2.35                     | 0.42              |
| 5:E:7:ASP:OD1    | 5:E:11:ASN:O      | 2.37                     | 0.42              |
| 5:E:218:VAL:CG1  | 37:E:8419:HOH:O   | 2.67                     | 0.42              |
| 8:H:33:THR:HG21  | 8:H:59:ILE:O      | 2.20                     | 0.42              |
| 9:I:64:ASN:N     | 9:I:64:ASN:ND2    | 2.68                     | 0.42              |
| 15:O:43:VAL:HG13 | 15:O:118:ILE:HD11 | 2.02                     | 0.42              |
| 15:O:110:THR:HB  | 15:O:113:SER:OG   | 2.19                     | 0.42              |
| 16:P:32:ARG:HE   | 16:P:35:LYS:HD2   | 1.85                     | 0.42              |
| 18:R:30:VAL:O    | 18:R:30:VAL:HG12  | 2.20                     | 0.42              |
| 21:U:27:LEU:HD23 | 21:U:98:VAL:HB    | 2.02                     | 0.42              |
| 22:V:31:PHE:CG   | 22:V:37:GLU:HG2   | 2.55                     | 0.42              |
| 27:1:39:CYS:HA   | 27:1:40:PRO:HD3   | 1.95                     | 0.42              |
| 1:A:201:G:N1     | 1:A:202:U:C4      | 2.88                     | 0.42              |
| 1:A:332:G:O2'    | 1:A:333:G:H5'     | 2.20                     | 0.42              |
| 1:A:441:A:H1'    | 1:A:442:A:N7      | 2.35                     | 0.42              |
| 1:A:731:U:H2'    | 1:A:732:C:C6      | 2.55                     | 0.42              |
| 1:A:858:U:H2'    | 1:A:859:C:C6      | 2.54                     | 0.42              |
| 1:A:1391:G:C6    | 1:A:1435:U:C5     | 3.08                     | 0.42              |
| 1:A:1772:C:H5'   | 1:A:1773:G:C5     | 2.55                     | 0.42              |
| 1:A:2012:U:H2'   | 1:A:2013:G:OP1    | 2.19                     | 0.42              |
| 1:A:2247:C:C5'   | 37:A:6916:HOH:O   | 2.67                     | 0.42              |
| 1:A:2591:C:H2'   | 1:A:2592:G:O4'    | 2.20                     | 0.42              |
| 1:A:2791:U:C1'   | 1:A:2792:A:H5''   | 2.50                     | 0.42              |
| 2:B:3057:A:N3    | 2:B:3057:A:H5'    | 2.35                     | 0.42              |
| 4:D:14:GLY:CA    | 4:D:15:PRO:C      | 2.93                     | 0.42              |
| 4:D:41:PHE:CZ    | 4:D:79:MET:HG3    | 2.55                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:149:GLU:OE1  | 7:G:168:ILE:HG12  | 2.20                     | 0.42              |
| 9:I:63:ARG:O     | 9:I:67:LEU:HG     | 2.20                     | 0.42              |
| 9:I:73:ASP:C     | 37:I:2994:HOH:O   | 2.62                     | 0.42              |
| 11:K:42:GLU:O    | 11:K:131:THR:HG23 | 2.19                     | 0.42              |
| 12:L:27:ARG:HD2  | 37:L:4747:HOH:O   | 2.19                     | 0.42              |
| 29:3:40:ARG:HG3  | 29:3:45:ASN:CB    | 2.50                     | 0.42              |
| 29:3:41:HIS:O    | 29:3:45:ASN:HB2   | 2.20                     | 0.42              |
| 1:A:154:C:C2     | 1:A:155:C:C6      | 3.08                     | 0.41              |
| 1:A:634:G:O2'    | 1:A:1358:A:OP1    | 2.33                     | 0.41              |
| 1:A:902:G:N7     | 13:M:18:HIS:CD2   | 2.85                     | 0.41              |
| 1:A:1191:A:N1    | 1:A:1206:U:O4     | 2.53                     | 0.41              |
| 1:A:1351:G:OP1   | 5:E:96:LYS:NZ     | 2.41                     | 0.41              |
| 1:A:1496:G:H5'   | 1:A:1572:A:H1'    | 2.02                     | 0.41              |
| 1:A:1862:C:N4    | 1:A:1868:G:C6     | 2.88                     | 0.41              |
| 1:A:2362:A:H2'   | 1:A:2363:G:C8     | 2.55                     | 0.41              |
| 1:A:2503:A:OP1   | 10:J:147:ARG:NH2  | 2.48                     | 0.41              |
| 1:A:2570:G:H5''  | 37:A:4485:HOH:O   | 2.20                     | 0.41              |
| 1:A:2912:C:H2'   | 1:A:2913:A:O4'    | 2.20                     | 0.41              |
| 4:D:32:ASP:HA    | 37:D:8575:HOH:O   | 2.19                     | 0.41              |
| 4:D:130:ASP:HB2  | 37:D:8599:HOH:O   | 2.19                     | 0.41              |
| 10:J:126:HIS:O   | 10:J:127:GLY:C    | 2.62                     | 0.41              |
| 14:N:95:LYS:HG2  | 14:N:99:ARG:HB3   | 2.02                     | 0.41              |
| 16:P:96:VAL:CG1  | 16:P:97:SER:N     | 2.82                     | 0.41              |
| 21:U:40:VAL:HG23 | 21:U:119:ALA:C    | 2.45                     | 0.41              |
| 1:A:79:G:N2      | 1:A:80:A:N6       | 2.68                     | 0.41              |
| 1:A:464:G:N2     | 1:A:475:G:H2'     | 2.34                     | 0.41              |
| 1:A:834:G:H3'    | 1:A:835:U:H4'     | 2.03                     | 0.41              |
| 1:A:1164:U:O5'   | 1:A:1164:U:H6     | 2.03                     | 0.41              |
| 1:A:1182:C:H1'   | 1:A:1192:A:C8     | 2.52                     | 0.41              |
| 1:A:1829:A:H2'   | 1:A:1830:C:H5'    | 2.02                     | 0.41              |
| 1:A:2120:U:H2'   | 1:A:2121:G:O4'    | 2.19                     | 0.41              |
| 1:A:2438:G:H5'   | 37:4:8552:HOH:O   | 2.21                     | 0.41              |
| 1:A:2473:U:O3'   | 1:A:2474:A:H3'    | 2.19                     | 0.41              |
| 1:A:2498:C:O2'   | 1:A:2499:U:H5'    | 2.20                     | 0.41              |
| 1:A:2825:C:H4'   | 1:A:2826:G:O5'    | 2.20                     | 0.41              |
| 1:A:2896:A:OP1   | 37:A:3447:HOH:O   | 2.22                     | 0.41              |
| 3:C:105:VAL:HG13 | 3:C:155:THR:O     | 2.20                     | 0.41              |
| 3:C:111:SER:O    | 3:C:112:PRO:C     | 2.63                     | 0.41              |
| 4:D:80:ARG:HD3   | 37:D:8608:HOH:O   | 2.20                     | 0.41              |
| 4:D:267:LYS:NZ   | 4:D:300:SER:O     | 2.52                     | 0.41              |
| 5:E:7:ASP:C      | 5:E:9:ASP:H       | 2.29                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:27:ARG:CG     | 5:E:29:ASP:OD1    | 2.66                     | 0.41              |
| 6:F:174:VAL:CG1   | 37:F:6555:HOH:O   | 2.64                     | 0.41              |
| 7:G:126:ILE:HB    | 7:G:131:LEU:CD2   | 2.50                     | 0.41              |
| 12:L:118:ALA:C    | 12:L:120:ARG:H    | 2.29                     | 0.41              |
| 13:M:62:ALA:HB2   | 13:M:103:ALA:CB   | 2.50                     | 0.41              |
| 15:O:42:HIS:CG    | 15:O:62:HIS:HE1   | 2.38                     | 0.41              |
| 15:O:154:LEU:CG   | 15:O:155:GLU:N    | 2.81                     | 0.41              |
| 21:U:113:GLU:O    | 21:U:114:SER:C    | 2.62                     | 0.41              |
| 26:Z:106:THR:HG22 | 26:Z:107:PRO:O    | 2.20                     | 0.41              |
| 26:Z:150:LEU:O    | 26:Z:151:SER:C    | 2.64                     | 0.41              |
| 1:A:160:A:C4      | 1:A:177:A:C2      | 3.09                     | 0.41              |
| 1:A:226:A:H1'     | 1:A:393:G:C5      | 2.55                     | 0.41              |
| 1:A:398:U:H2'     | 1:A:399:C:C6      | 2.55                     | 0.41              |
| 1:A:415:A:O2'     | 1:A:416:G:H5'     | 2.20                     | 0.41              |
| 1:A:588:G:O6      | 24:X:154:ARG:NH1  | 2.53                     | 0.41              |
| 1:A:835:U:OP2     | 1:A:1753:C:O2'    | 2.34                     | 0.41              |
| 1:A:1565:C:O4'    | 1:A:2738:G:H1'    | 2.21                     | 0.41              |
| 1:A:1707:G:N2     | 1:A:1709:G:H3'    | 2.36                     | 0.41              |
| 6:F:170:TYR:N     | 6:F:170:TYR:CD1   | 2.89                     | 0.41              |
| 11:K:46:ILE:HA    | 37:K:1123:HOH:O   | 2.19                     | 0.41              |
| 11:K:56:LYS:NZ    | 35:K:8516:CL:CL   | 2.78                     | 0.41              |
| 14:N:122:GLU:HB2  | 14:N:126:HIS:O    | 2.20                     | 0.41              |
| 15:O:67:ALA:HA    | 15:O:71:TRP:HB3   | 2.02                     | 0.41              |
| 15:O:175:LEU:CD1  | 37:O:8539:HOH:O   | 2.68                     | 0.41              |
| 17:Q:13:VAL:HG11  | 17:Q:40:VAL:HG11  | 2.02                     | 0.41              |
| 29:3:19:SER:HB3   | 37:3:4479:HOH:O   | 2.19                     | 0.41              |
| 1:A:1477:C:C5'    | 1:A:1868:G:H5''   | 2.50                     | 0.41              |
| 1:A:1603:A:H5'    | 1:A:1605:G:C4'    | 2.49                     | 0.41              |
| 1:A:1758:U:H2'    | 1:A:1759:A:O4'    | 2.21                     | 0.41              |
| 1:A:2506:A:H1'    | 37:A:5633:HOH:O   | 2.20                     | 0.41              |
| 1:A:2838:A:H2'    | 1:A:2839:C:O4'    | 2.20                     | 0.41              |
| 37:A:4923:HOH:O   | 21:U:3:GLN:HG2    | 2.19                     | 0.41              |
| 37:A:5825:HOH:O   | 22:V:56:ARG:HD3   | 2.19                     | 0.41              |
| 2:B:3053:G:O2'    | 2:B:3054:A:H5'    | 2.20                     | 0.41              |
| 6:F:23:VAL:HG23   | 6:F:41:LEU:HD22   | 2.01                     | 0.41              |
| 6:F:81:GLU:O      | 6:F:83:PHE:N      | 2.54                     | 0.41              |
| 7:G:34:TRP:O      | 11:K:127:ILE:HD11 | 2.19                     | 0.41              |
| 8:H:13:GLU:OE2    | 8:H:78:GLU:HG2    | 2.21                     | 0.41              |
| 10:J:47:GLU:CB    | 10:J:133:ILE:CD1  | 2.93                     | 0.41              |
| 10:J:83:PHE:CE1   | 10:J:146:TRP:NE1  | 2.88                     | 0.41              |
| 14:N:3:SER:O      | 14:N:6:SER:OG     | 2.36                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:1:82:ALA:C    | 37:1:8420:HOH:O   | 2.63                     | 0.41              |
| 1:A:1003:U:O2'   | 10:J:90:PHE:HE1   | 2.03                     | 0.41              |
| 1:A:1494:A:O2'   | 1:A:1505:U:O2     | 2.33                     | 0.41              |
| 1:A:1614:G:H2'   | 37:A:4202:HOH:O   | 2.21                     | 0.41              |
| 1:A:1677:U:OP2   | 29:3:8:LYS:NZ     | 2.48                     | 0.41              |
| 1:A:1843:A:C8    | 1:A:1843:A:O5'    | 2.73                     | 0.41              |
| 1:A:1854:C:O2'   | 1:A:1858:A:N3     | 2.45                     | 0.41              |
| 1:A:2252:A:C5    | 1:A:2253:G:H1'    | 2.55                     | 0.41              |
| 4:D:79:MET:HE3   | 4:D:144:THR:HG21  | 2.03                     | 0.41              |
| 4:D:132:HIS:CE1  | 4:D:171:VAL:CG2   | 3.04                     | 0.41              |
| 4:D:275:GLY:C    | 4:D:291:ASP:HA    | 2.46                     | 0.41              |
