



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:36 AM UTC

PDB ID : 1S72 / pdb\_00001s72  
Title : REFINED CRYSTAL STRUCTURE OF THE HALOARCUA MARISMORTUI LARGE RIBOSOMAL SUBUNIT AT 2.4 ANGSTROM RESOLUTION  
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2004-01-28  
Resolution : 2.40 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                                                              |
| 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                                                             |

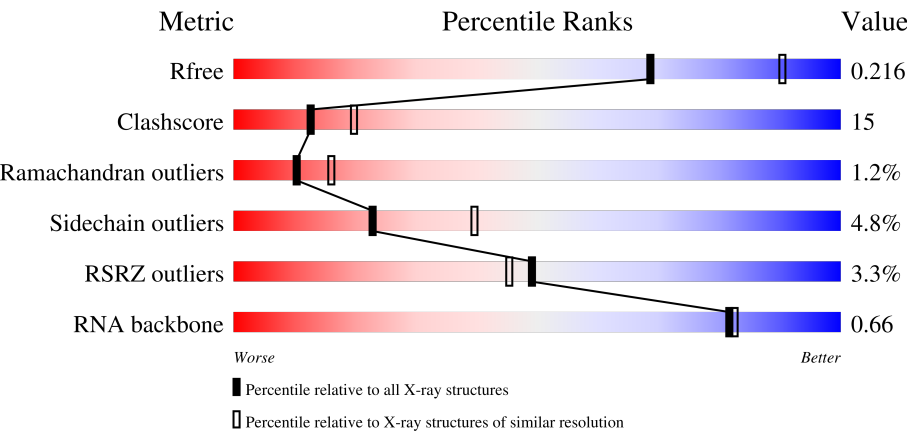
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 4912 (2.40-2.40)                                      |
| Clashscore            | 190562                      | 5391 (2.40-2.40)                                      |
| Ramachandran outliers | 187476                      | 5320 (2.40-2.40)                                      |
| Sidechain outliers    | 187428                      | 5321 (2.40-2.40)                                      |
| RSRZ outliers         | 180081                      | 4916 (2.40-2.40)                                      |
| RNA backbone          | 3983                        | 1155 (2.70-2.10)                                      |

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   | 0     | 2922   | <div><div>2%</div><div><div></div><div>65%</div><div>24%</div><div>5%</div><div>6%</div></div></div> |
| 2   | 9     | 122    | <div><div>3%</div><div><div></div><div>55%</div><div>36%</div><div>7%</div><div></div></div></div>   |
| 3   | A     | 240    | <div><div>2%</div><div><div></div><div>60%</div><div>32%</div><div>6%</div><div></div></div></div>   |
| 4   | B     | 338    | <div><div></div><div><div></div><div>54%</div><div>38%</div><div>7%</div><div></div></div></div>     |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | C     | 246    |                  |
| 6   | D     | 177    |                  |
| 7   | E     | 178    |                  |
| 8   | F     | 120    |                  |
| 9   | G     | 348    |                  |
| 10  | H     | 171    |                  |
| 11  | I     | 162    |                  |
| 12  | J     | 145    |                  |
| 13  | K     | 132    |                  |
| 14  | L     | 165    |                  |
| 15  | M     | 194    |                  |
| 16  | N     | 187    |                  |
| 17  | O     | 116    |                  |
| 18  | P     | 149    |                  |
| 19  | Q     | 96     |                  |
| 20  | R     | 155    |                  |
| 21  | S     | 85     |                  |
| 22  | T     | 120    |                  |
| 23  | U     | 66     |                  |
| 24  | V     | 71     |                  |
| 25  | W     | 154    |                  |
| 26  | X     | 92     |                  |
| 27  | Y     | 241    |                  |
| 28  | Z     | 73     |                  |
| 29  | 1     | 57     |                  |

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| Mol | Chain | Length | Quality of chain                                                             |
|-----|-------|--------|------------------------------------------------------------------------------|
| 30  | 2     | 50     | <div><div></div><div>4%</div><div>54%</div><div>36%</div><div>8%</div></div> |
| 31  | 3     | 92     | <div><div></div><div>2%</div><div>62%</div><div>30%</div><div>7%</div></div> |

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99039 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 ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | 0     | 2754     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 59021 | 26350 | 10878 | 19048 | 2745 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| 0     | 560     | C        | U      | conflict         | GB 3377779 |
| 0     | 628     | 1MA      | A      | modified residue | GB 3377779 |
| 0     | 2587    | OMU      | U      | modified residue | GB 3377779 |
| 0     | 2588    | OMG      | G      | modified residue | GB 3377779 |
| 0     | 2619    | UR3      | U      | modified residue | GB 3377779 |
| 0     | 2621    | PSU      | U      | modified residue | GB 3377779 |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | 9     | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2600  | 1160 | 472 | 847 | 121 |         |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | A     | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1753  | 1072 | 352 | 324 | 5 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 85      | SER      | ASP    | conflict | UNP P20276 |
| A     | 160     | ALA      | GLY    | conflict | UNP P20276 |

- Molecule 4 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | B     | 337      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2625  | 1616 | 493 | 511 | 5 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 310     | ARG      | PRO    | conflict | UNP P20279 |

- Molecule 5 is a protein called 50S ribosomal protein L4E.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | C     | 246      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1859  | 1131 | 344 | 383 | 1 |         |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | F     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 890   | 551 | 141 | 197 | 1 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 103     | GLU      | ALA    | conflict | UNP P12743 |
| F     | 105     | ASP      | ALA    | conflict | UNP P12743 |
| F     | 106     | ALA      | THR    | conflict | UNP P12743 |
| F     | 107     | ASP      | VAL    | conflict | UNP P12743 |
| F     | 108     | VAL      | LEU    | conflict | UNP P12743 |
| F     | 110     | ASP      | GLU    | conflict | UNP P12743 |

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 10 is a protein called 50S ribosomal protein L10e.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | H     | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1266  | 785 | 237 | 238 | 6 |         |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L11P.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 11  | I     | 70       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 519   | 323 | 81 | 114 | 1 |         |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | J     | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1120  | 696 | 199 | 222 | 3 |         |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | K     | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 992   | 609 | 187 | 192 | 4 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| K     | 44      | LEU      | HIS    | conflict | UNP P22450 |

- Molecule 14 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | L     | 145      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1118  | 670 | 222 | 226 |         |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | M     | 194      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1560  | 943 | 332 | 284 | 1 |         |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | N     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 895 | 262 | 286 | 2 |         |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17  | O     | 115      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 865   | 529 | 161 | 175 |  |         |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L19E.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 18  | P     | 143      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1136  | 683 | 229 | 224 |  |         |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 19  | Q     | 95       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 735   | 450 | 141 | 144 |  |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | R     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1149  | 713 | 209 | 223 | 4 |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | S     | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 641   | 389 | 111 | 138 | 3 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L24P.



| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 22  | T     | 119      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 950   | 568 | 180 | 202 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L24E.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 23  | U     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 410   | 244 | 75 | 86 | 5 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 24  | V     | 65       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 499   | 304 | 94 | 100 | 1 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | W     | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1196  | 737 | 209 | 244 | 6 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | X     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 654   | 402 | 129 | 122 | 1 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L32E.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 27  | Y     | 142      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1130  | 686 | 228 | 216 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | Z     | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 579   | 346 | 116 | 112 | 5 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29  | 1     | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 431   | 258 | 86 | 83 | 4 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | 2     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 396   | 239 | 89 | 67 | 1 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | 3     | 92       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 458 | 153 | 137 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32  | 0     | 109      | Total | Mg  | 0       | 0       |
|     |       |          | 109   | 109 |         |         |
| 32  | 9     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | A     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | B     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | K     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | T     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | Y     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 32  | 3     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 33  | 0     | 2        | Total | K | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

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

| Mol | Chain | Residues | Atoms             | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 34  | 0     | 72       | Total Na<br>72 72 | 0       | 0       |
| 34  | 9     | 2        | Total Na<br>2 2   | 0       | 0       |
| 34  | A     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | C     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | H     | 2        | Total Na<br>2 2   | 0       | 0       |
| 34  | J     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | L     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | M     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | Q     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | R     | 2        | Total Na<br>2 2   | 0       | 0       |
| 34  | S     | 1        | Total Na<br>1 1   | 0       | 0       |
| 34  | T     | 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  | 0     | 10       | Total Cl<br>10 10 | 0       | 0       |
| 35  | A     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | B     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | J     | 3        | Total Cl<br>3 3   | 0       | 0       |
| 35  | L     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | M     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | N     | 1        | Total Cl<br>1 1   | 0       | 0       |
| 35  | O     | 1        | Total Cl<br>1 1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 35  | R     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 35  | Y     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 35  | 3     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 36  | O     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 36  | U     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 36  | Z     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 36  | 1     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 36  | 3     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 37 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 37  | 0     | 5893     | Total | O    | 0       | 0       |
|     |       |          | 5893  | 5893 |         |         |
| 37  | 9     | 136      | Total | O    | 0       | 0       |
|     |       |          | 136   | 136  |         |         |
| 37  | A     | 127      | Total | O    | 0       | 0       |
|     |       |          | 127   | 127  |         |         |
| 37  | B     | 153      | Total | O    | 0       | 0       |
|     |       |          | 153   | 153  |         |         |
| 37  | C     | 172      | Total | O    | 0       | 0       |
|     |       |          | 172   | 172  |         |         |
| 37  | D     | 49       | Total | O    | 0       | 0       |
|     |       |          | 49    | 49   |         |         |
| 37  | E     | 44       | Total | O    | 0       | 0       |
|     |       |          | 44    | 44   |         |         |
| 37  | F     | 25       | Total | O    | 0       | 0       |
|     |       |          | 25    | 25   |         |         |
| 37  | G     | 20       | Total | O    | 0       | 0       |
|     |       |          | 20    | 20   |         |         |