| 5:E:192:ILE:CG2  | 5:E:234:VAL:HG12  | 2.51                     | 0.41              |
| 7:G:125:GLU:O    | 7:G:132:THR:HG22  | 2.20                     | 0.41              |
| 9:I:23:ILE:O     | 9:I:27:ILE:HG13   | 2.20                     | 0.41              |
| 13:M:90:ARG:NH1  | 13:M:119:THR:HG21 | 2.35                     | 0.41              |
| 16:P:26:TRP:HA   | 16:P:26:TRP:CE3   | 2.56                     | 0.41              |
| 16:P:97:SER:HB3  | 16:P:100:GLN:HE21 | 1.85                     | 0.41              |
| 17:Q:7:LYS:CD    | 17:Q:21:VAL:CG2   | 2.99                     | 0.41              |
| 30:4:30:GLN:HE21 | 30:4:30:GLN:HB3   | 1.69                     | 0.41              |
| 1:A:249:G:O2'    | 1:A:266:G:H5'     | 2.20                     | 0.41              |
| 1:A:419:A:C2     | 1:A:2449:G:C2     | 3.08                     | 0.41              |
| 1:A:820:G:C6     | 3:C:171:LYS:HB2   | 2.56                     | 0.41              |
| 1:A:1327:G:N1    | 1:A:1331:A:C6     | 2.88                     | 0.41              |
| 1:A:1690:C:C5    | 1:A:1692:C:C4     | 3.09                     | 0.41              |
| 1:A:2321:A:C4    | 1:A:2323:G:N7     | 2.89                     | 0.41              |
| 4:D:101:TRP:HB2  | 4:D:119:HIS:CD2   | 2.56                     | 0.41              |
| 4:D:177:HIS:NE2  | 4:D:181:ILE:HD11  | 2.36                     | 0.41              |
| 5:E:5:ILE:HD13   | 37:E:8426:HOH:O   | 2.20                     | 0.41              |
| 7:G:66:GLN:O     | 7:G:70:GLU:HG3    | 2.21                     | 0.41              |
| 8:H:20:LEU:O     | 8:H:23:ALA:HB3    | 2.20                     | 0.41              |
| 13:M:65:ASP:CG   | 13:M:111:ALA:HB3  | 2.45                     | 0.41              |
| 13:M:125:PHE:CE1 | 13:M:140:VAL:HG13 | 2.56                     | 0.41              |
| 17:Q:103:THR:O   | 17:Q:106:ARG:HB3  | 2.21                     | 0.41              |
| 1:A:97:G:C2      | 21:U:107:LYS:HD2  | 2.55                     | 0.41              |
| 1:A:329:A:H5'    | 1:A:347:A:H1'     | 2.03                     | 0.41              |
| 1:A:876:A:N3     | 1:A:876:A:C2'     | 2.83                     | 0.41              |
| 1:A:1051:C:H2'   | 1:A:1052:G:O4'    | 2.21                     | 0.41              |
| 1:A:1268:C:H2'   | 1:A:1269:G:H8     | 1.86                     | 0.41              |
| 1:A:1409:G:H5'   | 37:A:3305:HOH:O   | 2.21                     | 0.41              |
| 1:A:1626:A:H2'   | 1:A:1627:G:H5'    | 2.02                     | 0.41              |
| 1:A:1661:A:O2'   | 1:A:1662:C:H5'    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1706:G:C5     | 1:A:1707:G:C6     | 3.09                     | 0.41              |
| 1:A:1791:U:H2'    | 1:A:1792:C:C6     | 2.56                     | 0.41              |
| 1:A:1943:C:O4'    | 3:C:212:PRO:HA    | 2.20                     | 0.41              |
| 1:A:2779:G:H21    | 7:G:143:GLN:HE22  | 1.64                     | 0.41              |
| 1:A:2890:A:H1'    | 22:V:56:ARG:HH21  | 1.82                     | 0.41              |
| 9:I:71:LEU:C      | 9:I:73:ASP:N      | 2.78                     | 0.41              |
| 10:J:84:ARG:NH2   | 10:J:135:TRP:CH2  | 2.81                     | 0.41              |
| 10:J:111:MET:O    | 10:J:114:PRO:HD3  | 2.21                     | 0.41              |
| 15:O:143:ARG:NH1  | 15:O:173:ASP:CG   | 2.79                     | 0.41              |
| 17:Q:38:GLU:CA    | 17:Q:41:ARG:NH1   | 2.82                     | 0.41              |
| 21:U:111:ARG:HB3  | 21:U:119:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:1246:A:C4     | 1:A:1248:A:C8     | 3.09                     | 0.41              |
| 1:A:2281:C:H2'    | 1:A:2282:U:H5'    | 2.03                     | 0.41              |
| 1:A:2304:G:C6     | 1:A:2305:A:C6     | 3.08                     | 0.41              |
| 1:A:2323:G:H5'    | 37:A:6592:HOH:O   | 2.20                     | 0.41              |
| 1:A:2432:C:OP1    | 13:M:48:LYS:NZ    | 2.38                     | 0.41              |
| 1:A:2515:C:H2'    | 1:A:2516:G:O4'    | 2.20                     | 0.41              |
| 7:G:35:TYR:HA     | 11:K:127:ILE:HD12 | 2.03                     | 0.41              |
| 14:N:187:LEU:HD23 | 14:N:187:LEU:HA   | 1.91                     | 0.41              |
| 15:O:87:LEU:CD1   | 15:O:186:LEU:HD21 | 2.44                     | 0.41              |
| 15:O:152:GLU:C    | 15:O:154:LEU:N    | 2.78                     | 0.41              |
| 23:W:27:LEU:O     | 23:W:28:LEU:C     | 2.64                     | 0.41              |
| 24:X:14:HIS:HB2   | 24:X:17:ILE:HG13  | 2.02                     | 0.41              |
| 28:2:38:GLY:O     | 28:2:39:PHE:C     | 2.64                     | 0.41              |
| 1:A:87:C:H2'      | 29:3:28:LYS:O     | 2.21                     | 0.41              |
| 1:A:303:C:O2'     | 1:A:304:G:H5'     | 2.21                     | 0.41              |
| 1:A:383:A:C2      | 1:A:407:A:C4      | 3.08                     | 0.41              |
| 1:A:445:U:H2'     | 1:A:446:G:H8      | 1.85                     | 0.41              |
| 1:A:524:A:C5'     | 19:S:29:LYS:HE2   | 2.50                     | 0.41              |
| 1:A:774:C:H5'     | 28:2:46:ARG:HH21  | 1.86                     | 0.41              |
| 1:A:875:A:C2      | 3:C:194:MET:SD    | 3.14                     | 0.41              |
| 1:A:963:C:O5'     | 1:A:963:C:H6      | 2.04                     | 0.41              |
| 1:A:1067:A:O2'    | 24:X:12:ASN:OD1   | 2.36                     | 0.41              |
| 1:A:1218:U:H2'    | 1:A:1219:U:H6     | 1.86                     | 0.41              |
| 1:A:1456:C:H2'    | 1:A:1457:U:C6     | 2.56                     | 0.41              |
| 1:A:1588:G:C6     | 1:A:1589:G:C6     | 3.09                     | 0.41              |
| 1:A:1675:C:H5''   | 29:3:5:LYS:HD2    | 2.03                     | 0.41              |
| 1:A:1695:G:C6     | 1:A:1696:U:C4     | 3.09                     | 0.41              |
| 1:A:1947:G:N2     | 1:A:1966:U:O2     | 2.53                     | 0.41              |
| 1:A:2497:A:H2'    | 1:A:2498:C:H6     | 1.86                     | 0.41              |
| 1:A:2727:A:C6     | 1:A:2756:U:C4     | 3.08                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 37:A:6976:HOH:O   | 21:U:2:LYS:HE2   | 2.19                     | 0.41              |
| 2:B:3057:A:O2'    | 6:F:152:PRO:HD2  | 2.21                     | 0.41              |
| 3:C:211:LYS:HD3   | 37:C:8614:HOH:O  | 2.19                     | 0.41              |
| 4:D:23:THR:CG2    | 4:D:162:MET:HE3  | 2.51                     | 0.41              |
| 4:D:84:LEU:HD13   | 4:D:84:LEU:C     | 2.46                     | 0.41              |
| 4:D:146:THR:C     | 4:D:148:PRO:HD3  | 2.45                     | 0.41              |
| 4:D:156:LYS:NZ    | 4:D:160:ASP:OD2  | 2.49                     | 0.41              |
| 5:E:27:ARG:HD2    | 5:E:29:ASP:OD1   | 2.21                     | 0.41              |
| 6:F:15:GLU:O      | 6:F:16:PRO:O     | 2.39                     | 0.41              |
| 8:H:27:GLY:HA3    | 37:H:5413:HOH:O  | 2.21                     | 0.41              |
| 8:H:60:VAL:O      | 8:H:60:VAL:CG1   | 2.69                     | 0.41              |
| 8:H:91:VAL:CG1    | 8:H:92:GLY:N     | 2.80                     | 0.41              |
| 11:K:42:GLU:HG2   | 11:K:43:ARG:HG3  | 2.02                     | 0.41              |
| 15:O:113:SER:C    | 37:O:8559:HOH:O  | 2.64                     | 0.41              |
| 15:O:115:VAL:HG23 | 37:O:8559:HOH:O  | 2.19                     | 0.41              |
| 15:O:159:TYR:CE2  | 15:O:163:PHE:HE2 | 2.37                     | 0.41              |
| 15:O:175:LEU:HD12 | 15:O:175:LEU:HA  | 1.89                     | 0.41              |
| 18:R:16:ASN:HD22  | 18:R:16:ASN:HA   | 1.55                     | 0.41              |
| 26:Z:112:GLU:O    | 26:Z:116:LEU:HG  | 2.21                     | 0.41              |
| 26:Z:149:GLN:HE21 | 26:Z:149:GLN:HB3 | 1.73                     | 0.41              |
| 26:Z:216:ARG:CD   | 37:Z:8157:HOH:O  | 2.64                     | 0.41              |
| 29:3:11:LEU:HD23  | 29:3:11:LEU:HA   | 1.86                     | 0.41              |
| 30:4:7:PHE:CD1    | 30:4:7:PHE:C     | 2.99                     | 0.41              |
| 1:A:454:U:C2      | 37:A:8623:HOH:O  | 2.57                     | 0.41              |
| 1:A:821:U:H2'     | 1:A:822:C:C6     | 2.56                     | 0.41              |
| 1:A:951:A:H2'     | 1:A:952:G:H5'    | 2.03                     | 0.41              |
| 1:A:1037:G:C2     | 1:A:1038:G:C8    | 3.09                     | 0.41              |
| 1:A:1055:G:OP2    | 10:J:94:ARG:NH1  | 2.54                     | 0.41              |
| 1:A:1168:C:H5     | 37:A:7071:HOH:O  | 2.04                     | 0.41              |
| 1:A:1211:G:O2'    | 1:A:1212:C:H5'   | 2.20                     | 0.41              |
| 1:A:1261:A:O5'    | 1:A:1261:A:C8    | 2.74                     | 0.41              |
| 1:A:1427:A:H61    | 1:A:1440:U:H1'   | 1.86                     | 0.41              |
| 1:A:1804:A:H2'    | 1:A:1805:G:H8    | 1.86                     | 0.41              |
| 1:A:2090:G:N2     | 1:A:2655:U:C2    | 2.89                     | 0.41              |
| 1:A:2093:G:H5''   | 37:A:9062:HOH:O  | 2.21                     | 0.41              |
| 1:A:2453:G:H4'    | 13:M:50:GLY:C    | 2.46                     | 0.41              |
| 1:A:2637:A:H5'    | 37:A:3941:HOH:O  | 2.20                     | 0.41              |
| 1:A:2727:A:N1     | 1:A:2756:U:C2    | 2.89                     | 0.41              |
| 2:B:3003:A:N6     | 2:B:3022:G:H1'   | 2.36                     | 0.41              |
| 4:D:69:VAL:HA     | 4:D:70:PRO:HD3   | 1.90                     | 0.41              |
| 6:F:128:LEU:C     | 6:F:128:LEU:HD23 | 2.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:68:ALA:HB2   | 10:J:149:ALA:HB2  | 2.03                     | 0.41              |
| 10:J:82:LYS:HB2   | 10:J:82:LYS:HZ2   | 1.86                     | 0.41              |
| 10:J:136:VAL:HG23 | 37:J:8344:HOH:O   | 2.20                     | 0.41              |
| 13:M:73:VAL:HG11  | 13:M:118:LEU:HD21 | 2.03                     | 0.41              |
| 14:N:5:TYR:O      | 14:N:6:SER:C      | 2.64                     | 0.41              |
| 26:Z:130:ARG:HB2  | 26:Z:142:SER:O    | 2.20                     | 0.41              |
| 27:1:31:ILE:O     | 27:1:35:LYS:HG3   | 2.20                     | 0.41              |
| 1:A:12:U:H2'      | 1:A:13:G:H5'      | 2.02                     | 0.40              |
| 1:A:70:A:H4'      | 1:A:71:G:O5'      | 2.21                     | 0.40              |
| 1:A:154:C:P       | 14:N:188:ARG:HH12 | 2.44                     | 0.40              |
| 1:A:262:A:OP2     | 8:H:91:VAL:HG11   | 2.22                     | 0.40              |
| 1:A:685:C:O2      | 1:A:748:C:H4'     | 2.20                     | 0.40              |
| 1:A:778:C:C4      | 1:A:779:U:C4      | 3.09                     | 0.40              |
| 1:A:784:A:O2'     | 1:A:1458:A:N3     | 2.45                     | 0.40              |
| 1:A:1024:G:C5     | 1:A:1025:C:C4     | 3.09                     | 0.40              |
| 1:A:1634:G:H2'    | 1:A:1635:U:H6     | 1.86                     | 0.40              |
| 1:A:1681:G:H4'    | 1:A:1682:A:N3     | 2.36                     | 0.40              |
| 1:A:2455:A:H2'    | 1:A:2456:A:O4'    | 2.21                     | 0.40              |
| 2:B:3050:G:C6     | 2:B:3051:A:N6     | 2.89                     | 0.40              |
| 2:B:3057:A:C8     | 6:F:141:VAL:HG21  | 2.56                     | 0.40              |
| 3:C:107:ASN:OD1   | 3:C:116:GLY:HA3   | 2.21                     | 0.40              |
| 3:C:140:LEU:HB3   | 3:C:141:PRO:HD2   | 2.03                     | 0.40              |
| 4:D:51:VAL:HG21   | 4:D:327:VAL:HG13  | 2.03                     | 0.40              |
| 4:D:92:TYR:CD1    | 4:D:92:TYR:N      | 2.89                     | 0.40              |
| 5:E:39:GLN:O      | 5:E:43:LYS:HD3    | 2.21                     | 0.40              |
| 5:E:127:ARG:CZ    | 5:E:225:PRO:HG2   | 2.49                     | 0.40              |
| 13:M:104:ASP:HB2  | 37:M:8448:HOH:O   | 2.21                     | 0.40              |
| 14:N:37:VAL:HG21  | 14:N:108:LYS:CG   | 2.51                     | 0.40              |
| 15:O:72:GLU:H     | 15:O:171:HIS:CE1  | 2.39                     | 0.40              |
| 16:P:22:GLY:CA    | 37:P:2823:HOH:O   | 2.69                     | 0.40              |
| 19:S:61:GLN:CD    | 37:S:8540:HOH:O   | 2.64                     | 0.40              |
| 19:S:72:VAL:HG11  | 19:S:75:TRP:HB3   | 2.02                     | 0.40              |
| 19:S:149:GLU:HA   | 19:S:150:PRO:HD3  | 1.87                     | 0.40              |
| 1:A:432:G:O2'     | 1:A:433:C:H5'     | 2.21                     | 0.40              |
| 1:A:709:G:O2'     | 16:P:25:VAL:HG12  | 2.21                     | 0.40              |
| 1:A:840:U:O2      | 1:A:2055:A:H1'    | 2.22                     | 0.40              |
| 1:A:958:G:H2'     | 1:A:959:C:C6      | 2.55                     | 0.40              |
| 1:A:1141:U:H2'    | 1:A:1142:C:H6     | 1.86                     | 0.40              |
| 1:A:1309:U:O2'    | 1:A:1310:U:H5'    | 2.22                     | 0.40              |
| 1:A:2001:G:C2'    | 1:A:2002:C:H5'    | 2.52                     | 0.40              |
| 1:A:2038:A:OP2    | 4:D:224:LYS:NZ    | 2.43                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:2090:G:H2'   | 1:A:2091:G:C8     | 2.56                     | 0.40              |
| 1:A:2441:U:H4'   | 13:M:53:ARG:HD2   | 2.03                     | 0.40              |
| 1:A:2502:C:H4'   | 10:J:151:MET:HG2  | 2.03                     | 0.40              |
| 2:B:3045:A:H2'   | 2:B:3046:C:H6     | 1.86                     | 0.40              |
| 2:B:3091:C:H2'   | 2:B:3092:G:O4'    | 2.21                     | 0.40              |
| 3:C:126:ALA:HB1  | 3:C:138:VAL:CG1   | 2.51                     | 0.40              |
| 4:D:7:ARG:NH2    | 4:D:250:THR:O     | 2.54                     | 0.40              |
| 7:G:139:GLU:CG   | 37:G:5919:HOH:O   | 2.69                     | 0.40              |
| 10:J:132:PHE:C   | 10:J:133:ILE:HG12 | 2.47                     | 0.40              |
| 16:P:44:ASN:OD1  | 16:P:65:LEU:HB2   | 2.21                     | 0.40              |
| 24:X:5:VAL:O     | 24:X:52:VAL:HG22  | 2.21                     | 0.40              |
| 24:X:58:SER:O    | 24:X:59:GLN:C     | 2.63                     | 0.40              |
| 29:3:18:ASN:ND2  | 29:3:40:ARG:H     | 2.15                     | 0.40              |
| 30:4:84:ARG:HD3  | 37:4:8551:HOH:O   | 2.21                     | 0.40              |
| 1:A:466:A:H2'    | 1:A:467:G:O4'     | 2.22                     | 0.40              |
| 1:A:1016:U:O2'   | 1:A:2303:A:N7     | 2.40                     | 0.40              |
| 1:A:1058:A:H2'   | 1:A:1060:C:C5'    | 2.49                     | 0.40              |
| 1:A:1068:C:OP2   | 37:A:3868:HOH:O   | 2.22                     | 0.40              |
| 1:A:1495:C:C1'   | 1:A:1573:A:H1'    | 2.52                     | 0.40              |
| 1:A:1593:C:O2'   | 1:A:1594:C:H5'    | 2.22                     | 0.40              |
| 1:A:1613:C:H2'   | 1:A:1614:G:O4'    | 2.21                     | 0.40              |
| 1:A:1827:G:H2'   | 1:A:1828:G:C8     | 2.56                     | 0.40              |
| 1:A:2453:G:H5''  | 37:M:8415:HOH:O   | 2.20                     | 0.40              |
| 1:A:2456:A:H2'   | 1:A:2457:U:H6     | 1.84                     | 0.40              |
| 3:C:30:ARG:HE    | 3:C:30:ARG:HB3    | 1.70                     | 0.40              |
| 3:C:130:THR:HG22 | 3:C:131:HIS:O     | 2.20                     | 0.40              |
| 4:D:162:MET:HE2  | 4:D:310:ARG:CG    | 2.52                     | 0.40              |
| 11:K:52:GLN:CG   | 11:K:53:ILE:N     | 2.85                     | 0.40              |
| 12:L:87:ARG:NE   | 37:L:4854:HOH:O   | 2.53                     | 0.40              |
| 14:N:49:ALA:C    | 14:N:54:TYR:HB3   | 2.46                     | 0.40              |
| 16:P:4:ASN:HB3   | 16:P:7:LEU:HB3    | 2.04                     | 0.40              |
| 18:R:42:LYS:HA   | 18:R:42:LYS:HD2   | 1.93                     | 0.40              |
| 21:U:23:VAL:C    | 21:U:93:THR:HG21  | 2.46                     | 0.40              |
| 25:Y:74:ALA:CB   | 25:Y:85:VAL:HG22  | 2.52                     | 0.40              |
| 1:A:282:C:H2'    | 1:A:283:U:O4'     | 2.20                     | 0.40              |
| 1:A:327:A:OP1    | 5:E:149:LYS:NZ    | 2.41                     | 0.40              |
| 1:A:538:C:H5''   | 1:A:539:G:C8      | 2.56                     | 0.40              |
| 1:A:1730:G:C5'   | 1:A:1731:C:C6     | 3.04                     | 0.40              |
| 1:A:1859:A:N6    | 37:A:9721:HOH:O   | 2.42                     | 0.40              |
| 1:A:2121:G:O2'   | 1:A:2122:C:H5'    | 2.21                     | 0.40              |
| 1:A:2550:U:O2'   | 1:A:2551:C:H5'    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:108:GLU:HB3   | 4:D:111:ARG:HD2  | 2.03                     | 0.40              |
| 6:F:104:PHE:CE2   | 6:F:166:ILE:HD13 | 2.57                     | 0.40              |
| 7:G:83:GLY:O      | 7:G:169:THR:N    | 2.41                     | 0.40              |
| 14:N:115:LEU:HD13 | 14:N:115:LEU:C   | 2.46                     | 0.40              |
| 15:O:143:ARG:NH1  | 15:O:173:ASP:OD2 | 2.40                     | 0.40              |
| 16:P:99:GLU:CG    | 37:P:6044:HOH:O  | 2.68                     | 0.40              |
| 16:P:99:GLU:HG3   | 37:P:6044:HOH:O  | 2.21                     | 0.40              |
| 21:U:44:ALA:HA    | 21:U:62:VAL:HG12 | 2.03                     | 0.40              |
| 25:Y:71:ARG:HD2   | 37:Y:7542:HOH:O  | 2.22                     | 0.40              |
| 1:A:1224:G:H2'    | 1:A:1225:C:C6    | 2.56                     | 0.40              |
| 1:A:1416:G:H2'    | 1:A:1417:G:H5'   | 2.03                     | 0.40              |
| 1:A:1594:C:C5     | 17:Q:120:ARG:CZ  | 3.04                     | 0.40              |
| 1:A:1706:G:C6     | 1:A:1707:G:C6    | 3.09                     | 0.40              |
| 1:A:1815:A:H2'    | 1:A:1816:C:O4'   | 2.21                     | 0.40              |
| 1:A:2270:G:C4'    | 3:C:223:ARG:HH12 | 2.31                     | 0.40              |
| 1:A:2552:C:C6     | 1:A:2577:A:N7    | 2.89                     | 0.40              |
| 1:A:2564:G:OP2    | 1:A:2565:C:H5''  | 2.22                     | 0.40              |
| 1:A:2598:U:H2'    | 1:A:2600:A:OP2   | 2.22                     | 0.40              |
| 1:A:2812:A:H1'    | 37:A:5365:HOH:O  | 2.21                     | 0.40              |
| 1:A:2823:G:H4'    | 1:A:2827:A:O4'   | 2.21                     | 0.40              |
| 4:D:195:ARG:NH1   | 4:D:324:ASP:OD1  | 2.52                     | 0.40              |
| 6:F:173:GLU:HG3   | 6:F:174:VAL:N    | 2.37                     | 0.40              |
| 7:G:138:ILE:HG23  | 7:G:139:GLU:N    | 2.36                     | 0.40              |
| 8:H:26:THR:HG21   | 8:H:103:ALA:CB   | 2.52                     | 0.40              |
| 10:J:163:PRO:HG2  | 37:J:8339:HOH:O  | 2.21                     | 0.40              |
| 11:K:130:VAL:CG1  | 11:K:131:THR:N   | 2.84                     | 0.40              |
| 12:L:22:ASP:CG    | 12:L:24:THR:HG23 | 2.46                     | 0.40              |
| 12:L:78:LYS:HA    | 12:L:79:PRO:HD3  | 1.80                     | 0.40              |
| 15:O:24:LEU:O     | 15:O:25:ARG:C    | 2.62                     | 0.40              |
| 15:O:149:GLU:O    | 15:O:152:GLU:HB2 | 2.22                     | 0.40              |
| 23:W:45:ARG:C     | 23:W:47:LYS:N    | 2.78                     | 0.40              |
| 27:1:17:ARG:O     | 27:1:18:TYR:HB2  | 2.21                     | 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 X-ray entries followed by that with respect to entries

of similar resolution.

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 |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3   | C     | 235/239 (98%)   | 204 (87%)  | 26 (11%) | 5 (2%)   | 5           | 31  |
| 4   | D     | 335/337 (99%)   | 303 (90%)  | 23 (7%)  | 9 (3%)   | 4           | 25  |
| 5   | E     | 244/246 (99%)   | 220 (90%)  | 23 (9%)  | 1 (0%)   | 30          | 62  |
| 6   | F     | 134/176 (76%)   | 94 (70%)   | 26 (19%) | 14 (10%) | 0           | 2   |
| 7   | G     | 170/177 (96%)   | 160 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 8   | H     | 117/119 (98%)   | 103 (88%)  | 12 (10%) | 2 (2%)   | 7           | 35  |
| 9   | I     | 25/348 (7%)     | 24 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 10  | J     | 152/167 (91%)   | 130 (86%)  | 17 (11%) | 5 (3%)   | 3           | 21  |