*Continued on next page...*

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 37  | H     | 71       | Total<br>71  | O<br>71  | 0       | 0       |
| 37  | I     | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 37  | J     | 55       | Total<br>55  | O<br>55  | 0       | 0       |
| 37  | K     | 61       | Total<br>61  | O<br>61  | 0       | 0       |
| 37  | L     | 85       | Total<br>85  | O<br>85  | 0       | 0       |
| 37  | M     | 121      | Total<br>121 | O<br>121 | 0       | 0       |
| 37  | N     | 64       | Total<br>64  | O<br>64  | 0       | 0       |
| 37  | O     | 44       | Total<br>44  | O<br>44  | 0       | 0       |
| 37  | P     | 65       | Total<br>65  | O<br>65  | 0       | 0       |
| 37  | Q     | 52       | Total<br>52  | O<br>52  | 0       | 0       |
| 37  | R     | 83       | Total<br>83  | O<br>83  | 0       | 0       |
| 37  | S     | 33       | Total<br>33  | O<br>33  | 0       | 0       |
| 37  | T     | 40       | Total<br>40  | O<br>40  | 0       | 0       |
| 37  | U     | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 37  | V     | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 37  | W     | 67       | Total<br>67  | O<br>67  | 0       | 0       |
| 37  | X     | 28       | Total<br>28  | O<br>28  | 0       | 0       |
| 37  | Y     | 96       | Total<br>96  | O<br>96  | 0       | 0       |
| 37  | Z     | 29       | Total<br>29  | O<br>29  | 0       | 0       |
| 37  | 1     | 51       | Total<br>51  | O<br>51  | 0       | 0       |
| 37  | 2     | 40       | Total<br>40  | O<br>40  | 0       | 0       |

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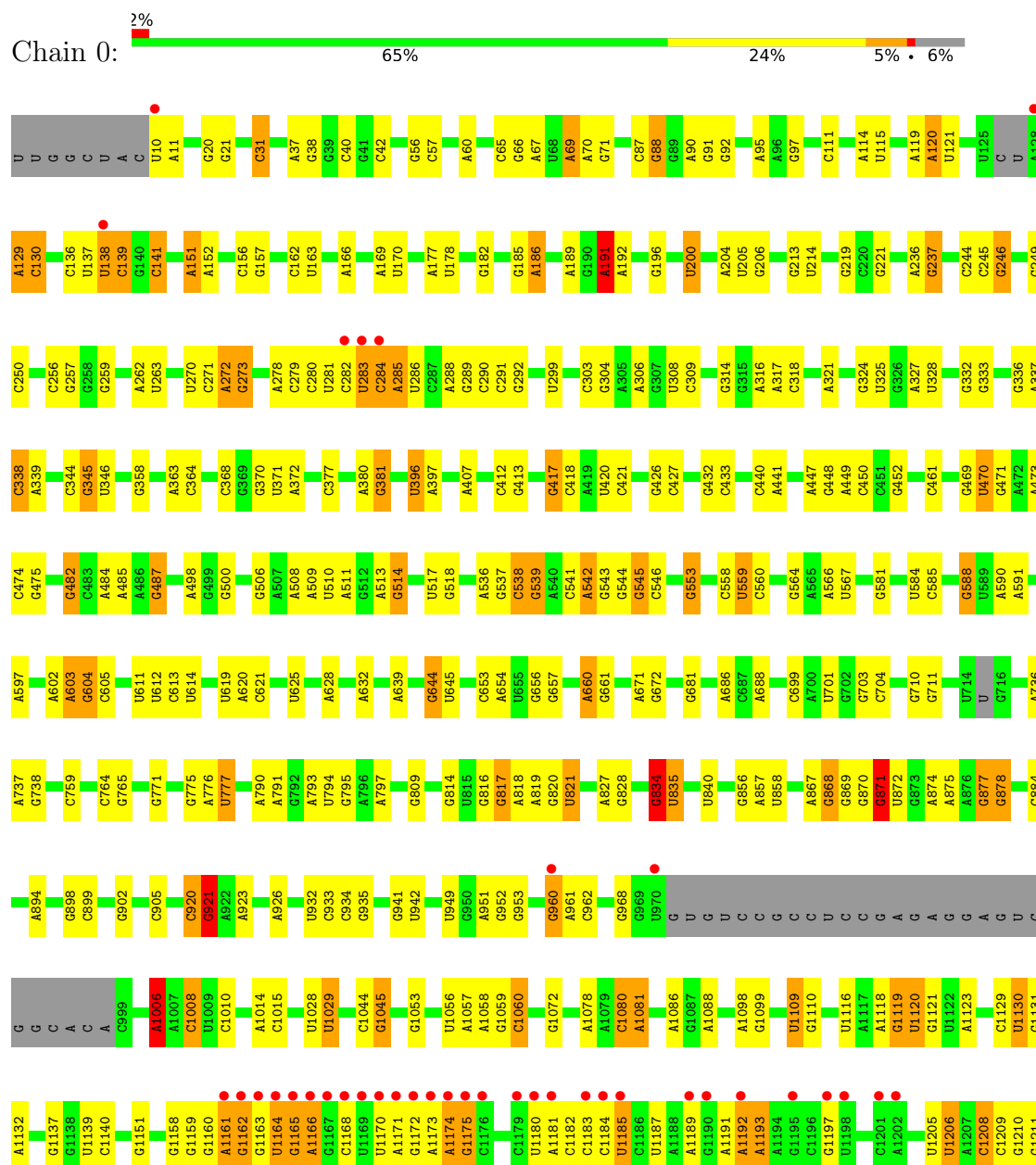
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 37  | 3     | 71       | Total | O  | 0       | 0       |
|     |       |          | 71    | 71 |         |         |

### 3 Residue-property plots

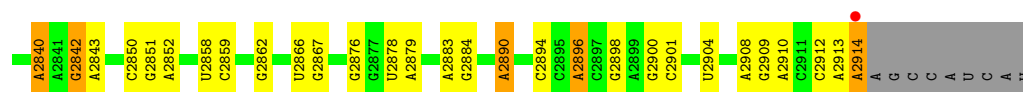
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ribosomal RNA