| 11  | K     | 140/145 (97%)   | 130 (93%)  | 7 (5%)   | 3 (2%)   | 5           | 31  |
| 12  | L     | 130/132 (98%)   | 116 (89%)  | 12 (9%)  | 2 (2%)   | 8           | 37  |
| 13  | M     | 141/164 (86%)   | 119 (84%)  | 20 (14%) | 2 (1%)   | 9           | 39  |
| 14  | N     | 192/194 (99%)   | 174 (91%)  | 15 (8%)  | 3 (2%)   | 7           | 36  |
| 15  | O     | 184/186 (99%)   | 164 (89%)  | 13 (7%)  | 7 (4%)   | 2           | 18  |
| 16  | P     | 113/115 (98%)   | 108 (96%)  | 4 (4%)   | 1 (1%)   | 14          | 47  |
| 17  | Q     | 141/148 (95%)   | 135 (96%)  | 5 (4%)   | 1 (1%)   | 18          | 52  |
| 18  | R     | 93/95 (98%)     | 86 (92%)   | 6 (6%)   | 1 (1%)   | 11          | 43  |
| 19  | S     | 148/154 (96%)   | 139 (94%)  | 8 (5%)   | 1 (1%)   | 18          | 52  |
| 20  | T     | 79/84 (94%)     | 74 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 21  | U     | 117/119 (98%)   | 107 (92%)  | 9 (8%)   | 1 (1%)   | 14          | 47  |
| 22  | V     | 51/66 (77%)     | 46 (90%)   | 4 (8%)   | 1 (2%)   | 6           | 31  |
| 23  | W     | 63/70 (90%)     | 57 (90%)   | 4 (6%)   | 2 (3%)   | 3           | 21  |
| 24  | X     | 152/154 (99%)   | 145 (95%)  | 6 (4%)   | 1 (1%)   | 18          | 52  |
| 25  | Y     | 80/91 (88%)     | 71 (89%)   | 8 (10%)  | 1 (1%)   | 9           | 40  |
| 26  | Z     | 140/240 (58%)   | 137 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 27  | 1     | 71/73 (97%)     | 61 (86%)   | 8 (11%)  | 2 (3%)   | 4           | 25  |
| 28  | 2     | 54/56 (96%)     | 52 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 29  | 3     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 30  | 4     | 90/92 (98%)     | 84 (93%)   | 4 (4%)   | 2 (2%)   | 5           | 29  |
| All | All   | 3633/4235 (86%) | 3285 (90%) | 281 (8%) | 67 (2%)  | 6           | 34  |

All (67) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 139 | ASP  |
| 6   | F     | 93  | LEU  |
| 6   | F     | 95  | THR  |
| 6   | F     | 173 | GLU  |
| 8   | H     | 101 | ALA  |
| 10  | J     | 162 | SER  |
| 10  | J     | 164 | ALA  |
| 11  | K     | 143 | LYS  |
| 13  | M     | 21  | ARG  |
| 13  | M     | 80  | ASP  |
| 15  | O     | 154 | LEU  |
| 15  | O     | 164 | ASP  |
| 15  | O     | 183 | ASP  |
| 23  | W     | 43  | PRO  |
| 24  | X     | 77  | ALA  |
| 3   | C     | 34  | ASP  |
| 3   | C     | 37  | VAL  |
| 3   | C     | 132 | ASP  |
| 4   | D     | 34  | GLY  |
| 4   | D     | 169 | GLY  |
| 4   | D     | 184 | ASP  |
| 6   | F     | 16  | PRO  |
| 6   | F     | 20  | LYS  |
| 6   | F     | 61  | PHE  |
| 6   | F     | 171 | ASP  |
| 10  | J     | 40  | PRO  |
| 10  | J     | 138 | PRO  |
| 11  | K     | 5   | GLU  |
| 14  | N     | 140 | ALA  |
| 14  | N     | 165 | SER  |
| 15  | O     | 162 | ASP  |
| 15  | O     | 181 | ASP  |
| 22  | V     | 7   | ASP  |
| 30  | 4     | 57  | GLY  |
| 4   | D     | 107 | SER  |
| 5   | E     | 8   | LEU  |
| 6   | F     | 36  | ASN  |
| 6   | F     | 137 | PRO  |
| 6   | F     | 147 | ALA  |
| 12  | L     | 119 | GLN  |
| 25  | Y     | 77  | PHE  |
| 6   | F     | 11  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 82  | GLU  |
| 6   | F     | 170 | TYR  |
| 11  | K     | 7   | ASP  |
| 14  | N     | 18  | GLY  |
| 15  | O     | 65  | ASP  |
| 15  | O     | 167 | ASP  |
| 17  | Q     | 116 | SER  |
| 27  | 1     | 81  | LYS  |
| 30  | 4     | 56  | PRO  |
| 3   | C     | 69  | LEU  |
| 3   | C     | 119 | ALA  |
| 4   | D     | 206 | THR  |
| 4   | D     | 291 | ASP  |
| 6   | F     | 96  | SER  |
| 8   | H     | 64  | PRO  |
| 12  | L     | 126 | SER  |
| 16  | P     | 20  | SER  |
| 4   | D     | 2   | GLN  |
| 4   | D     | 185 | GLY  |
| 21  | U     | 53  | GLY  |
| 10  | J     | 72  | VAL  |
| 23  | W     | 40  | PRO  |
| 27  | 1     | 41  | VAL  |
| 19  | S     | 81  | PRO  |
| 18  | R     | 54  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3   | C     | 179/181 (99%)  | 168 (94%) | 11 (6%)  | 17          | 49 |
| 4   | D     | 282/282 (100%) | 264 (94%) | 18 (6%)  | 16          | 48 |
| 5   | E     | 193/193 (100%) | 175 (91%) | 18 (9%)  | 8           | 33 |
| 6   | F     | 117/147 (80%)  | 109 (93%) | 8 (7%)   | 14          | 46 |
| 7   | G     | 152/155 (98%)  | 147 (97%) | 5 (3%)   | 33          | 65 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8   | H     | 92/92 (100%)    | 89 (97%)   | 3 (3%)   | 33          | 65  |
| 9   | I     | 27/283 (10%)    | 27 (100%)  | 0        | 100         | 100 |
| 10  | J     | 122/122 (100%)  | 107 (88%)  | 15 (12%) | 4           | 22  |
| 11  | K     | 118/121 (98%)   | 110 (93%)  | 8 (7%)   | 14          | 46  |
| 12  | L     | 106/106 (100%)  | 103 (97%)  | 3 (3%)   | 38          | 68  |
| 13  | M     | 112/126 (89%)   | 109 (97%)  | 3 (3%)   | 39          | 68  |
| 14  | N     | 166/166 (100%)  | 159 (96%)  | 7 (4%)   | 26          | 60  |
| 15  | O     | 149/149 (100%)  | 142 (95%)  | 7 (5%)   | 23          | 57  |
| 16  | P     | 93/93 (100%)    | 88 (95%)   | 5 (5%)   | 20          | 53  |
| 17  | Q     | 113/116 (97%)   | 110 (97%)  | 3 (3%)   | 39          | 68  |
| 18  | R     | 79/79 (100%)    | 75 (95%)   | 4 (5%)   | 21          | 54  |
| 19  | S     | 117/121 (97%)   | 114 (97%)  | 3 (3%)   | 40          | 69  |
| 20  | T     | 71/73 (97%)     | 70 (99%)   | 1 (1%)   | 59          | 77  |
| 21  | U     | 105/105 (100%)  | 100 (95%)  | 5 (5%)   | 23          | 56  |
| 22  | V     | 44/52 (85%)     | 44 (100%)  | 0        | 100         | 100 |
| 23  | W     | 51/56 (91%)     | 50 (98%)   | 1 (2%)   | 48          | 72  |
| 24  | X     | 130/130 (100%)  | 120 (92%)  | 10 (8%)  | 12          | 41  |
| 25  | Y     | 66/73 (90%)     | 61 (92%)   | 5 (8%)   | 12          | 42  |
| 26  | Z     | 120/195 (62%)   | 112 (93%)  | 8 (7%)   | 15          | 47  |
| 27  | 1     | 56/56 (100%)    | 54 (96%)   | 2 (4%)   | 31          | 63  |
| 28  | 2     | 46/46 (100%)    | 46 (100%)  | 0        | 100         | 100 |
| 29  | 3     | 42/44 (96%)     | 41 (98%)   | 1 (2%)   | 43          | 70  |
| 30  | 4     | 79/79 (100%)    | 76 (96%)   | 3 (4%)   | 29          | 62  |
| All | All   | 3027/3441 (88%) | 2870 (95%) | 157 (5%) | 21          | 54  |

All (157) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 3   | ARG  |
| 3   | C     | 36  | ASP  |
| 3   | C     | 55  | VAL  |
| 3   | C     | 68  | ILE  |
| 3   | C     | 69  | LEU  |
| 3   | C     | 94  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 131 | HIS  |
| 3   | C     | 153 | ARG  |
| 3   | C     | 175 | LYS  |
| 3   | C     | 179 | MET  |
| 3   | C     | 217 | ARG  |
| 4   | D     | 7   | ARG  |
| 4   | D     | 11  | LEU  |
| 4   | D     | 27  | ASN  |
| 4   | D     | 33  | ASP  |
| 4   | D     | 63  | GLU  |
| 4   | D     | 84  | LEU  |
| 4   | D     | 97  | LEU  |
| 4   | D     | 98  | THR  |
| 4   | D     | 103 | ASP  |
| 4   | D     | 195 | ARG  |
| 4   | D     | 245 | SER  |
| 4   | D     | 251 | VAL  |
| 4   | D     | 254 | GLN  |
| 4   | D     | 256 | GLN  |
| 4   | D     | 264 | GLU  |
| 4   | D     | 304 | PRO  |
| 4   | D     | 307 | ARG  |
| 4   | D     | 312 | ARG  |
| 5   | E     | 2   | GLN  |
| 5   | E     | 27  | ARG  |
| 5   | E     | 67  | GLN  |
| 5   | E     | 78  | ARG  |
| 5   | E     | 91  | PRO  |
| 5   | E     | 94  | THR  |
| 5   | E     | 101 | ASP  |
| 5   | E     | 115 | LEU  |
| 5   | E     | 136 | VAL  |
| 5   | E     | 187 | ARG  |
| 5   | E     | 214 | THR  |
| 5   | E     | 222 | ASP  |
| 5   | E     | 223 | LEU  |
| 5   | E     | 234 | VAL  |
| 5   | E     | 236 | THR  |
| 5   | E     | 240 | LEU  |
| 5   | E     | 243 | VAL  |
| 5   | E     | 246 | ARG  |
| 6   | F     | 24  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 50  | VAL  |
| 6   | F     | 95  | THR  |
| 6   | F     | 99  | ASP  |
| 6   | F     | 131 | THR  |
| 6   | F     | 136 | ARG  |
| 6   | F     | 137 | PRO  |
| 6   | F     | 149 | ARG  |
| 7   | G     | 7   | ILE  |
| 7   | G     | 36  | PRO  |
| 7   | G     | 54  | ASP  |
| 7   | G     | 86  | VAL  |
| 7   | G     | 102 | VAL  |
| 8   | H     | 1   | PRO  |
| 8   | H     | 12  | LEU  |
| 8   | H     | 46  | GLU  |
| 10  | J     | 1   | LYS  |
| 10  | J     | 18  | GLU  |
| 10  | J     | 30  | GLN  |
| 10  | J     | 59  | ASN  |
| 10  | J     | 61  | LEU  |
| 10  | J     | 72  | VAL  |
| 10  | J     | 73  | GLN  |
| 10  | J     | 82  | LYS  |
| 10  | J     | 85  | ILE  |
| 10  | J     | 86  | ARG  |
| 10  | J     | 93  | ILE  |
| 10  | J     | 94  | ARG  |
| 10  | J     | 142 | VAL  |
| 10  | J     | 150 | LYS  |
| 10  | J     | 166 | ASN  |
| 11  | K     | 46  | ILE  |
| 11  | K     | 52  | GLN  |
| 11  | K     | 74  | ARG  |
| 11  | K     | 93  | ARG  |
| 11  | K     | 120 | SER  |
| 11  | K     | 125 | SER  |
| 11  | K     | 127 | ILE  |
| 11  | K     | 131 | THR  |
| 12  | L     | 7   | ASP  |
| 12  | L     | 10  | GLN  |
| 12  | L     | 98  | VAL  |
| 13  | M     | 35  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 117 | GLU  |
| 13  | M     | 140 | VAL  |
| 14  | N     | 38  | VAL  |
| 14  | N     | 46  | LEU  |
| 14  | N     | 48  | ARG  |
| 14  | N     | 81  | ARG  |
| 14  | N     | 87  | MET  |
| 14  | N     | 93  | ARG  |
| 14  | N     | 164 | THR  |
| 15  | O     | 26  | LEU  |
| 15  | O     | 43  | VAL  |
| 15  | O     | 47  | LEU  |
| 15  | O     | 127 | LEU  |
| 15  | O     | 128 | ASP  |
| 15  | O     | 152 | GLU  |
| 15  | O     | 163 | PHE  |
| 16  | P     | 3   | THR  |
| 16  | P     | 28  | ASP  |
| 16  | P     | 97  | SER  |
| 16  | P     | 98  | LEU  |
| 16  | P     | 111 | VAL  |
| 17  | Q     | 52  | LYS  |
| 17  | Q     | 91  | LYS  |
| 17  | Q     | 98  | ILE  |
| 18  | R     | 11  | ARG  |
| 18  | R     | 16  | ASN  |
| 18  | R     | 57  | ASP  |
| 18  | R     | 95  | GLU  |
| 19  | S     | 13  | THR  |
| 19  | S     | 39  | THR  |
| 19  | S     | 82  | GLU  |
| 20  | T     | 10  | VAL  |
| 21  | U     | 39  | ASN  |
| 21  | U     | 46  | ASP  |
| 21  | U     | 47  | THR  |
| 21  | U     | 48  | VAL  |
| 21  | U     | 96  | VAL  |
| 23  | W     | 43  | PRO  |
| 24  | X     | 4   | LEU  |
| 24  | X     | 35  | VAL  |
| 24  | X     | 45  | VAL  |
| 24  | X     | 52  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | X     | 73  | LEU  |
| 24  | X     | 120 | PRO  |
| 24  | X     | 122 | ARG  |
| 24  | X     | 142 | ASP  |
| 24  | X     | 146 | ILE  |
| 24  | X     | 154 | ARG  |
| 25  | Y     | 15  | ARG  |
| 25  | Y     | 49  | ARG  |
| 25  | Y     | 52  | PRO  |
| 25  | Y     | 66  | THR  |
| 25  | Y     | 72  | VAL  |
| 26  | Z     | 103 | THR  |
| 26  | Z     | 154 | ARG  |
| 26  | Z     | 163 | THR  |
| 26  | Z     | 172 | THR  |
| 26  | Z     | 189 | ASN  |
| 26  | Z     | 200 | THR  |
| 26  | Z     | 203 | VAL  |
| 26  | Z     | 235 | GLU  |
| 27  | 1     | 11  | THR  |
| 27  | 1     | 64  | ILE  |
| 29  | 3     | 18  | ASN  |
| 30  | 4     | 42  | ARG  |
| 30  | 4     | 56  | PRO  |
| 30  | 4     | 65  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 5   | GLN  |
| 3   | C     | 47  | HIS  |
| 3   | C     | 92  | ASN  |
| 3   | C     | 127 | GLN  |
| 3   | C     | 199 | HIS  |
| 3   | C     | 218 | ASN  |
| 4   | D     | 2   | GLN  |
| 4   | D     | 27  | ASN  |
| 4   | D     | 55  | ASN  |
| 4   | D     | 94  | GLN  |
| 4   | D     | 145 | HIS  |
| 4   | D     | 221 | GLN  |
| 4   | D     | 238 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 260 | HIS  |
| 4   | D     | 318 | ASN  |
| 4   | D     | 332 | ASN  |
| 5   | E     | 2   | GLN  |
| 5   | E     | 39  | GLN  |
| 5   | E     | 67  | GLN  |
| 5   | E     | 108 | GLN  |
| 5   | E     | 129 | HIS  |
| 5   | E     | 163 | HIS  |
| 6   | F     | 103 | ASN  |
| 6   | F     | 133 | ASN  |
| 7   | G     | 96  | ASN  |
| 7   | G     | 106 | ASN  |
| 7   | G     | 119 | HIS  |
| 7   | G     | 143 | GLN  |
| 8   | H     | 79  | GLN  |
| 9   | I     | 17  | GLN  |
| 9   | I     | 64  | ASN  |
| 10  | J     | 8   | ASN  |
| 10  | J     | 30  | GLN  |
| 10  | J     | 35  | ASN  |
| 10  | J     | 45  | GLN  |
| 10  | J     | 55  | GLN  |
| 10  | J     | 58  | HIS  |
| 10  | J     | 59  | ASN  |
| 10  | J     | 74  | ASN  |
| 10  | J     | 80  | ASN  |
| 10  | J     | 91  | HIS  |
| 10  | J     | 129 | ASN  |
| 10  | J     | 130 | HIS  |
| 10  | J     | 137 | ASN  |
| 10  | J     | 166 | ASN  |
| 11  | K     | 52  | GLN  |
| 11  | K     | 107 | ASN  |
| 12  | L     | 10  | GLN  |
| 13  | M     | 18  | HIS  |
| 13  | M     | 41  | HIS  |
| 13  | M     | 42  | ASN  |
| 13  | M     | 58  | GLN  |
| 13  | M     | 116 | HIS  |
| 14  | N     | 19  | GLN  |
| 14  | N     | 58  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 89  | ASN  |
| 14  | N     | 176 | GLN  |
| 15  | O     | 107 | ASN  |
| 15  | O     | 153 | GLN  |
| 16  | P     | 53  | GLN  |
| 16  | P     | 100 | GLN  |
| 16  | P     | 105 | ASN  |
| 17  | Q     | 50  | GLN  |
| 17  | Q     | 66  | GLN  |
| 17  | Q     | 73  | HIS  |
| 17  | Q     | 118 | GLN  |
| 18  | R     | 16  | ASN  |
| 18  | R     | 40  | HIS  |
| 18  | R     | 67  | GLN  |
| 19  | S     | 61  | GLN  |
| 19  | S     | 94  | ASN  |
| 19  | S     | 98  | ASN  |
| 19  | S     | 113 | HIS  |
| 19  | S     | 117 | HIS  |
| 19  | S     | 140 | GLN  |
| 20  | T     | 25  | GLN  |
| 20  | T     | 53  | ASN  |
| 20  | T     | 55  | GLN  |
| 20  | T     | 56  | ASN  |
| 21  | U     | 11  | GLN  |
| 21  | U     | 39  | ASN  |
| 21  | U     | 73  | HIS  |
| 22  | V     | 39  | ASN  |
| 23  | W     | 60  | GLN  |
| 24  | X     | 28  | HIS  |
| 24  | X     | 110 | GLN  |
| 24  | X     | 119 | HIS  |
| 24  | X     | 125 | HIS  |
| 24  | X     | 141 | HIS  |
| 25  | Y     | 23  | HIS  |
| 26  | Z     | 133 | HIS  |
| 26  | Z     | 134 | HIS  |
| 26  | Z     | 149 | GLN  |
| 26  | Z     | 189 | ASN  |
| 27  | 1     | 33  | HIS  |
| 27  | 1     | 70  | GLN  |
| 28  | 2     | 8   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | 2     | 16  | HIS  |
| 28  | 2     | 28  | HIS  |
| 29  | 3     | 16  | ASN  |
| 29  | 3     | 18  | ASN  |
| 29  | 3     | 37  | HIS  |
| 29  | 3     | 41  | HIS  |
| 29  | 3     | 45  | ASN  |
| 30  | 4     | 30  | GLN  |
| 30  | 4     | 48  | ASN  |
| 30  | 4     | 78  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 2747/2922 (94%) | 252 (9%)          | 36 (1%)         |
| 2   | B     | 121/122 (99%)   | 16 (13%)          | 6 (4%)          |
| All | All   | 2868/3044 (94%) | 268 (9%)          | 42 (1%)         |

All (268) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | A    |
| 1   | A     | 31  | C    |
| 1   | A     | 60  | A    |
| 1   | A     | 67  | A    |
| 1   | A     | 69  | A    |
| 1   | A     | 70  | A    |
| 1   | A     | 71  | G    |
| 1   | A     | 87  | C    |
| 1   | A     | 88  | G    |
| 1   | A     | 115 | U    |
| 1   | A     | 120 | A    |
| 1   | A     | 130 | C    |
| 1   | A     | 139 | C    |
| 1   | A     | 141 | C    |
| 1   | A     | 151 | A    |
| 1   | A     | 166 | A    |
| 1   | A     | 169 | A    |
| 1   | A     | 186 | A    |
| 1   | A     | 191 | A    |
| 1   | A     | 192 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 200 | U    |
| 1   | A     | 219 | G    |
| 1   | A     | 237 | G    |
| 1   | A     | 271 | C    |
| 1   | A     | 272 | A    |
| 1   | A     | 273 | G    |
| 1   | A     | 283 | U    |
| 1   | A     | 284 | C    |
| 1   | A     | 285 | A    |
| 1   | A     | 308 | U    |
| 1   | A     | 309 | C    |
| 1   | A     | 318 | C    |
| 1   | A     | 336 | G    |
| 1   | A     | 337 | A    |
| 1   | A     | 345 | G    |
| 1   | A     | 358 | G    |
| 1   | A     | 381 | G    |
| 1   | A     | 397 | A    |
| 1   | A     | 417 | G    |
| 1   | A     | 461 | C    |
| 1   | A     | 487 | G    |
| 1   | A     | 498 | A    |
| 1   | A     | 510 | U    |
| 1   | A     | 511 | A    |
| 1   | A     | 514 | G    |
| 1   | A     | 537 | G    |
| 1   | A     | 538 | C    |
| 1   | A     | 539 | G    |
| 1   | A     | 542 | A    |
| 1   | A     | 545 | G    |
| 1   | A     | 553 | G    |
| 1   | A     | 559 | U    |
| 1   | A     | 588 | G    |
| 1   | A     | 604 | G    |
| 1   | A     | 620 | A    |
| 1   | A     | 632 | A    |
| 1   | A     | 644 | G    |
| 1   | A     | 645 | U    |
| 1   | A     | 660 | A    |
| 1   | A     | 688 | A    |
| 1   | A     | 701 | U    |
| 1   | A     | 717 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 759  | C    |
| 1   | A     | 777  | U    |
| 1   | A     | 809  | G    |
| 1   | A     | 821  | U    |
| 1   | A     | 835  | U    |
| 1   | A     | 840  | U    |
| 1   | A     | 857  | A    |
| 1   | A     | 858  | U    |
| 1   | A     | 868  | G    |
| 1   | A     | 869  | G    |
| 1   | A     | 871  | G    |
| 1   | A     | 872  | U    |
| 1   | A     | 875  | A    |
| 1   | A     | 877  | G    |
| 1   | A     | 878  | G    |
| 1   | A     | 882  | A    |
| 1   | A     | 884  | C    |
| 1   | A     | 885  | G    |
| 1   | A     | 905  | C    |
| 1   | A     | 920  | C    |
| 1   | A     | 921  | G    |
| 1   | A     | 923  | A    |
| 1   | A     | 953  | G    |
| 1   | A     | 960  | G    |
| 1   | A     | 961  | A    |
| 1   | A     | 1006 | A    |
| 1   | A     | 1008 | C    |
| 1   | A     | 1029 | U    |
| 1   | A     | 1045 | G    |
| 1   | A     | 1059 | G    |
| 1   | A     | 1060 | C    |
| 1   | A     | 1072 | G    |
| 1   | A     | 1081 | A    |
| 1   | A     | 1083 | C    |
| 1   | A     | 1087 | G    |
| 1   | A     | 1088 | A    |
| 1   | A     | 1109 | U    |
| 1   | A     | 1110 | G    |
| 1   | A     | 1119 | G    |
| 1   | A     | 1130 | U    |
| 1   | A     | 1137 | G    |
| 1   | A     | 1151 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1161 | A    |
| 1   | A     | 1162 | G    |
| 1   | A     | 1164 | U    |
| 1   | A     | 1165 | G    |
| 1   | A     | 1166 | A    |
| 1   | A     | 1171 | A    |
| 1   | A     | 1174 | A    |
| 1   | A     | 1175 | G    |
| 1   | A     | 1177 | A    |
| 1   | A     | 1185 | U    |
| 1   | A     | 1192 | A    |
| 1   | A     | 1193 | A    |
| 1   | A     | 1206 | U    |
| 1   | A     | 1216 | G    |
| 1   | A     | 1234 | U    |
| 1   | A     | 1237 | U    |
| 1   | A     | 1238 | C    |
| 1   | A     | 1239 | G    |
| 1   | A     | 1261 | A    |
| 1   | A     | 1262 | C    |
| 1   | A     | 1279 | U    |
| 1   | A     | 1289 | C    |
| 1   | A     | 1342 | C    |
| 1   | A     | 1353 | C    |
| 1   | A     | 1360 | C    |
| 1   | A     | 1377 | C    |
| 1   | A     | 1407 | A    |
| 1   | A     | 1409 | G    |
| 1   | A     | 1451 | C    |
| 1   | A     | 1474 | C    |
| 1   | A     | 1488 | U    |
| 1   | A     | 1505 | U    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1524 | U    |
| 1   | A     | 1525 | G    |
| 1   | A     | 1526 | A    |
| 1   | A     | 1564 | C    |
| 1   | A     | 1580 | A    |
| 1   | A     | 1592 | G    |
| 1   | A     | 1625 | U    |
| 1   | A     | 1626 | A    |
| 1   | A     | 1633 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1634 | G    |
| 1   | A     | 1656 | A    |
| 1   | A     | 1667 | A    |
| 1   | A     | 1668 | U    |
| 1   | A     | 1682 | A    |
| 1   | A     | 1684 | A    |
| 1   | A     | 1685 | A    |
| 1   | A     | 1692 | C    |
| 1   | A     | 1701 | A    |
| 1   | A     | 1710 | A    |
| 1   | A     | 1722 | U    |
| 1   | A     | 1723 | G    |
| 1   | A     | 1725 | C    |
| 1   | A     | 1731 | C    |
| 1   | A     | 1752 | G    |
| 1   | A     | 1778 | A    |
| 1   | A     | 1798 | C    |
| 1   | A     | 1820 | G    |
| 1   | A     | 1829 | A    |
| 1   | A     | 1856 | C    |
| 1   | A     | 1879 | U    |
| 1   | A     | 1904 | A    |
| 1   | A     | 1919 | A    |
| 1   | A     | 1942 | A    |
| 1   | A     | 1943 | C    |
| 1   | A     | 1971 | G    |
| 1   | A     | 1973 | A    |
| 1   | A     | 1974 | G    |
| 1   | A     | 1978 | A    |
| 1   | A     | 1980 | U    |
| 1   | A     | 1982 | C    |
| 1   | A     | 1996 | U    |
| 1   | A     | 2006 | C    |
| 1   | A     | 2008 | U    |
| 1   | A     | 2011 | A    |
| 1   | A     | 2012 | U    |
| 1   | A     | 2013 | G    |
| 1   | A     | 2033 | G    |
| 1   | A     | 2034 | U    |
| 1   | A     | 2064 | U    |
| 1   | A     | 2072 | G    |
| 1   | A     | 2073 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2074 | A    |
| 1   | A     | 2096 | A    |
| 1   | A     | 2101 | A    |
| 1   | A     | 2102 | G    |
| 1   | A     | 2110 | G    |
| 1   | A     | 2238 | A    |
| 1   | A     | 2258 | A    |
| 1   | A     | 2271 | G    |
| 1   | A     | 2272 | G    |
| 1   | A     | 2291 | A    |
| 1   | A     | 2317 | C    |
| 1   | A     | 2321 | A    |
| 1   | A     | 2346 | C    |
| 1   | A     | 2354 | A    |
| 1   | A     | 2361 | A    |
| 1   | A     | 2369 | A    |
| 1   | A     | 2422 | U    |
| 1   | A     | 2462 | G    |
| 1   | A     | 2465 | A    |
| 1   | A     | 2467 | A    |
| 1   | A     | 2469 | A    |
| 1   | A     | 2476 | C    |
| 1   | A     | 2483 | A    |
| 1   | A     | 2507 | G    |
| 1   | A     | 2511 | A    |
| 1   | A     | 2526 | C    |
| 1   | A     | 2527 | U    |
| 1   | A     | 2533 | C    |