|       |       |       |       |       |   |   |   |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|---|---|---|-------|-------|-------|-------|-------|-------|-------|
| G2738 | G2634 | A2521 | A2414 | A2302 | A | G | U | G2033 | G1923 | U1766 | C1633 | G1497 | C1343 | C1212 |
| A2741 | A2635 | G2524 | A2415 | C2309 | G | U | G | U2034 | G1926 | A1767 | G1634 | G1497 | G1351 | G1216 |
| G2742 | G2636 | G2525 | G2416 | G2310 | G | U | G | A1927 | A1927 | C1769 | U1635 | U1500 | C1352 | G1217 |
| C2747 | A2637 | C2526 | U2419 | A2311 | A | C | C | G2044 | C1928 | A1778 | G1636 | U1503 | C1353 | U1218 |
| G2748 | G2638 | U2527 | G2420 | C2313 | A | C | C | G2050 | G1929 | A1779 | A1637 | A1504 | C1360 | U1219 |
| U2749 | G2642 | C2533 | C2421 | G2314 | U | C | C | A2054 | C1940 | C1787 | A1641 | U1505 | C1229 | C1229 |
| G2750 | G2643 | C2534 | G2422 | G2315 | A | A | A | A2061 | A1941 | U1788 | A1642 | U1506 | A1367 | A1232 |
| U2756 | A2649 | U2537 | G2426 | C2316 | C | U | U | C2062 | C1942 | G1789 | A1656 | A1515 | U1368 | A1233 |
| A2761 | U2652 | U2541 | A2434 | C2317 | A | G | G | A2063 | C1943 | G1794 | A1657 | C1516 | U1234 | U1235 |
| C2762 | A2653 | G2542 | G2438 | U2320 | C | U | U | U2064 | G1947 | C1798 | A1658 | G1523 | A1372 | A1236 |
| A2768 | A2654 | G2543 | C2443 | A2321 | C | A | A | G2072 | G1948 | C1798 | C1666 | U1524 | C1377 | A1237 |
| C2769 | A2664 | C2544 | G2443 | U2326 | G | G | G | G2073 | G1951 | G1809 | A1667 | G1525 | G1378 | C1238 |
| G2770 | A     | C2547 | G2453 | C2329 | U | C | A | A2074 | U     | G1819 | U1668 | A1526 | G1384 | G1239 |
| G2777 | U     | C2548 | A2456 | U2330 | G | A | A | U2078 | A     | G1820 | G1670 | A1528 | G1385 | A1242 |
| A2778 | G2667 | C2552 | U2457 | G2336 | U | C | C | A2081 | C     | A1845 | C1679 | G1545 | A1406 | G1243 |
| G2779 | U2669 | A2553 | G2462 | A     | U | C | A | G2082 | U     | U     | C1680 | C1546 | A1407 | C1244 |
| C2780 | G2670 | C2559 | G2465 | C     | A | C | C | U2083 | A     | C     | G1681 | U1527 | U1408 | C1245 |
| U2781 | U2671 | C2560 | A2466 | A     | U | A | A | A2089 | G     | U     | A1682 | A1529 | G1409 | A1246 |
| G2782 | C2672 | C2561 | A2467 | G2344 | C | C | C | G2090 | U     | A     | G1683 | G1555 | A1413 | A1247 |
| A2783 | U2673 | G2562 | A2468 | A2345 | C | A | A | G2091 | C     | C     | A1684 | A1559 | A1414 | U1249 |
| G2786 | C2676 | U2563 | A2469 | C2346 | G | C | C | A2095 | U     | U     | A1685 | U     | C1250 | C1251 |
| C2787 | G2679 | C2564 | A2472 | G2347 | G | A | A | A2096 | C     | C     | C1692 | C1562 | G1417 | U1266 |
| C2790 | A2680 | G2565 | C2476 | U2241 | C | C | C | G2094 | C1965 | A1845 | C1693 | G1563 | U1418 | U1267 |
| U2791 | A2681 | C2570 | C2477 | U2242 | A | U | U | A2096 | U     | G1848 | A1693 | C1564 | U1419 | C1267 |
| A2792 | C2682 | G2578 | G2478 | C2247 | U | C | A | U2097 | C1966 | C1853 | C1699 | C1565 | G1423 | G1268 |
| C2795 | U2690 | U2586 | A2479 | G2251 | C | C | C | G2102 | U1967 | C1856 | G1700 | C1566 | A1424 | G1269 |
| U2796 | A2691 | U2587 | G2480 | A2252 | G | C | C | G2109 | G1970 | A1857 | U1702 | A1580 | G1430 | C1273 |
| A2800 | A2694 | G2588 | A2483 | A2255 | C | C | C | G2110 | U1972 | C1862 | A1710 | G1582 | G1439 | U1279 |
| U2807 | U2710 | U2589 | A2488 | G2256 | G | G | A | A2112 | G1974 | G1863 | A1717 | C1593 | U1440 | U1279 |
| A2811 | G2711 | U2590 | G2489 | G2257 | C | C | C | G2113 | A1978 | U1867 | C1730 | C1594 | G1289 | C1289 |
| A2812 | G2712 | G2592 | A2490 | A2258 | U | U | U | C2114 | G1979 | G1868 | A1732 | G1595 | G1290 | G1290 |
| A2813 | G2716 | A2601 | C2493 | U2265 | A | G | G | U2115 | U1980 | U1874 | G1723 | A1597 | G1291 | G1291 |
| A2814 | C2717 | G2602 | C2502 | A2266 | C | C | C | U2116 | U1996 | C1877 | C1725 | A1598 | C1451 | U1298 |
| G2815 | A2718 | G2603 | G2503 | G2267 | G | G | G | G2128 | A1997 | U1877 | G1730 | A1603 | A1458 | G1299 |
| A2820 | C2720 | A2604 | A2504 | G2270 | C | C | A | G2136 | G2001 | U1878 | C1731 | G1604 | C1462 | U1306 |
| C2821 | U2721 | U2607 | G2505 | G2271 | C | C | G | A     | C2002 | U1879 | A1733 | G1605 | A1463 | U1306 |
| C2825 | G2723 | C2608 | A2606 | G2272 | A | A | U | C     | U2003 | U1883 | G1734 | G1610 | A1470 | U1314 |
| G2826 | U2724 | G2613 | C2507 | C2281 | C | C | C | G     | G2005 | G1884 | C1735 | C1613 | G1327 | G1327 |
| A2827 | G2725 | G2616 | C2508 | U2282 | G | A | A | U     | U2008 | G1902 | A1736 | G1614 | A1328 | A1328 |
| G2828 | U2726 | C2619 | A2509 | G2289 | A | G | G | C     | G2009 | U1903 | U1741 | A1615 | A1329 | A1329 |
| G2829 | A2727 | C2616 | C2510 | G2289 | G | G | A | U     | A2010 | A1904 | A1742 | C1477 | U1478 | U1333 |
| U2830 | C2728 | U2619 | A2511 | U2290 | U | U | C | C     | A2011 | A1909 | U1625 | U1625 | C1334 | C1334 |
| C2831 | G2729 | U2620 | C2403 | A2301 | C | C | A | C     | U2012 | A1909 | G1751 | A1626 | G1484 | U1340 |
| C2832 | G2730 | U2621 | G2412 | A2300 | A | A | A | C     | G2013 | A1919 | C1752 | G1627 | A1485 | G1340 |
| U2837 | G2731 | G2630 | A2413 | A2301 | C | C | C | A     | A2019 | A1919 | C1753 | A1630 | A1488 | C1342 |





• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2P

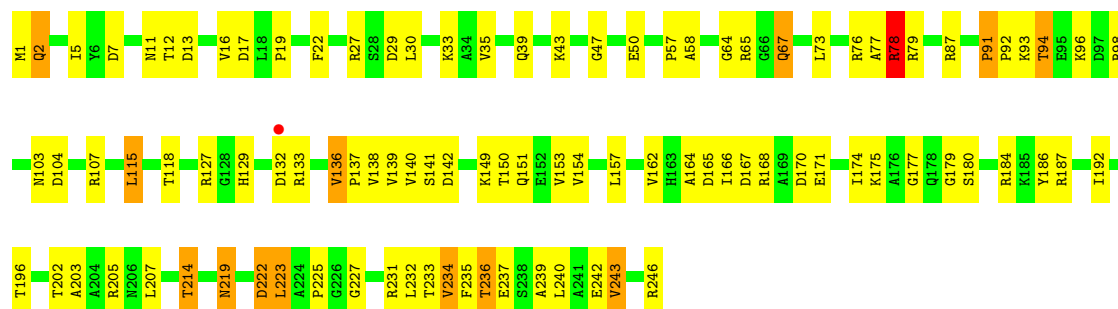


• Molecule 4: 50S ribosomal protein L3P

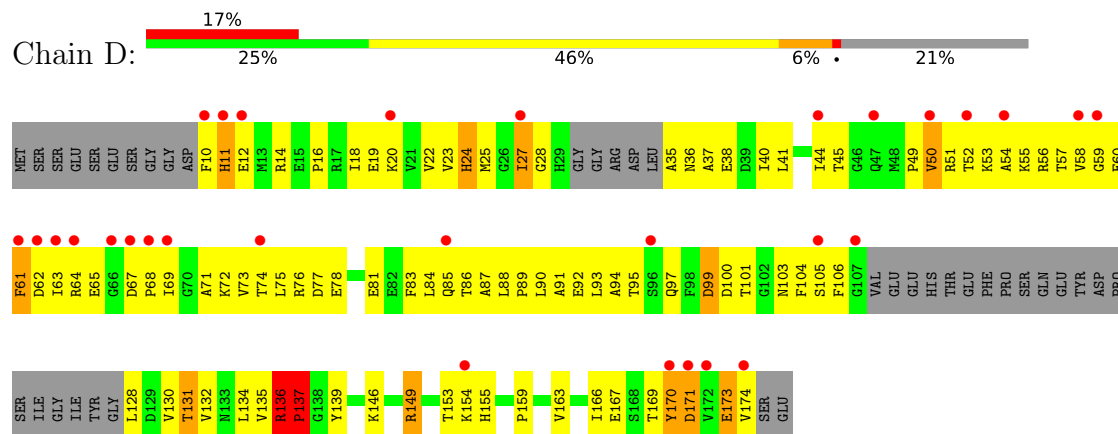


• Molecule 5: 50S ribosomal protein L4E

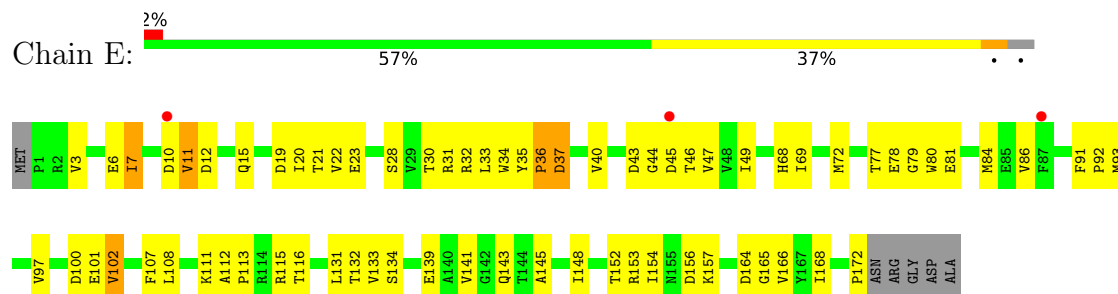




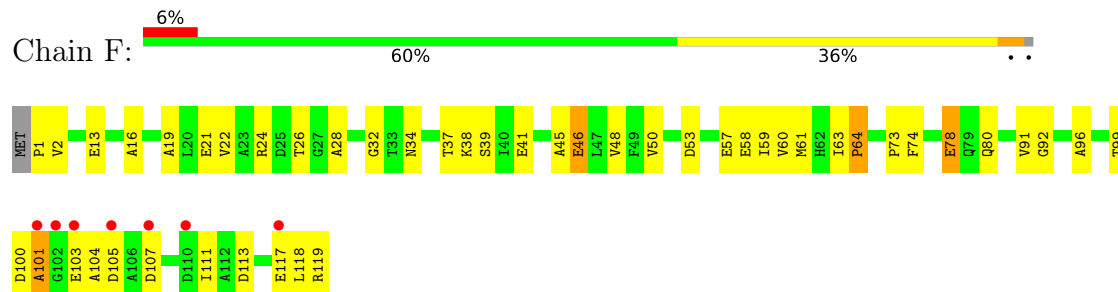
• Molecule 6: 50S ribosomal protein L5P



• Molecule 7: 50S ribosomal protein L6P



• Molecule 8: 50S ribosomal protein L7Ae

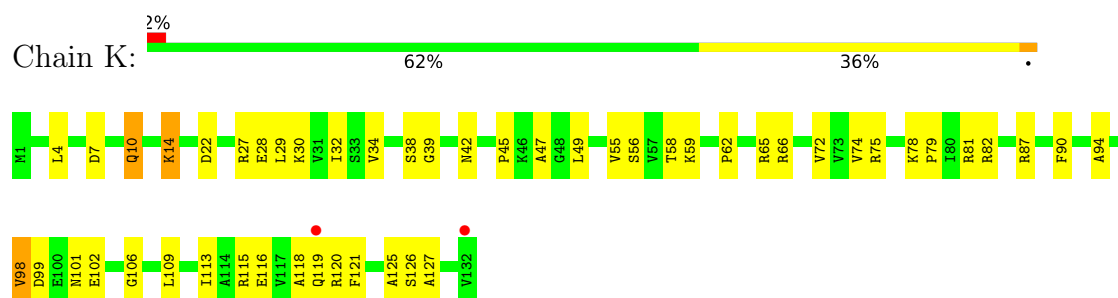


• Molecule 9: Acidic ribosomal protein P0 homolog

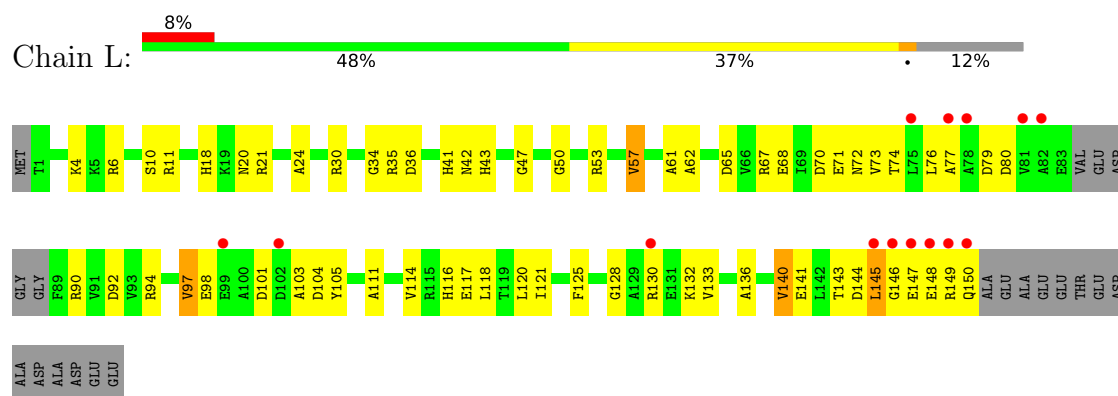




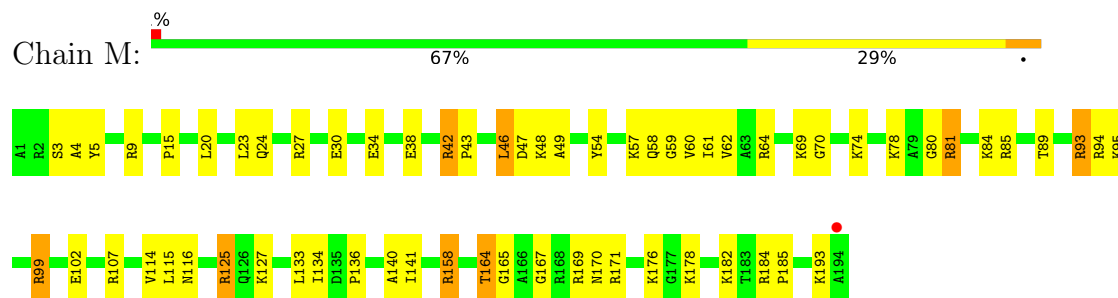
- Molecule 13: 50S ribosomal protein L14P



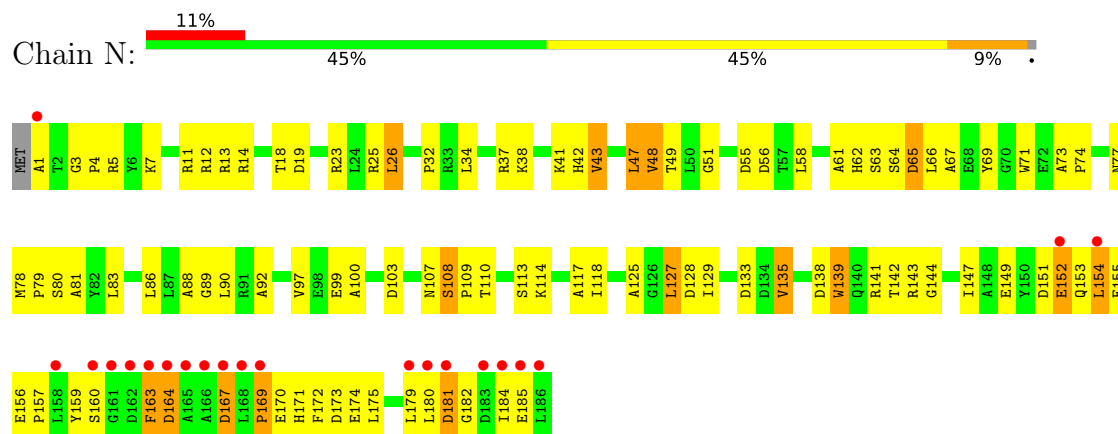
- Molecule 14: 50S ribosomal protein L15P



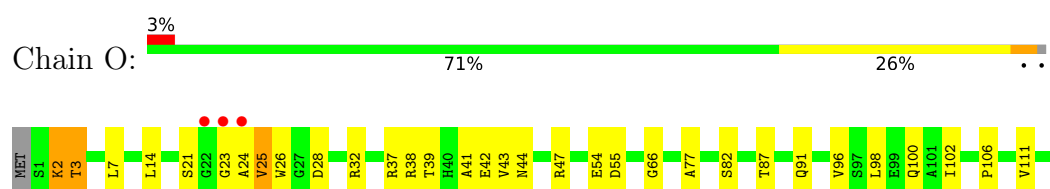
- Molecule 15: 50S ribosomal protein L15e



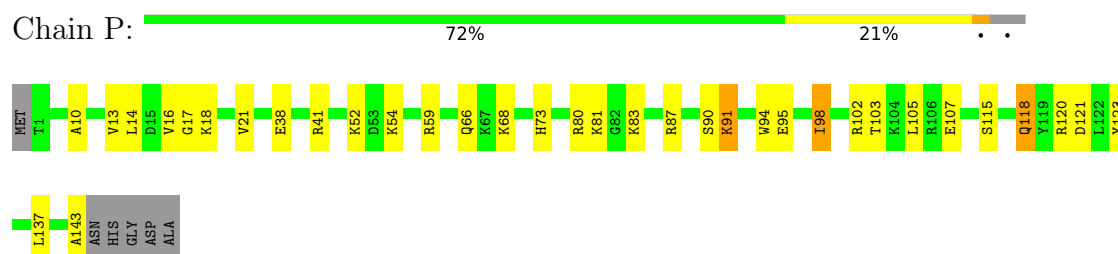
- Molecule 16: 50S ribosomal protein L18P



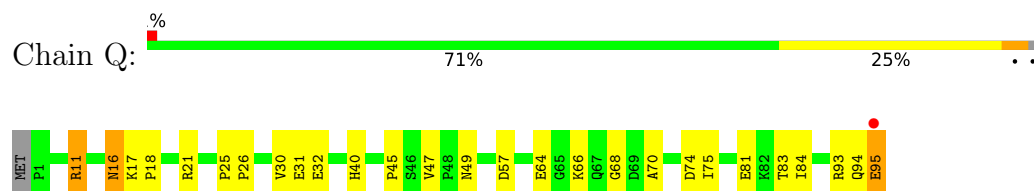
- Molecule 17: 50S ribosomal protein L18e



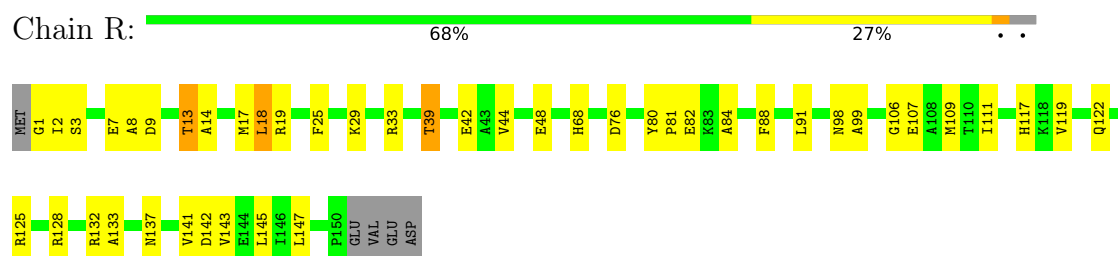
- Molecule 18: 50S ribosomal protein L19E



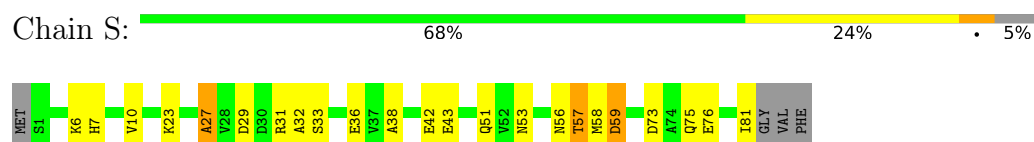
- Molecule 19: 50S ribosomal protein L21e



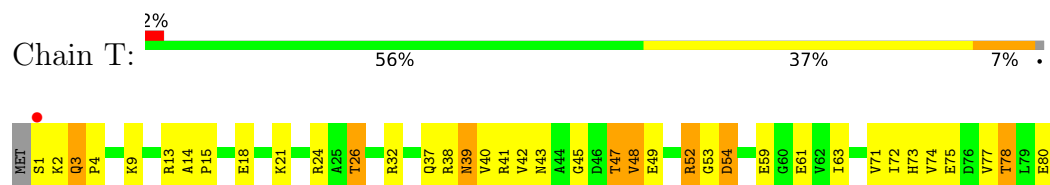
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P

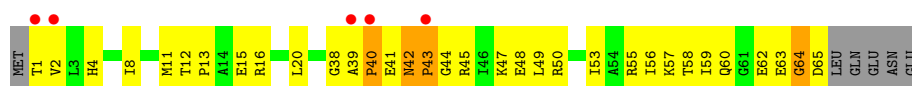




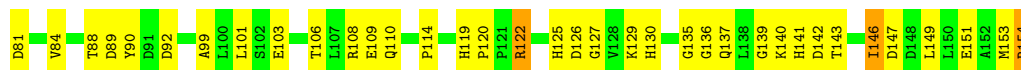
- Molecule 23: 50S ribosomal protein L24E



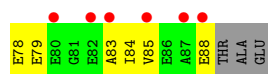
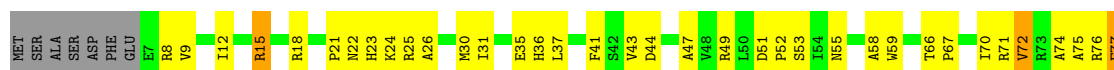
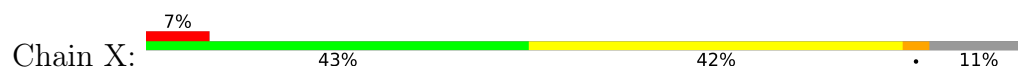
- Molecule 24: 50S ribosomal protein L29P



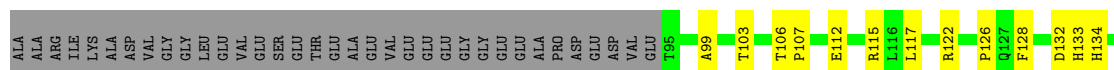
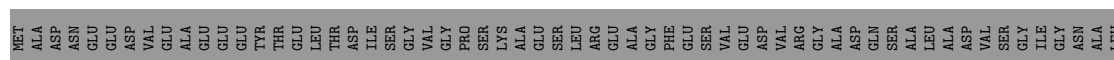
- Molecule 25: 50S ribosomal protein L30P

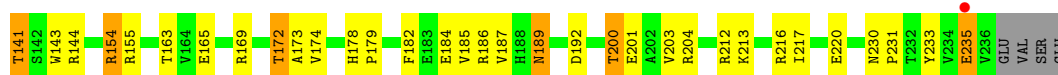


- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E





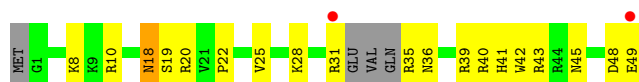
- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.66Å 299.67Å 573.77Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 15.00 – 2.40<br>15.00 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.2 (15.00-2.40)<br>90.2 (15.00-2.40)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.37 (at 2.40Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.188 , 0.222<br>0.183 , 0.216                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6547 reflections (0.98%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.263                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 52.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 99039                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 44.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: CD, UR3, CL, OMG, OMU, MG, PSU, 1MA, NA, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                   |
|-----|-------|--------------|-------------|-------------|-------------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$       |
| 1   | 0     | 0.38         | 0/65959     | 0.62        | 34/102870 (0.0%)  |
| 2   | 9     | 0.38         | 0/2905      | 0.65        | 5/4528 (0.1%)     |
| 3   | A     | 0.44         | 0/1786      | 1.00        | 7/2408 (0.3%)     |
| 4   | B     | 0.43         | 0/2690      | 1.00        | 12/3652 (0.3%)    |
| 5   | C     | 0.48         | 0/1884      | 0.99        | 9/2551 (0.4%)     |
| 6   | D     | 0.36         | 0/1111      | 0.94        | 5/1498 (0.3%)     |
| 7   | E     | 0.38         | 0/1382      | 0.87        | 2/1880 (0.1%)     |
| 8   | F     | 0.43         | 0/901       | 0.89        | 1/1224 (0.1%)     |
| 9   | G     | 0.36         | 0/241       | 0.77        | 0/324             |
| 10  | H     | 0.38         | 0/1287      | 0.99        | 7/1725 (0.4%)     |
| 11  | I     | 0.43         | 0/526       | 0.93        | 1/716 (0.1%)      |
| 12  | J     | 0.41         | 0/1136      | 0.93        | 4/1530 (0.3%)     |
| 13  | K     | 0.42         | 0/1001      | 0.99        | 3/1347 (0.2%)     |
| 14  | L     | 0.40         | 0/1130      | 1.02        | 7/1509 (0.5%)     |
| 15  | M     | 0.44         | 0/1584      | 0.93        | 6/2119 (0.3%)     |
| 16  | N     | 0.46         | 0/1474      | 1.12        | 17/1999 (0.9%)    |
| 17  | O     | 0.42         | 0/874       | 0.93        | 3/1181 (0.3%)     |
| 18  | P     | 0.41         | 0/1147      | 0.84        | 2/1528 (0.1%)     |
| 19  | Q     | 0.44         | 0/749       | 1.06        | 5/1005 (0.5%)     |
| 20  | R     | 0.45         | 0/1172      | 0.98        | 5/1578 (0.3%)     |
| 21  | S     | 0.39         | 0/648       | 0.90        | 3/875 (0.3%)      |
| 22  | T     | 0.39         | 0/958       | 0.96        | 5/1289 (0.4%)     |
| 23  | U     | 0.37         | 0/417       | 0.86        | 0/562             |
| 24  | V     | 0.39         | 0/502       | 0.98        | 3/675 (0.4%)      |
| 25  | W     | 0.47         | 0/1219      | 1.00        | 5/1655 (0.3%)     |
| 26  | X     | 0.43         | 0/664       | 0.99        | 1/895 (0.1%)      |
| 27  | Y     | 0.43         | 0/1146      | 0.96        | 3/1536 (0.2%)     |
| 28  | Z     | 0.39         | 0/590       | 0.96        | 1/787 (0.1%)      |
| 29  | 1     | 0.49         | 0/438       | 0.98        | 3/578 (0.5%)      |
| 30  | 2     | 0.44         | 0/401       | 0.75        | 0/529             |
| 31  | 3     | 0.42         | 0/771       | 0.96        | 5/1024 (0.5%)     |
| All | All   | 0.40         | 0/98693     | 0.73        | 164/147577 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 0     | 1                   | 60                  |
| 2   | 9     | 0                   | 2                   |
| All | All   | 1                   | 62                  |

There are no bond length outliers.