| 1   | A     | 2537 | G    |
| 1   | A     | 2541 | U    |
| 1   | A     | 2553 | A    |
| 1   | A     | 2564 | G    |
| 1   | A     | 2589 | U    |
| 1   | A     | 2601 | A    |
| 1   | A     | 2602 | G    |
| 1   | A     | 2608 | C    |
| 1   | A     | 2613 | G    |
| 1   | A     | 2638 | G    |
| 1   | A     | 2649 | A    |
| 1   | A     | 2664 | A    |
| 1   | A     | 2681 | A    |
| 1   | A     | 2682 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2718 | C    |
| 1   | A     | 2719 | A    |
| 1   | A     | 2726 | U    |
| 1   | A     | 2747 | C    |
| 1   | A     | 2748 | G    |
| 1   | A     | 2749 | U    |
| 1   | A     | 2750 | G    |
| 1   | A     | 2762 | C    |
| 1   | A     | 2768 | A    |
| 1   | A     | 2786 | G    |
| 1   | A     | 2792 | A    |
| 1   | A     | 2800 | A    |
| 1   | A     | 2811 | A    |
| 1   | A     | 2812 | A    |
| 1   | A     | 2825 | C    |
| 1   | A     | 2840 | A    |
| 1   | A     | 2850 | C    |
| 1   | A     | 2876 | G    |
| 1   | A     | 2890 | A    |
| 1   | A     | 2896 | A    |
| 1   | A     | 2903 | C    |
| 1   | A     | 2914 | A    |
| 2   | B     | 3002 | U    |
| 2   | B     | 3003 | A    |
| 2   | B     | 3014 | G    |
| 2   | B     | 3022 | G    |
| 2   | B     | 3024 | U    |
| 2   | B     | 3041 | C    |
| 2   | B     | 3043 | G    |
| 2   | B     | 3044 | A    |
| 2   | B     | 3052 | A    |
| 2   | B     | 3057 | A    |
| 2   | B     | 3066 | G    |
| 2   | B     | 3077 | A    |
| 2   | B     | 3103 | A    |
| 2   | B     | 3104 | A    |
| 2   | B     | 3114 | G    |
| 2   | B     | 3122 | C    |

All (42) RNA pucker outliers are listed below:

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

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 10   | U    |
| 1   | A     | 69   | A    |
| 1   | A     | 129  | A    |
| 1   | A     | 284  | C    |
| 1   | A     | 338  | C    |
| 1   | A     | 603  | A    |
| 1   | A     | 644  | G    |
| 1   | A     | 699  | C    |
| 1   | A     | 716  | G    |
| 1   | A     | 834  | G    |
| 1   | A     | 857  | A    |
| 1   | A     | 871  | G    |
| 1   | A     | 877  | G    |
| 1   | A     | 1080 | C    |
| 1   | A     | 1164 | U    |
| 1   | A     | 1237 | U    |
| 1   | A     | 1261 | A    |
| 1   | A     | 1352 | A    |
| 1   | A     | 1450 | C    |
| 1   | A     | 1563 | G    |
| 1   | A     | 1667 | A    |
| 1   | A     | 1692 | C    |
| 1   | A     | 1814 | G    |
| 1   | A     | 1856 | C    |
| 1   | A     | 1942 | A    |
| 1   | A     | 1979 | G    |
| 1   | A     | 2005 | G    |
| 1   | A     | 2011 | A    |
| 1   | A     | 2313 | C    |
| 1   | A     | 2467 | A    |
| 1   | A     | 2526 | C    |
| 1   | A     | 2536 | C    |
| 1   | A     | 2649 | A    |
| 1   | A     | 2718 | C    |
| 1   | A     | 2761 | A    |
| 1   | A     | 2791 | U    |
| 2   | B     | 3023 | U    |
| 2   | B     | 3024 | U    |
| 2   | B     | 3025 | G    |
| 2   | B     | 3043 | G    |
| 2   | B     | 3065 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 3103 | A    |

## 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 233 ligands modelled in this entry, 232 are 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 |
| 31  | ZIT  | A     | 8600 | -    | 54,54,54     | 1.80 | 10 (18%) | 82,83,83    | 1.29 | 8 (9%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 31  | ZIT  | A     | 8600 | -    | -       | 1/72/107/107 | 0/3/3/3 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 31  | A     | 8600 | ZIT  | C2-C3   | 4.65 | 1.65        | 1.54     |
| 31  | A     | 8600 | ZIT  | C7-C6   | 4.53 | 1.61        | 1.54     |
| 31  | A     | 8600 | ZIT  | C3A-N3A | 4.36 | 1.57        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 31  | A     | 8600 | ZIT  | C11-N10 | 3.48 | 1.54        | 1.49     |
| 31  | A     | 8600 | ZIT  | C2B-C3B | 3.36 | 1.60        | 1.52     |
| 31  | A     | 8600 | ZIT  | C4A-C5A | 3.04 | 1.57        | 1.52     |
| 31  | A     | 8600 | ZIT  | C13-C14 | 2.67 | 1.59        | 1.55     |
| 31  | A     | 8600 | ZIT  | O5A-C5A | 2.59 | 1.49        | 1.44     |
| 31  | A     | 8600 | ZIT  | C4-C5   | 2.54 | 1.61        | 1.54     |
| 31  | A     | 8600 | ZIT  | C4A-C3A | 2.19 | 1.58        | 1.53     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31  | A     | 8600 | ZIT  | C6-C5-C4    | -3.82 | 108.35      | 113.89   |
| 31  | A     | 8600 | ZIT  | O1A-C5-C6   | 3.16  | 110.17      | 106.40   |
| 31  | A     | 8600 | ZIT  | C17-C2-C3   | 2.56  | 118.73      | 113.00   |
| 31  | A     | 8600 | ZIT  | O1B-C3-C4   | 2.41  | 111.08      | 108.23   |
| 31  | A     | 8600 | ZIT  | C21-N10-C9  | 2.39  | 113.83      | 110.26   |
| 31  | A     | 8600 | ZIT  | O5A-C5A-C6A | -2.29 | 102.60      | 106.88   |
| 31  | A     | 8600 | ZIT  | C9-N10-C11  | -2.29 | 108.26      | 112.06   |
| 31  | A     | 8600 | ZIT  | C2A-C3A-N3A | 2.16  | 117.17      | 110.94   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 31  | A     | 8600 | ZIT  | C4A-C3A-N3A-C8A |

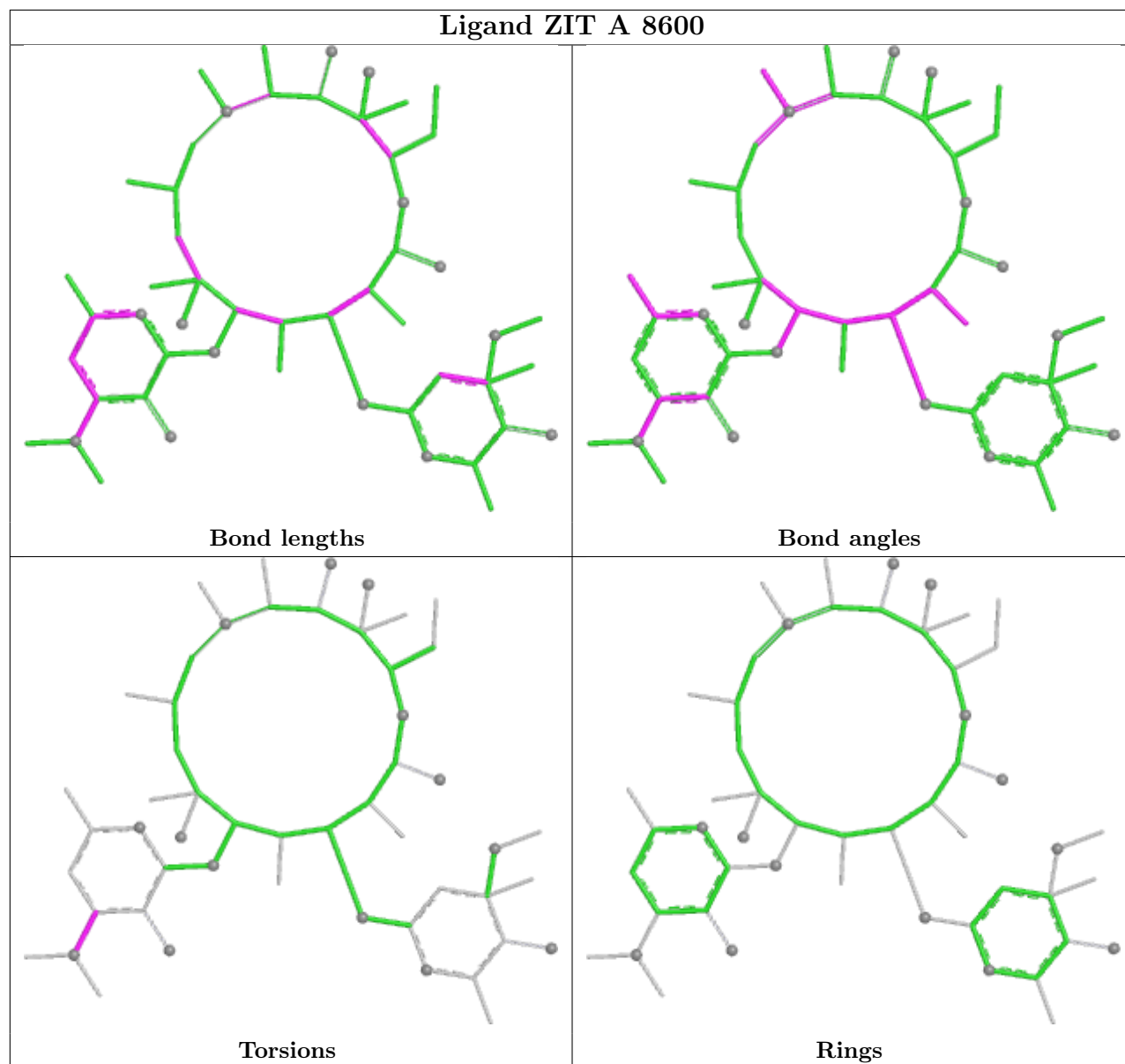
There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 31  | A     | 8600 | ZIT  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 2754/2922 (94%) | -0.40  | 30 (1%) 78 61 | 27, 56, 101, 149      | 0     |
| 2   | B     | 122/122 (100%)  | -0.00  | 4 (3%) 49 30  | 43, 71, 98, 158       | 0     |
| 3   | C     | 237/239 (99%)   | -0.21  | 2 (0%) 82 67  | 38, 62, 93, 114       | 0     |
| 4   | D     | 337/337 (100%)  | -0.17  | 2 (0%) 85 73  | 29, 64, 90, 99        | 0     |
| 5   | E     | 246/246 (100%)  | -0.28  | 0 100 100     | 30, 58, 81, 92        | 0     |
| 6   | F     | 140/176 (79%)   | 0.64   | 8 (5%) 29 19  | 61, 108, 124, 131     | 0     |
| 7   | G     | 172/177 (97%)   | 0.10   | 4 (2%) 61 41  | 50, 76, 97, 102       | 0     |
| 8   | H     | 119/119 (100%)  | 0.13   | 0 100 100     | 62, 82, 106, 110      | 0     |
| 9   | I     | 29/348 (8%)     | 1.37   | 5 (17%) 4 3   | 80, 100, 109, 109     | 0     |
| 10  | J     | 156/167 (93%)   | 0.09   | 6 (3%) 44 27  | 43, 65, 94, 101       | 0     |
| 11  | K     | 142/145 (97%)   | -0.20  | 0 100 100     | 45, 57, 80, 97        | 0     |
| 12  | L     | 132/132 (100%)  | -0.28  | 0 100 100     | 38, 58, 80, 87        | 0     |
| 13  | M     | 145/164 (88%)   | -0.00  | 2 (1%) 73 54  | 33, 77, 113, 123      | 0     |
| 14  | N     | 194/194 (100%)  | -0.22  | 2 (1%) 79 63  | 42, 56, 73, 84        | 0     |
| 15  | O     | 186/186 (100%)  | 0.32   | 8 (4%) 40 24  | 52, 74, 114, 124      | 0     |
| 16  | P     | 115/115 (100%)  | -0.10  | 0 100 100     | 52, 66, 84, 88        | 0     |
| 17  | Q     | 143/148 (96%)   | -0.19  | 0 100 100     | 45, 65, 80, 89        | 0     |
| 18  | R     | 95/95 (100%)    | -0.31  | 1 (1%) 78 61  | 38, 54, 70, 82        | 0     |
| 19  | S     | 150/154 (97%)   | -0.35  | 0 100 100     | 40, 54, 74, 82        | 0     |
| 20  | T     | 81/84 (96%)     | -0.13  | 0 100 100     | 55, 71, 90, 97        | 0     |
| 21  | U     | 119/119 (100%)  | -0.00  | 1 (0%) 82 67  | 52, 69, 92, 103       | 0     |
| 22  | V     | 53/66 (80%)     | -0.07  | 0 100 100     | 51, 64, 82, 89        | 0     |
| 23  | W     | 65/70 (92%)     | 0.16   | 2 (3%) 51 32  | 62, 83, 118, 124      | 0     |
| 24  | X     | 154/154 (100%)  | -0.39  | 0 100 100     | 38, 56, 76, 85        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 25  | Y     | 82/91 (90%)     | 0.01   | 2 (2%) 59 40  | 53, 67, 91, 107       | 0     |
| 26  | Z     | 142/240 (59%)   | -0.27  | 1 (0%) 84 69  | 33, 56, 77, 94        | 0     |
| 27  | 1     | 73/73 (100%)    | 0.16   | 1 (1%) 73 54  | 59, 71, 87, 94        | 0     |
| 28  | 2     | 56/56 (100%)    | -0.45  | 0 100 100     | 35, 46, 51, 52        | 0     |
| 29  | 3     | 46/48 (95%)     | 0.03   | 0 100 100     | 44, 72, 96, 106       | 0     |
| 30  | 4     | 92/92 (100%)    | -0.02  | 0 100 100     | 44, 66, 79, 90        | 0     |
| All | All   | 6577/7279 (90%) | -0.21  | 81 (1%) 76 58 | 27, 62, 101, 158      | 0     |

All (81) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1173 | A    | 5.8  |
| 1   | A     | 1175 | G    | 5.4  |
| 23  | W     | 1    | THR  | 4.7  |
| 1   | A     | 1176 | C    | 4.4  |
| 7   | G     | 10   | ASP  | 3.9  |
| 1   | A     | 1193 | A    | 3.8  |
| 4   | D     | 1    | PRO  | 3.7  |
| 2   | B     | 3001 | U    | 3.7  |
| 2   | B     | 3025 | G    | 3.6  |
| 1   | A     | 1190 | G    | 3.6  |
| 6   | F     | 10   | PHE  | 3.5  |
| 1   | A     | 1161 | A    | 3.5  |
| 1   | A     | 1177 | A    | 3.2  |
| 1   | A     | 1184 | C    | 3.2  |
| 1   | A     | 1160 | G    | 3.2  |
| 15  | O     | 147  | ILE  | 3.1  |
| 1   | A     | 1165 | G    | 3.1  |
| 9   | I     | 26   | MET  | 3.0  |
| 9   | I     | 27   | ILE  | 3.0  |
| 1   | A     | 10   | U    | 3.0  |
| 1   | A     | 1168 | C    | 3.0  |
| 7   | G     | 45   | ASP  | 2.9  |
| 13  | M     | 83   | GLU  | 2.9  |
| 1   | A     | 1174 | A    | 2.9  |
| 1   | A     | 1964 | U    | 2.8  |
| 15  | O     | 167  | ASP  | 2.8  |
| 1   | A     | 1186 | C    | 2.8  |
| 1   | A     | 2345 | A    | 2.8  |
| 15  | O     | 162  | ASP  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | O     | 168  | LEU  | 2.7  |
| 15  | O     | 186  | LEU  | 2.7  |
| 2   | B     | 3024 | U    | 2.7  |
| 2   | B     | 3023 | U    | 2.6  |
| 1   | A     | 1166 | A    | 2.6  |
| 1   | A     | 1171 | A    | 2.6  |
| 1   | A     | 1172 | G    | 2.5  |
| 15  | O     | 148  | ALA  | 2.5  |
| 9   | I     | 29   | SER  | 2.5  |
| 1   | A     | 1169 | U    | 2.5  |
| 6   | F     | 21   | VAL  | 2.5  |
| 7   | G     | 87   | PHE  | 2.4  |
| 6   | F     | 131  | THR  | 2.4  |
| 9   | I     | 71   | LEU  | 2.4  |
| 1   | A     | 1185 | U    | 2.4  |
| 4   | D     | 337  | GLY  | 2.3  |
| 6   | F     | 63   | ILE  | 2.3  |
| 3   | C     | 31   | LYS  | 2.3  |
| 10  | J     | 38   | ALA  | 2.3  |
| 1   | A     | 1167 | G    | 2.3  |
| 14  | N     | 87   | MET  | 2.3  |
| 6   | F     | 171  | ASP  | 2.3  |
| 25  | Y     | 88   | GLU  | 2.2  |
| 1   | A     | 138  | U    | 2.2  |
| 1   | A     | 1192 | A    | 2.2  |
| 1   | A     | 735  | C    | 2.2  |
| 1   | A     | 1206 | U    | 2.2  |
| 10  | J     | 40   | PRO  | 2.2  |
| 15  | O     | 1    | ALA  | 2.2  |
| 21  | U     | 1    | SER  | 2.2  |
| 15  | O     | 179  | LEU  | 2.2  |
| 14  | N     | 194  | ALA  | 2.2  |
| 6   | F     | 26   | GLY  | 2.2  |
| 27  | 1     | 22   | ILE  | 2.1  |
| 7   | G     | 81   | GLU  | 2.1  |
| 13  | M     | 82   | ALA  | 2.1  |
| 1   | A     | 1162 | G    | 2.1  |