All (164) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 0     | 1563 | G    | C2'-C3'-O3' | 14.02 | 130.53      | 109.50   |
| 1   | 0     | 1979 | G    | C2'-C3'-O3' | 11.54 | 126.82      | 109.50   |
| 1   | 0     | 1942 | A    | C5'-C4'-C3' | 10.04 | 131.06      | 116.00   |
| 6   | D     | 11   | HIS  | N-CA-C      | 9.18  | 120.98      | 110.97   |
| 31  | 3     | 55   | VAL  | CA-C-N      | 9.17  | 131.31      | 119.84   |
| 31  | 3     | 55   | VAL  | C-N-CA      | 9.17  | 131.31      | 119.84   |
| 1   | 0     | 1563 | G    | C4'-C3'-O3' | 9.13  | 123.10      | 109.40   |
| 16  | N     | 135  | VAL  | N-CA-C      | -9.06 | 104.32      | 113.47   |
| 19  | Q     | 17   | LYS  | N-CA-C      | -8.71 | 98.76       | 109.83   |
| 6   | D     | 136  | ARG  | CA-C-N      | 8.69  | 130.71      | 119.84   |
| 6   | D     | 136  | ARG  | C-N-CA      | 8.69  | 130.71      | 119.84   |
| 16  | N     | 163  | PHE  | N-CA-C      | -8.58 | 100.28      | 110.41   |
| 4   | B     | 157  | LYS  | N-CA-C      | -8.28 | 103.77      | 114.04   |
| 16  | N     | 169  | PRO  | N-CA-C      | -8.24 | 100.73      | 114.75   |
| 14  | L     | 57   | VAL  | N-CA-C      | -7.96 | 105.10      | 112.43   |
| 1   | 0     | 1819 | G    | C5'-C4'-C3' | 7.87  | 127.80      | 116.00   |
| 26  | X     | 22   | ASN  | N-CA-C      | 7.84  | 120.81      | 111.33   |
| 20  | R     | 141  | VAL  | N-CA-C      | 7.64  | 118.81      | 108.11   |
| 2   | 9     | 39   | U    | N1-C1'-C2'  | 7.63  | 123.44      | 112.00   |
| 7   | E     | 11   | VAL  | N-CA-C      | 7.60  | 120.84      | 108.99   |
| 19  | Q     | 49   | ASN  | N-CA-C      | 7.55  | 120.27      | 110.53   |
| 1   | 0     | 871  | G    | C5'-C4'-O4' | -7.26 | 98.91       | 109.80   |
| 3   | A     | 222  | GLY  | N-CA-C      | -7.14 | 105.37      | 114.37   |
| 24  | V     | 42   | ASN  | CA-C-N      | 7.13  | 128.75      | 119.84   |
| 24  | V     | 42   | ASN  | C-N-CA      | 7.13  | 128.75      | 119.84   |
| 12  | J     | 68   | GLY  | N-CA-C      | 7.05  | 121.01      | 112.48   |
| 10  | H     | 160  | SER  | N-CA-C      | -7.03 | 100.08      | 110.48   |
| 22  | T     | 54   | ASP  | N-CA-C      | -6.99 | 104.22      | 112.89   |
| 1   | 0     | 2316 | G    | C5'-C4'-C3' | -6.91 | 104.83      | 115.20   |
| 29  | 1     | 43   | ALA  | N-CA-C      | -6.89 | 103.85      | 111.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 16  | N     | 3    | GLY  | CA-C-N      | 6.85  | 126.82      | 119.28   |
| 16  | N     | 3    | GLY  | C-N-CA      | 6.85  | 126.82      | 119.28   |
| 1   | O     | 206  | G    | C5'-C4'-C3' | -6.82 | 105.77      | 116.00   |
| 21  | S     | 27   | ALA  | N-CA-C      | -6.82 | 97.62       | 108.73   |
| 15  | M     | 89   | THR  | N-CA-C      | 6.79  | 118.34      | 111.07   |
| 27  | Y     | 143  | TRP  | N-CA-C      | 6.72  | 120.12      | 110.10   |
| 1   | O     | 1504 | A    | N9-C1'-C2'  | 6.72  | 122.07      | 112.00   |
| 15  | M     | 70   | GLY  | N-CA-C      | 6.70  | 121.54      | 112.17   |
| 1   | O     | 2291 | A    | N9-C1'-C2'  | 6.63  | 121.95      | 112.00   |
| 1   | O     | 920  | C    | C2'-C3'-O3' | -6.62 | 103.77      | 113.70   |
| 14  | L     | 145  | LEU  | N-CA-C      | -6.60 | 104.11      | 111.71   |
| 4   | B     | 323  | LEU  | N-CA-C      | 6.59  | 119.06      | 110.43   |
| 20  | R     | 122  | GLN  | N-CA-C      | -6.55 | 98.52       | 108.67   |
| 20  | R     | 3    | SER  | N-CA-C      | -6.55 | 99.35       | 109.24   |
| 16  | N     | 133  | ASP  | N-CA-C      | 6.52  | 119.22      | 111.33   |
| 14  | L     | 47   | GLY  | N-CA-C      | 6.49  | 118.73      | 111.85   |
| 4   | B     | 222  | LYS  | N-CA-C      | -6.29 | 100.66      | 110.42   |
| 1   | O     | 834  | G    | C2'-C3'-O3' | -6.28 | 104.29      | 113.70   |
| 28  | Z     | 42   | CYS  | N-CA-C      | -6.26 | 100.43      | 109.31   |
| 1   | O     | 1450 | C    | C2'-C3'-O3' | -6.25 | 104.32      | 113.70   |
| 14  | L     | 20   | ASN  | N-CA-C      | 6.25  | 120.73      | 111.04   |
| 21  | S     | 59   | ASP  | N-CA-C      | -6.24 | 105.61      | 113.72   |
| 1   | O     | 1559 | A    | C2'-C3'-O3' | 6.24  | 123.05      | 113.70   |
| 5   | C     | 175  | LYS  | N-CA-C      | 6.22  | 118.32      | 110.24   |
| 19  | Q     | 47   | VAL  | CA-C-N      | 6.21  | 125.43      | 118.97   |
| 19  | Q     | 47   | VAL  | C-N-CA      | 6.21  | 125.43      | 118.97   |
| 31  | 3     | 67   | LEU  | N-CA-C      | 6.20  | 119.64      | 109.85   |
| 5   | C     | 205  | ARG  | N-CA-C      | 6.20  | 118.83      | 111.33   |
| 3   | A     | 70   | ALA  | N-CA-C      | 6.19  | 118.58      | 109.42   |
| 22  | T     | 52   | ARG  | N-CA-C      | 6.18  | 123.97      | 110.80   |
| 11  | I     | 121  | LEU  | N-CA-C      | -6.14 | 105.05      | 112.54   |
| 10  | H     | 159  | PRO  | N-CA-C      | 6.12  | 119.79      | 111.22   |
| 6   | D     | 100  | ASP  | N-CA-C      | -6.12 | 105.81      | 113.28   |
| 4   | B     | 154  | VAL  | CA-C-N      | 6.10  | 126.28      | 119.32   |
| 4   | B     | 154  | VAL  | C-N-CA      | 6.10  | 126.28      | 119.32   |
| 17  | O     | 66   | GLY  | N-CA-C      | 6.09  | 125.59      | 115.66   |
| 20  | R     | 137  | ASN  | N-CA-C      | 6.01  | 119.36      | 110.46   |
| 3   | A     | 228  | ILE  | N-CA-C      | 6.00  | 116.76      | 108.84   |
| 4   | B     | 265  | LEU  | N-CA-C      | 5.99  | 118.63      | 110.55   |
| 16  | N     | 51   | GLY  | CA-C-N      | 5.95  | 125.82      | 119.28   |
| 16  | N     | 51   | GLY  | C-N-CA      | 5.95  | 125.82      | 119.28   |
| 10  | H     | 116  | ALA  | N-CA-C      | 5.94  | 119.79      | 112.54   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | S     | 57   | THR  | N-CA-C      | 5.92  | 118.55      | 110.55   |
| 25  | W     | 68   | THR  | N-CA-C      | 5.88  | 117.77      | 111.36   |
| 1   | 0     | 1592 | G    | N9-C1'-C2'  | 5.87  | 120.80      | 112.00   |
| 16  | N     | 117  | ALA  | N-CA-C      | -5.85 | 104.98      | 111.36   |
| 5   | C     | 177  | GLY  | N-CA-C      | 5.85  | 118.00      | 112.04   |
| 1   | 0     | 1942 | A    | C5'-C4'-O4' | 5.83  | 118.55      | 109.80   |
| 15  | M     | 74   | LYS  | N-CA-C      | 5.83  | 118.97      | 109.59   |
| 1   | 0     | 1120 | U    | C5'-C4'-C3' | -5.82 | 107.28      | 116.00   |
| 25  | W     | 143  | THR  | N-CA-C      | -5.81 | 105.08      | 111.82   |
| 17  | O     | 82   | SER  | N-CA-C      | -5.80 | 102.87      | 110.53   |
| 24  | V     | 64   | GLY  | N-CA-C      | -5.78 | 106.99      | 115.72   |
| 4   | B     | 111  | ARG  | N-CA-C      | -5.76 | 106.26      | 113.28   |
| 20  | R     | 18   | LEU  | N-CA-C      | -5.75 | 100.81      | 109.95   |
| 12  | J     | 36   | VAL  | N-CA-C      | 5.73  | 116.73      | 108.48   |
| 22  | T     | 3    | GLN  | CA-C-N      | 5.72  | 125.84      | 119.32   |
| 22  | T     | 3    | GLN  | C-N-CA      | 5.72  | 125.84      | 119.32   |
| 1   | 0     | 2726 | U    | N1-C1'-C2'  | 5.70  | 120.55      | 112.00   |
| 17  | O     | 2    | LYS  | N-CA-C      | -5.70 | 102.85      | 110.55   |
| 1   | 0     | 2526 | C    | N1-C1'-C2'  | 5.69  | 120.54      | 112.00   |
| 16  | N     | 153  | GLN  | N-CA-C      | -5.68 | 105.48      | 113.20   |
| 22  | T     | 78   | THR  | N-CA-C      | 5.68  | 117.24      | 109.18   |
| 5   | C     | 64   | GLY  | N-CA-C      | 5.67  | 119.65      | 113.58   |
| 1   | 0     | 1942 | A    | C4'-C3'-C2' | -5.67 | 96.93       | 102.60   |
| 2   | 9     | 103  | A    | C5'-C4'-O4' | 5.66  | 118.30      | 109.80   |
| 10  | H     | 88   | ARG  | N-CA-C      | 5.66  | 120.03      | 113.18   |
| 18  | P     | 118  | GLN  | N-CA-C      | -5.65 | 105.04      | 111.14   |
| 3   | A     | 38   | ILE  | N-CA-C      | 5.63  | 116.54      | 108.93   |
| 25  | W     | 9    | GLY  | N-CA-C      | 5.63  | 119.80      | 112.25   |
| 2   | 9     | 65   | A    | N9-C1'-C2'  | 5.61  | 120.41      | 112.00   |
| 29  | 1     | 54   | ALA  | N-CA-C      | 5.60  | 117.83      | 111.11   |
| 2   | 9     | 39   | U    | C4'-C3'-O3' | -5.55 | 104.67      | 113.00   |
| 7   | E     | 37   | ASP  | N-CA-C      | 5.54  | 119.33      | 112.24   |
| 27  | Y     | 230  | ASN  | CA-C-N      | 5.53  | 125.73      | 120.31   |
| 27  | Y     | 230  | ASN  | C-N-CA      | 5.53  | 125.73      | 120.31   |
| 13  | K     | 78   | LYS  | CA-C-N      | 5.53  | 125.84      | 119.92   |
| 13  | K     | 78   | LYS  | C-N-CA      | 5.53  | 125.84      | 119.92   |
| 4   | B     | 175  | LEU  | N-CA-C      | -5.52 | 105.17      | 111.07   |
| 29  | 1     | 21   | ARG  | N-CA-C      | 5.51  | 118.47      | 111.69   |
| 1   | 0     | 1819 | G    | C4'-C3'-C2' | -5.47 | 97.13       | 102.60   |
| 15  | M     | 125  | ARG  | N-CA-C      | 5.45  | 120.62      | 112.94   |
| 4   | B     | 114  | ASP  | N-CA-C      | -5.37 | 97.88       | 107.98   |
| 5   | C     | 91   | PRO  | N-CA-C      | 5.37  | 117.25      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | W     | 35   | VAL  | CA-C-N      | 5.36  | 125.30      | 119.78   |
| 25  | W     | 35   | VAL  | C-N-CA      | 5.36  | 125.30      | 119.78   |
| 16  | N     | 181  | ASP  | N-CA-C      | -5.36 | 103.07      | 110.35   |
| 31  | 3     | 43   | ASN  | N-CA-C      | 5.35  | 119.66      | 113.18   |
| 1   | 0     | 874  | A    | C4'-C3'-O3' | -5.35 | 104.97      | 113.00   |
| 14  | L     | 43   | HIS  | N-CA-C      | -5.32 | 100.72      | 109.40   |
| 16  | N     | 48   | VAL  | N-CA-C      | 5.32  | 116.24      | 108.53   |
| 5   | C     | 78   | ARG  | N-CA-C      | 5.32  | 116.88      | 108.96   |
| 8   | F     | 118  | LEU  | N-CA-C      | -5.29 | 106.89      | 113.19   |
| 1   | 0     | 1504 | A    | C1'-O4'-C4' | -5.28 | 104.62      | 109.90   |
| 5   | C     | 179  | GLY  | N-CA-C      | -5.26 | 106.34      | 113.24   |
| 1   | 0     | 2664 | A    | N9-C1'-C2'  | 5.26  | 119.89      | 112.00   |
| 16  | N     | 13   | ARG  | N-CA-C      | -5.26 | 105.14      | 112.45   |
| 1   | 0     | 1878 | G    | O4'-C1'-C2' | -5.26 | 102.34      | 107.60   |
| 10  | H     | 118  | GLY  | N-CA-C      | 5.26  | 119.27      | 112.54   |
| 1   | 0     | 2291 | A    | C4'-C3'-O3' | -5.26 | 105.11      | 113.00   |
| 1   | 0     | 129  | A    | C2'-C3'-O3' | 5.26  | 121.59      | 113.70   |
| 16  | N     | 185  | GLU  | CA-C-N      | -5.22 | 112.30      | 121.70   |
| 16  | N     | 185  | GLU  | C-N-CA      | -5.22 | 112.30      | 121.70   |
| 6   | D     | 137  | PRO  | N-CA-C      | 5.22  | 123.22      | 112.47   |
| 5   | C     | 219  | ASN  | N-CA-C      | 5.21  | 117.20      | 109.69   |
| 1   | 0     | 2313 | C    | C5'-C4'-C3' | 5.17  | 123.76      | 116.00   |
| 5   | C     | 186  | TYR  | N-CA-C      | 5.16  | 118.42      | 110.42   |
| 16  | N     | 108  | SER  | CA-C-N      | 5.16  | 126.28      | 119.84   |
| 16  | N     | 108  | SER  | C-N-CA      | 5.16  | 126.28      | 119.84   |
| 31  | 3     | 60   | LYS  | N-CA-C      | -5.15 | 102.72      | 110.24   |
| 12  | J     | 105  | LEU  | N-CA-C      | -5.15 | 101.37      | 109.25   |
| 2   | 9     | 103  | A    | C4'-C3'-C2' | -5.15 | 97.45       | 102.60   |
| 1   | 0     | 1450 | C    | C4'-C3'-O3' | 5.14  | 120.72      | 113.00   |
| 13  | K     | 14   | LYS  | N-CA-C      | -5.14 | 102.45      | 110.10   |
| 1   | 0     | 921  | G    | N9-C1'-C2'  | 5.13  | 119.70      | 112.00   |
| 10  | H     | 158  | THR  | N-CA-C      | 5.13  | 121.16      | 109.81   |
| 1   | 0     | 2467 | A    | C1'-O4'-C4' | -5.12 | 104.58      | 109.70   |
| 3   | A     | 236  | GLY  | N-CA-C      | 5.11  | 117.34      | 111.36   |
| 18  | P     | 90   | SER  | N-CA-C      | 5.11  | 116.84      | 111.28   |
| 3   | A     | 122  | SER  | N-CA-C      | 5.10  | 117.74      | 110.24   |
| 14  | L     | 97   | VAL  | N-CA-C      | 5.08  | 116.23      | 109.37   |
| 4   | B     | 151  | VAL  | CA-C-N      | 5.07  | 124.25      | 118.97   |
| 4   | B     | 151  | VAL  | C-N-CA      | 5.07  | 124.25      | 118.97   |
| 1   | 0     | 1006 | A    | N9-C1'-C2'  | 5.07  | 119.61      | 112.00   |
| 3   | A     | 175  | LYS  | N-CA-C      | -5.07 | 105.64      | 111.07   |
| 15  | M     | 42   | ARG  | CA-C-N      | 5.07  | 124.83      | 119.76   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | M     | 42   | ARG  | C-N-CA      | 5.07  | 124.83      | 119.76   |
| 1   | 0     | 1615 | A    | C5'-C4'-C3' | 5.06  | 123.59      | 116.00   |
| 19  | Q     | 68   | GLY  | N-CA-C      | -5.05 | 102.78      | 111.47   |
| 4   | B     | 108  | GLU  | N-CA-C      | 5.04  | 118.97      | 111.87   |
| 10  | H     | 112  | GLY  | N-CA-C      | -5.04 | 101.24      | 113.18   |
| 12  | J     | 22   | VAL  | N-CA-C      | -5.04 | 105.94      | 110.82   |
| 14  | L     | 42   | ASN  | N-CA-C      | 5.02  | 118.67      | 112.24   |
| 1   | 0     | 138  | U    | C2'-C3'-O3' | -5.02 | 106.17      | 113.70   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | 0     | 1563 | G    | C3'  |