| 1   | A     | 1188 | A    | 2.1  |
| 1   | A     | 1189 | A    | 2.1  |
| 10  | J     | 114  | PRO  | 2.1  |
| 10  | J     | 167  | ALA  | 2.1  |
| 18  | R     | 95   | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1199 | A    | 2.1  |
| 3   | C     | 36   | ASP  | 2.1  |
| 25  | Y     | 87   | ALA  | 2.1  |
| 10  | J     | 110  | GLY  | 2.1  |
| 6   | F     | 104  | PHE  | 2.1  |
| 23  | W     | 2    | VAL  | 2.0  |
| 9   | I     | 22   | ALA  | 2.0  |
| 10  | J     | 39   | GLY  | 2.0  |
| 6   | F     | 174  | VAL  | 2.0  |
| 26  | Z     | 235  | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | NA   | A     | 8329 | 1/1   | 0.22 | 0.19 | 70,70,70,70                 | 0     |
| 34  | NA   | A     | 8340 | 1/1   | 0.56 | 0.16 | 56,56,56,56                 | 0     |
| 34  | NA   | A     | 8385 | 1/1   | 0.62 | 0.34 | 73,73,73,73                 | 0     |
| 34  | NA   | A     | 8363 | 1/1   | 0.67 | 0.47 | 79,79,79,79                 | 0     |
| 32  | MG   | A     | 8050 | 1/1   | 0.67 | 0.09 | 67,67,67,67                 | 0     |
| 35  | CL   | A     | 8515 | 1/1   | 0.68 | 0.36 | 110,110,110,110             | 0     |
| 34  | NA   | A     | 8384 | 1/1   | 0.71 | 0.15 | 90,90,90,90                 | 0     |
| 32  | MG   | A     | 8087 | 1/1   | 0.72 | 0.09 | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 8092 | 1/1   | 0.74 | 0.17 | 95,95,95,95                 | 0     |
| 34  | NA   | T     | 8312 | 1/1   | 0.75 | 0.06 | 51,51,51,51                 | 0     |
| 34  | NA   | A     | 8366 | 1/1   | 0.75 | 0.19 | 79,79,79,79                 | 0     |
| 34  | NA   | A     | 8310 | 1/1   | 0.76 | 0.14 | 29,29,29,29                 | 0     |
| 34  | NA   | B     | 8351 | 1/1   | 0.77 | 0.17 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | NA   | A     | 8326 | 1/1   | 0.78 | 0.34 | 92,92,92,92                 | 0     |
| 34  | NA   | E     | 8304 | 1/1   | 0.80 | 0.07 | 32,32,32,32                 | 0     |
| 34  | NA   | A     | 8341 | 1/1   | 0.80 | 0.10 | 63,63,63,63                 | 0     |
| 31  | ZIT  | A     | 8600 | 52/52 | 0.80 | 0.17 | 81,91,95,96                 | 0     |
| 34  | NA   | A     | 8357 | 1/1   | 0.81 | 0.23 | 64,64,64,64                 | 0     |
| 34  | NA   | A     | 8328 | 1/1   | 0.81 | 0.11 | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 8067 | 1/1   | 0.81 | 0.13 | 51,51,51,51                 | 0     |
| 35  | CL   | A     | 8522 | 1/1   | 0.81 | 0.47 | 83,83,83,83                 | 0     |
| 34  | NA   | A     | 8330 | 1/1   | 0.82 | 0.13 | 57,57,57,57                 | 0     |
| 34  | NA   | A     | 8305 | 1/1   | 0.83 | 0.14 | 46,46,46,46                 | 0     |
| 34  | NA   | A     | 8371 | 1/1   | 0.83 | 0.16 | 48,48,48,48                 | 0     |
| 34  | NA   | A     | 8336 | 1/1   | 0.83 | 0.07 | 85,85,85,85                 | 0     |
| 35  | CL   | O     | 8507 | 1/1   | 0.83 | 0.12 | 84,84,84,84                 | 0     |
| 34  | NA   | A     | 8360 | 1/1   | 0.84 | 0.22 | 59,59,59,59                 | 0     |
| 34  | NA   | A     | 8355 | 1/1   | 0.84 | 0.20 | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 8082 | 1/1   | 0.85 | 0.10 | 83,83,83,83                 | 0     |
| 32  | MG   | A     | 8101 | 1/1   | 0.85 | 0.17 | 60,60,60,60                 | 0     |
| 34  | NA   | A     | 8374 | 1/1   | 0.85 | 0.49 | 89,89,89,89                 | 0     |
| 35  | CL   | A     | 8513 | 1/1   | 0.85 | 0.12 | 67,67,67,67                 | 0     |
| 34  | NA   | A     | 8381 | 1/1   | 0.85 | 0.09 | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 8112 | 1/1   | 0.85 | 0.18 | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 8066 | 1/1   | 0.85 | 0.14 | 48,48,48,48                 | 0     |
| 34  | NA   | A     | 8327 | 1/1   | 0.86 | 0.17 | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 8106 | 1/1   | 0.86 | 0.07 | 71,71,71,71                 | 0     |
| 34  | NA   | S     | 8386 | 1/1   | 0.86 | 0.39 | 97,97,97,97                 | 0     |
| 34  | NA   | A     | 8356 | 1/1   | 0.86 | 0.29 | 78,78,78,78                 | 0     |
| 34  | NA   | A     | 8314 | 1/1   | 0.87 | 0.12 | 48,48,48,48                 | 0     |
| 34  | NA   | A     | 8372 | 1/1   | 0.87 | 0.38 | 87,87,87,87                 | 0     |
| 34  | NA   | A     | 8307 | 1/1   | 0.87 | 0.10 | 48,48,48,48                 | 0     |
| 32  | MG   | 1     | 8105 | 1/1   | 0.87 | 0.10 | 38,38,38,38                 | 0     |
| 34  | NA   | A     | 8344 | 1/1   | 0.87 | 0.05 | 39,39,39,39                 | 0     |
| 34  | NA   | A     | 8333 | 1/1   | 0.87 | 0.29 | 51,51,51,51                 | 0     |
| 34  | NA   | A     | 8367 | 1/1   | 0.87 | 0.09 | 38,38,38,38                 | 0     |
| 35  | CL   | R     | 8511 | 1/1   | 0.87 | 0.19 | 102,102,102,102             | 0     |
| 34  | NA   | A     | 8325 | 1/1   | 0.88 | 0.12 | 62,62,62,62                 | 0     |
| 35  | CL   | A     | 8517 | 1/1   | 0.88 | 0.08 | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 8116 | 1/1   | 0.88 | 0.07 | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 8094 | 1/1   | 0.88 | 0.15 | 66,66,66,66                 | 0     |
| 34  | NA   | A     | 8378 | 1/1   | 0.88 | 0.23 | 48,48,48,48                 | 0     |
| 32  | MG   | A     | 8102 | 1/1   | 0.89 | 0.13 | 75,75,75,75                 | 0     |
| 34  | NA   | A     | 8332 | 1/1   | 0.89 | 0.06 | 50,50,50,50                 | 0     |
| 34  | NA   | A     | 8379 | 1/1   | 0.89 | 0.15 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | NA   | S     | 8337 | 1/1   | 0.89 | 0.08 | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 8024 | 1/1   | 0.89 | 0.12 | 79,79,79,79                 | 0     |
| 34  | NA   | A     | 8364 | 1/1   | 0.89 | 0.13 | 52,52,52,52                 | 0     |
| 34  | NA   | A     | 8308 | 1/1   | 0.90 | 0.12 | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 8042 | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 34  | NA   | A     | 8382 | 1/1   | 0.90 | 0.19 | 74,74,74,74                 | 0     |
| 35  | CL   | A     | 8505 | 1/1   | 0.90 | 0.15 | 92,92,92,92                 | 0     |
| 34  | NA   | A     | 8342 | 1/1   | 0.90 | 0.13 | 51,51,51,51                 | 0     |
| 34  | NA   | A     | 8362 | 1/1   | 0.90 | 0.25 | 62,62,62,62                 | 0     |
| 34  | NA   | A     | 8334 | 1/1   | 0.90 | 0.06 | 45,45,45,45                 | 0     |
| 34  | NA   | B     | 8383 | 1/1   | 0.90 | 0.29 | 40,40,40,40                 | 0     |
| 35  | CL   | D     | 8519 | 1/1   | 0.90 | 0.12 | 65,65,65,65                 | 0     |
| 35  | CL   | K     | 8516 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 34  | NA   | A     | 8303 | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 34  | NA   | R     | 8348 | 1/1   | 0.90 | 0.05 | 39,39,39,39                 | 0     |
| 35  | CL   | 4     | 8504 | 1/1   | 0.90 | 0.08 | 93,93,93,93                 | 0     |
| 34  | NA   | A     | 8349 | 1/1   | 0.91 | 0.12 | 57,57,57,57                 | 0     |
| 35  | CL   | K     | 8502 | 1/1   | 0.91 | 0.11 | 87,87,87,87                 | 0     |
| 35  | CL   | A     | 8514 | 1/1   | 0.91 | 0.07 | 57,57,57,57                 | 0     |
| 35  | CL   | N     | 8518 | 1/1   | 0.91 | 0.08 | 65,65,65,65                 | 0     |
| 34  | NA   | A     | 8321 | 1/1   | 0.91 | 0.12 | 42,42,42,42                 | 0     |
| 34  | NA   | A     | 8370 | 1/1   | 0.91 | 0.11 | 42,42,42,42                 | 0     |
| 35  | CL   | S     | 8506 | 1/1   | 0.91 | 0.12 | 69,69,69,69                 | 0     |
| 34  | NA   | A     | 8365 | 1/1   | 0.91 | 0.26 | 76,76,76,76                 | 0     |
| 32  | MG   | A     | 8041 | 1/1   | 0.92 | 0.07 | 69,69,69,69                 | 0     |
| 34  | NA   | A     | 8369 | 1/1   | 0.92 | 0.17 | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 8111 | 1/1   | 0.92 | 0.05 | 62,62,62,62                 | 0     |
| 35  | CL   | A     | 8520 | 1/1   | 0.92 | 0.11 | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 8053 | 1/1   | 0.92 | 0.07 | 40,40,40,40                 | 0     |
| 34  | NA   | A     | 8361 | 1/1   | 0.92 | 0.09 | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 8049 | 1/1   | 0.92 | 0.07 | 74,74,74,74                 | 0     |
| 34  | NA   | A     | 8375 | 1/1   | 0.92 | 0.25 | 86,86,86,86                 | 0     |
| 35  | CL   | L     | 8512 | 1/1   | 0.92 | 0.11 | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 8090 | 1/1   | 0.92 | 0.09 | 47,47,47,47                 | 0     |
| 32  | MG   | A     | 8103 | 1/1   | 0.92 | 0.12 | 76,76,76,76                 | 0     |
| 34  | NA   | U     | 8343 | 1/1   | 0.92 | 0.15 | 38,38,38,38                 | 0     |
| 34  | NA   | A     | 8323 | 1/1   | 0.92 | 0.15 | 57,57,57,57                 | 0     |
| 34  | NA   | A     | 8324 | 1/1   | 0.92 | 0.36 | 48,48,48,48                 | 0     |
| 34  | NA   | A     | 8302 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 34  | NA   | A     | 8316 | 1/1   | 0.93 | 0.15 | 61,61,61,61                 | 0     |
| 34  | NA   | A     | 8368 | 1/1   | 0.93 | 0.19 | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 8114 | 1/1   | 0.93 | 0.10 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 8070 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 32  | MG   | B     | 8095 | 1/1   | 0.93 | 0.16 | 98,98,98,98                 | 0     |
| 32  | MG   | U     | 8073 | 1/1   | 0.93 | 0.05 | 62,62,62,62                 | 0     |
| 35  | CL   | P     | 8508 | 1/1   | 0.93 | 0.09 | 97,97,97,97                 | 0     |
| 34  | NA   | A     | 8373 | 1/1   | 0.93 | 0.11 | 67,67,67,67                 | 0     |
| 34  | NA   | A     | 8352 | 1/1   | 0.93 | 0.18 | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 8108 | 1/1   | 0.93 | 0.17 | 85,85,85,85                 | 0     |
| 32  | MG   | A     | 8057 | 1/1   | 0.94 | 0.07 | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 8047 | 1/1   | 0.94 | 0.09 | 81,81,81,81                 | 0     |
| 35  | CL   | K     | 8501 | 1/1   | 0.94 | 0.10 | 81,81,81,81                 | 0     |
| 32  | MG   | A     | 8088 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 34  | NA   | A     | 8313 | 1/1   | 0.94 | 0.06 | 66,66,66,66                 | 0     |
| 34  | NA   | A     | 8377 | 1/1   | 0.94 | 0.25 | 68,68,68,68                 | 0     |
| 36  | CD   | P     | 8405 | 1/1   | 0.94 | 0.07 | 152,152,152,152             | 0     |
| 35  | CL   | C     | 8509 | 1/1   | 0.95 | 0.14 | 69,69,69,69                 | 0     |
| 32  | MG   | A     | 8104 | 1/1   | 0.95 | 0.05 | 50,50,50,50                 | 0     |
| 34  | NA   | A     | 8335 | 1/1   | 0.95 | 0.18 | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 8045 | 1/1   | 0.95 | 0.06 | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 8096 | 1/1   | 0.95 | 0.06 | 64,64,64,64                 | 0     |
| 35  | CL   | K     | 8521 | 1/1   | 0.95 | 0.06 | 64,64,64,64                 | 0     |
| 34  | NA   | A     | 8301 | 1/1   | 0.95 | 0.09 | 42,42,42,42                 | 0     |
| 35  | CL   | A     | 8510 | 1/1   | 0.95 | 0.12 | 97,97,97,97                 | 0     |
| 32  | MG   | A     | 8099 | 1/1   | 0.95 | 0.07 | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 8075 | 1/1   | 0.95 | 0.06 | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 8052 | 1/1   | 0.95 | 0.08 | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 8085 | 1/1   | 0.95 | 0.09 | 68,68,68,68                 | 0     |
| 34  | NA   | J     | 8309 | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 34  | NA   | A     | 8353 | 1/1   | 0.95 | 0.11 | 46,46,46,46                 | 0     |
| 34  | NA   | A     | 8319 | 1/1   | 0.96 | 0.13 | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 8076 | 1/1   | 0.96 | 0.08 | 75,75,75,75                 | 0     |
| 34  | NA   | J     | 8322 | 1/1   | 0.96 | 0.20 | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 8063 | 1/1   | 0.96 | 0.12 | 92,92,92,92                 | 0     |
| 32  | MG   | A     | 8098 | 1/1   | 0.96 | 0.15 | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 8064 | 1/1   | 0.96 | 0.17 | 36,36,36,36                 | 0     |
| 34  | NA   | A     | 8306 | 1/1   | 0.96 | 0.14 | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 8100 | 1/1   | 0.96 | 0.16 | 88,88,88,88                 | 0     |
| 32  | MG   | A     | 8051 | 1/1   | 0.96 | 0.04 | 66,66,66,66                 | 0     |
| 34  | NA   | A     | 8350 | 1/1   | 0.96 | 0.20 | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 8117 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 8040 | 1/1   | 0.96 | 0.07 | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 8044 | 1/1   | 0.96 | 0.10 | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 8016 | 1/1   | 0.96 | 0.04 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | NA   | C     | 8345 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 8046 | 1/1   | 0.97 | 0.05 | 72,72,72,72                 | 0     |
| 34  | NA   | A     | 8358 | 1/1   | 0.97 | 0.29 | 107,107,107,107             | 0     |
| 32  | MG   | A     | 8093 | 1/1   | 0.97 | 0.06 | 59,59,59,59                 | 0     |
| 32  | MG   | A     | 8071 | 1/1   | 0.97 | 0.06 | 85,85,85,85                 | 0     |
| 32  | MG   | A     | 8113 | 1/1   | 0.97 | 0.07 | 53,53,53,53                 | 0     |
| 32  | MG   | A     | 8021 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 8097 | 1/1   | 0.97 | 0.11 | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 8060 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 8081 | 1/1   | 0.97 | 0.04 | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 8012 | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 32  | MG   | A     | 8043 | 1/1   | 0.97 | 0.05 | 56,56,56,56                 | 0     |
| 32  | MG   | 4     | 8078 | 1/1   | 0.97 | 0.07 | 54,54,54,54                 | 0     |
| 33  | K    | A     | 8202 | 1/1   | 0.97 | 0.13 | 61,61,61,61                 | 0     |
| 34  | NA   | K     | 8346 | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 8027 | 1/1   | 0.97 | 0.05 | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 8007 | 1/1   | 0.97 | 0.04 | 42,42,42,42                 | 0     |
| 34  | NA   | A     | 8354 | 1/1   | 0.97 | 0.08 | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 8089 | 1/1   | 0.97 | 0.06 | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 8068 | 1/1   | 0.97 | 0.04 | 56,56,56,56                 | 0     |
| 35  | CL   | A     | 8503 | 1/1   | 0.97 | 0.06 | 74,74,74,74                 | 0     |
| 34  | NA   | A     | 8376 | 1/1   | 0.97 | 0.20 | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 8084 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 34  | NA   | A     | 8359 | 1/1   | 0.98 | 0.14 | 75,75,75,75                 | 0     |
| 34  | NA   | A     | 8331 | 1/1   | 0.98 | 0.11 | 55,55,55,55                 | 0     |
| 32  | MG   | D     | 8055 | 1/1   | 0.98 | 0.05 | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 8062 | 1/1   | 0.98 | 0.03 | 61,61,61,61                 | 0     |
| 32  | MG   | Z     | 8109 | 1/1   | 0.98 | 0.03 | 61,61,61,61                 | 0     |
| 34  | NA   | A     | 8315 | 1/1   | 0.98 | 0.15 | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 8048 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 34  | NA   | A     | 8317 | 1/1   | 0.98 | 0.03 | 43,43,43,43                 | 0     |
| 34  | NA   | A     | 8318 | 1/1   | 0.98 | 0.13 | 45,45,45,45                 | 0     |
| 32  | MG   | A     | 8110 | 1/1   | 0.98 | 0.10 | 35,35,35,35                 | 0     |
| 34  | NA   | A     | 8320 | 1/1   | 0.98 | 0.03 | 32,32,32,32                 | 0     |
| 33  | K    | A     | 8201 | 1/1   | 0.98 | 0.10 | 70,70,70,70                 | 0     |
| 34  | NA   | N     | 8347 | 1/1   | 0.98 | 0.07 | 23,23,23,23                 | 0     |
| 32  | MG   | A     | 8072 | 1/1   | 0.98 | 0.04 | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 8039 | 1/1   | 0.98 | 0.03 | 67,67,67,67                 | 0     |
| 32  | MG   | A     | 8001 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 32  | MG   | A     | 8091 | 1/1   | 0.98 | 0.03 | 58,58,58,58                 | 0     |
| 32  | MG   | A     | 8115 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 8059 | 1/1   | 0.98 | 0.04 | 56,56,56,56                 | 0     |

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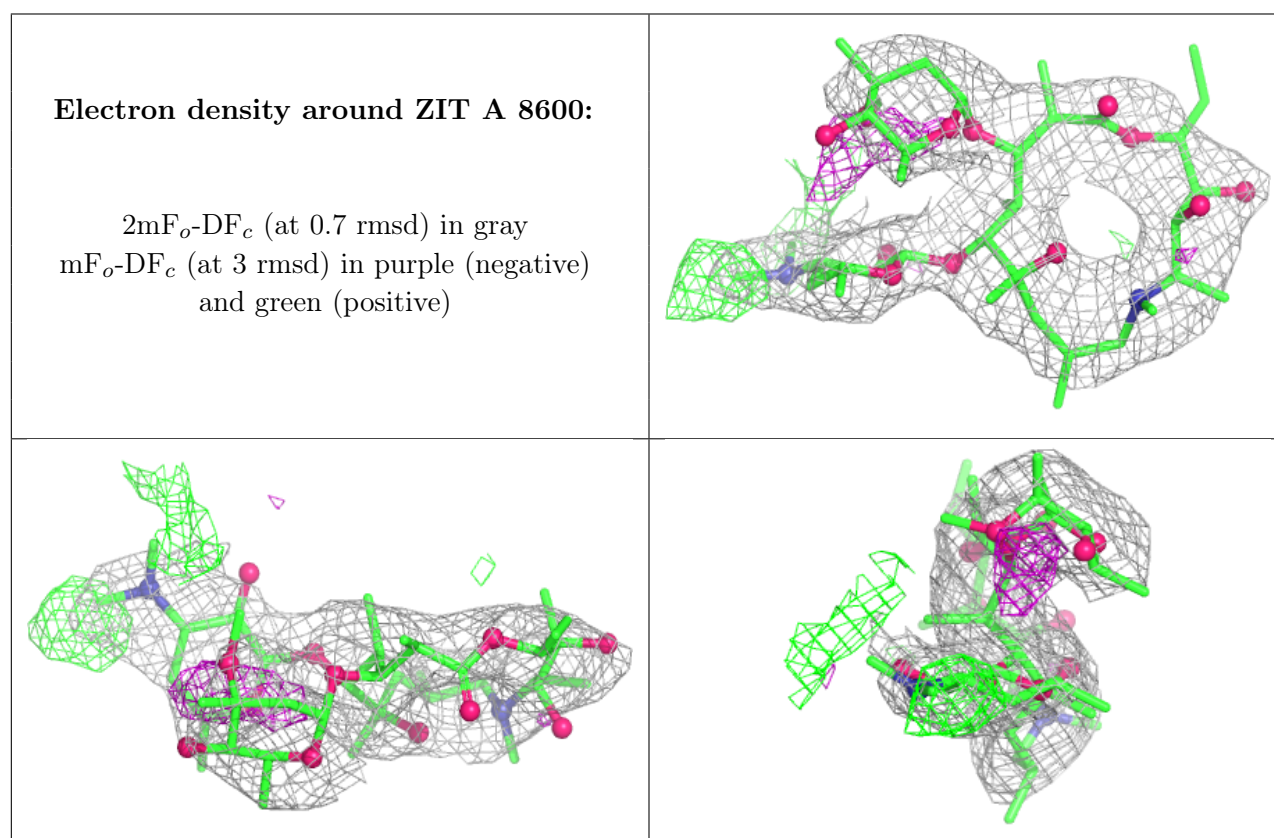
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 8006 | 1/1   | 0.98 | 0.04 | 54,54,54,54                 | 0     |
| 36  | CD   | 1     | 8403 | 1/1   | 0.98 | 0.03 | 77,77,77,77                 | 0     |
| 36  | CD   | 4     | 8404 | 1/1   | 0.98 | 0.03 | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 8011 | 1/1   | 0.99 | 0.03 | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 8002 | 1/1   | 0.99 | 0.02 | 43,43,43,43                 | 0     |
| 34  | NA   | M     | 8380 | 1/1   | 0.99 | 0.05 | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 8013 | 1/1   | 0.99 | 0.04 | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 8014 | 1/1   | 0.99 | 0.06 | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 8003 | 1/1   | 0.99 | 0.04 | 26,26,26,26                 | 0     |
| 34  | NA   | S     | 8338 | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 8017 | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 8019 | 1/1   | 0.99 | 0.09 | 24,24,24,24                 | 0     |
| 32  | MG   | A     | 8077 | 1/1   | 0.99 | 0.03 | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 8079 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 32  | MG   | A     | 8080 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 32  | MG   | A     | 8020 | 1/1   | 0.99 | 0.06 | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 8008 | 1/1   | 0.99 | 0.06 | 61,61,61,61                 | 0     |
| 32  | MG   | A     | 8083 | 1/1   | 0.99 | 0.07 | 51,51,51,51                 | 0     |
| 32  | MG   | A     | 8022 | 1/1   | 0.99 | 0.04 | 55,55,55,55                 | 0     |
| 32  | MG   | A     | 8023 | 1/1   | 0.99 | 0.06 | 33,33,33,33                 | 0     |
| 32  | MG   | L     | 8069 | 1/1   | 0.99 | 0.04 | 79,79,79,79                 | 0     |
| 32  | MG   | A     | 8086 | 1/1   | 0.99 | 0.07 | 56,56,56,56                 | 0     |
| 32  | MG   | A     | 8009 | 1/1   | 0.99 | 0.05 | 46,46,46,46                 | 0     |
| 32  | MG   | A     | 8025 | 1/1   | 0.99 | 0.04 | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 8026 | 1/1   | 0.99 | 0.03 | 49,49,49,49                 | 0     |
| 32  | MG   | A     | 8010 | 1/1   | 0.99 | 0.03 | 43,43,43,43                 | 0     |
| 32  | MG   | A     | 8056 | 1/1   | 0.99 | 0.04 | 61,61,61,61                 | 0     |
| 34  | NA   | A     | 8339 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 32  | MG   | A     | 8028 | 1/1   | 0.99 | 0.07 | 57,57,57,57                 | 0     |
| 32  | MG   | A     | 8058 | 1/1   | 0.99 | 0.04 | 62,62,62,62                 | 0     |
| 32  | MG   | A     | 8029 | 1/1   | 0.99 | 0.04 | 50,50,50,50                 | 0     |
| 32  | MG   | A     | 8032 | 1/1   | 0.99 | 0.02 | 63,63,63,63                 | 0     |
| 32  | MG   | A     | 8061 | 1/1   | 0.99 | 0.08 | 37,37,37,37                 | 0     |
| 32  | MG   | A     | 8033 | 1/1   | 0.99 | 0.04 | 36,36,36,36                 | 0     |
| 32  | MG   | A     | 8035 | 1/1   | 0.99 | 0.04 | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 8037 | 1/1   | 0.99 | 0.03 | 61,61,61,61                 | 0     |
| 34  | NA   | A     | 8311 | 1/1   | 0.99 | 0.05 | 63,63,63,63                 | 0     |
| 36  | CD   | 2     | 8402 | 1/1   | 0.99 | 0.03 | 70,70,70,70                 | 0     |
| 32  | MG   | A     | 8038 | 1/1   | 0.99 | 0.05 | 29,29,29,29                 | 0     |
| 32  | MG   | A     | 8107 | 1/1   | 1.00 | 0.01 | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 8074 | 1/1   | 1.00 | 0.02 | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 8036 | 1/1   | 1.00 | 0.03 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | A     | 8004 | 1/1   | 1.00 | 0.03 | 60,60,60,60                 | 0     |
| 32  | MG   | A     | 8054 | 1/1   | 1.00 | 0.04 | 52,52,52,52                 | 0     |
| 32  | MG   | A     | 8030 | 1/1   | 1.00 | 0.03 | 40,40,40,40                 | 0     |
| 32  | MG   | A     | 8031 | 1/1   | 1.00 | 0.04 | 44,44,44,44                 | 0     |
| 32  | MG   | A     | 8018 | 1/1   | 1.00 | 0.02 | 54,54,54,54                 | 0     |
| 32  | MG   | A     | 8015 | 1/1   | 1.00 | 0.03 | 57,57,57,57                 | 0     |
| 36  | CD   | V     | 8401 | 1/1   | 1.00 | 0.01 | 75,75,75,75                 | 0     |
| 32  | MG   | A     | 8034 | 1/1   | 1.00 | 0.08 | 32,32,32,32                 | 0     |
| 32  | MG   | A     | 8005 | 1/1   | 1.00 | 0.02 | 60,60,60,60                 | 0     |
| 32  | MG   | C     | 8065 | 1/1   | 1.00 | 0.06 | 40,40,40,40                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.