All (62) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | 0     | 1078 | A    | Sidechain |
| 1   | 0     | 1292 | G    | Sidechain |
| 1   | 0     | 1327 | G    | Sidechain |
| 1   | 0     | 1340 | G    | Sidechain |
| 1   | 0     | 1342 | C    | Sidechain |
| 1   | 0     | 1351 | G    | Sidechain |
| 1   | 0     | 1417 | G    | Sidechain |
| 1   | 0     | 1430 | G    | Sidechain |
| 1   | 0     | 1458 | A    | Sidechain |
| 1   | 0     | 1794 | G    | Sidechain |
| 1   | 0     | 1809 | G    | Sidechain |
| 1   | 0     | 1829 | A    | Sidechain |
| 1   | 0     | 1845 | A    | Sidechain |
| 1   | 0     | 1848 | G    | Sidechain |
| 1   | 0     | 1863 | G    | Sidechain |
| 1   | 0     | 1867 | G    | Sidechain |
| 1   | 0     | 1877 | G    | Sidechain |
| 1   | 0     | 1878 | G    | Sidechain |
| 1   | 0     | 191  | A    | Sidechain |
| 1   | 0     | 196  | G    | Sidechain |
| 1   | 0     | 1970 | G    | Sidechain |
| 1   | 0     | 1972 | U    | Sidechain |
| 1   | 0     | 1979 | G    | Sidechain |
| 1   | 0     | 2012 | U    | Sidechain |
| 1   | 0     | 2078 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | 0     | 221  | G    | Sidechain |
| 1   | 0     | 2316 | G    | Sidechain |
| 1   | 0     | 2386 | U    | Sidechain |
| 1   | 0     | 2395 | A    | Sidechain |
| 1   | 0     | 2412 | G    | Sidechain |
| 1   | 0     | 246  | G    | Sidechain |
| 1   | 0     | 2465 | A    | Sidechain |
| 1   | 0     | 2493 | C    | Sidechain |
| 1   | 0     | 2503 | A    | Sidechain |
| 1   | 0     | 2506 | A    | Sidechain |
| 1   | 0     | 2526 | C    | Sidechain |
| 1   | 0     | 2543 | G    | Sidechain |
| 1   | 0     | 2552 | C    | Sidechain |
| 1   | 0     | 2564 | G    | Sidechain |
| 1   | 0     | 2607 | U    | Sidechain |
| 1   | 0     | 2616 | G    | Sidechain |
| 1   | 0     | 2630 | G    | Sidechain |
| 1   | 0     | 270  | U    | Sidechain |
| 1   | 0     | 2842 | G    | Sidechain |
| 1   | 0     | 332  | G    | Sidechain |
| 1   | 0     | 333  | G    | Sidechain |
| 1   | 0     | 396  | U    | Sidechain |
| 1   | 0     | 452  | G    | Sidechain |
| 1   | 0     | 469  | G    | Sidechain |
| 1   | 0     | 470  | U    | Sidechain |
| 1   | 0     | 471  | G    | Sidechain |
| 1   | 0     | 482  | G    | Sidechain |
| 1   | 0     | 518  | G    | Sidechain |
| 1   | 0     | 619  | U    | Sidechain |
| 1   | 0     | 639  | A    | Sidechain |
| 1   | 0     | 771  | G    | Sidechain |
| 1   | 0     | 795  | G    | Sidechain |
| 1   | 0     | 817  | G    | Sidechain |
| 1   | 0     | 867  | A    | Sidechain |
| 1   | 0     | 868  | G    | Sidechain |
| 2   | 9     | 39   | U    | Sidechain |
| 2   | 9     | 87   | U    | Sidechain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 59021 | 0        | 29813    | 713     | 0            |
| 2   | 9     | 2600  | 0        | 1326     | 54      | 0            |
| 3   | A     | 1753  | 0        | 1766     | 106     | 0            |
| 4   | B     | 2625  | 0        | 2533     | 171     | 0            |
| 5   | C     | 1859  | 0        | 1816     | 111     | 0            |
| 6   | D     | 1094  | 0        | 1085     | 123     | 0            |
| 7   | E     | 1357  | 0        | 1266     | 80      | 0            |
| 8   | F     | 890   | 0        | 843      | 58      | 0            |
| 9   | G     | 240   | 0        | 231      | 17      | 0            |
| 10  | H     | 1266  | 0        | 1268     | 81      | 0            |
| 11  | I     | 519   | 0        | 500      | 74      | 0            |
| 12  | J     | 1120  | 0        | 1098     | 69      | 0            |
| 13  | K     | 992   | 0        | 1031     | 58      | 0            |
| 14  | L     | 1118  | 0        | 1076     | 57      | 0            |
| 15  | M     | 1560  | 0        | 1568     | 60      | 0            |
| 16  | N     | 1445  | 0        | 1401     | 118     | 0            |
| 17  | O     | 865   | 0        | 873      | 30      | 0            |
| 18  | P     | 1136  | 0        | 1123     | 35      | 0            |
| 19  | Q     | 735   | 0        | 728      | 18      | 0            |
| 20  | R     | 1149  | 0        | 1122     | 46      | 0            |
| 21  | S     | 641   | 0        | 605      | 20      | 0            |
| 22  | T     | 950   | 0        | 923      | 49      | 0            |
| 23  | U     | 410   | 0        | 364      | 31      | 0            |
| 24  | V     | 499   | 0        | 511      | 31      | 0            |
| 25  | W     | 1196  | 0        | 1137     | 102     | 0            |
| 26  | X     | 654   | 0        | 653      | 40      | 0            |
| 27  | Y     | 1130  | 0        | 1133     | 54      | 0            |
| 28  | Z     | 579   | 0        | 539      | 27      | 0            |
| 29  | 1     | 431   | 0        | 426      | 21      | 0            |
| 30  | 2     | 396   | 0        | 413      | 28      | 0            |
| 31  | 3     | 755   | 0        | 728      | 30      | 0            |
| 32  | 0     | 109   | 0        | 0        | 0       | 0            |
| 32  | 3     | 1     | 0        | 0        | 0       | 0            |
| 32  | 9     | 1     | 0        | 0        | 0       | 0            |
| 32  | A     | 1     | 0        | 0        | 0       | 0            |
| 32  | B     | 1     | 0        | 0        | 0       | 0            |
| 32  | K     | 1     | 0        | 0        | 0       | 0            |
| 32  | T     | 1     | 0        | 0        | 0       | 0            |
| 32  | Y     | 1     | 0        | 0        | 0       | 0            |
| 33  | 0     | 2     | 0        | 0        | 0       | 0            |
| 34  | 0     | 72    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34  | 9     | 2     | 0        | 0        | 0       | 0            |
| 34  | A     | 1     | 0        | 0        | 0       | 0            |
| 34  | C     | 1     | 0        | 0        | 0       | 0            |
| 34  | H     | 2     | 0        | 0        | 0       | 0            |
| 34  | J     | 1     | 0        | 0        | 0       | 0            |
| 34  | L     | 1     | 0        | 0        | 0       | 0            |
| 34  | M     | 1     | 0        | 0        | 0       | 0            |
| 34  | Q     | 1     | 0        | 0        | 0       | 0            |
| 34  | R     | 2     | 0        | 0        | 0       | 0            |
| 34  | S     | 1     | 0        | 0        | 0       | 0            |
| 34  | T     | 1     | 0        | 0        | 0       | 0            |
| 35  | 0     | 10    | 0        | 0        | 0       | 0            |
| 35  | 3     | 1     | 0        | 0        | 0       | 0            |
| 35  | A     | 1     | 0        | 0        | 0       | 0            |
| 35  | B     | 1     | 0        | 0        | 0       | 0            |
| 35  | J     | 3     | 0        | 0        | 1       | 0            |
| 35  | L     | 1     | 0        | 0        | 0       | 0            |
| 35  | M     | 1     | 0        | 0        | 0       | 0            |
| 35  | N     | 1     | 0        | 0        | 0       | 0            |
| 35  | O     | 1     | 0        | 0        | 0       | 0            |
| 35  | R     | 1     | 0        | 0        | 0       | 0            |
| 35  | Y     | 1     | 0        | 0        | 0       | 0            |
| 36  | 1     | 1     | 0        | 0        | 0       | 0            |
| 36  | 3     | 1     | 0        | 0        | 0       | 0            |
| 36  | O     | 1     | 0        | 0        | 0       | 0            |
| 36  | U     | 1     | 0        | 0        | 0       | 0            |
| 36  | Z     | 1     | 0        | 0        | 0       | 0            |
| 37  | 0     | 5893  | 0        | 0        | 146     | 0            |
| 37  | 1     | 51    | 0        | 0        | 1       | 0            |
| 37  | 2     | 40    | 0        | 0        | 5       | 0            |
| 37  | 3     | 71    | 0        | 0        | 9       | 0            |
| 37  | 9     | 136   | 0        | 0        | 8       | 0            |
| 37  | A     | 127   | 0        | 0        | 19      | 0            |
| 37  | B     | 153   | 0        | 0        | 28      | 0            |
| 37  | C     | 172   | 0        | 0        | 28      | 0            |
| 37  | D     | 49    | 0        | 0        | 20      | 0            |
| 37  | E     | 44    | 0        | 0        | 11      | 0            |
| 37  | F     | 25    | 0        | 0        | 7       | 0            |
| 37  | G     | 20    | 0        | 0        | 3       | 0            |
| 37  | H     | 71    | 0        | 0        | 16      | 0            |
| 37  | I     | 9     | 0        | 0        | 10      | 0            |
| 37  | J     | 55    | 0        | 0        | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37  | K     | 61    | 0        | 0        | 12      | 0            |
| 37  | L     | 85    | 0        | 0        | 17      | 0            |
| 37  | M     | 121   | 0        | 0        | 10      | 0            |
| 37  | N     | 64    | 0        | 0        | 13      | 0            |
| 37  | O     | 44    | 0        | 0        | 6       | 0            |
| 37  | P     | 65    | 0        | 0        | 3       | 0            |
| 37  | Q     | 52    | 0        | 0        | 2       | 0            |
| 37  | R     | 83    | 0        | 0        | 8       | 0            |
| 37  | S     | 33    | 0        | 0        | 5       | 0            |
| 37  | T     | 40    | 0        | 0        | 5       | 0            |
| 37  | U     | 25    | 0        | 0        | 4       | 0            |
| 37  | V     | 14    | 0        | 0        | 4       | 0            |
| 37  | W     | 67    | 0        | 0        | 10      | 0            |
| 37  | X     | 28    | 0        | 0        | 3       | 0            |
| 37  | Y     | 96    | 0        | 0        | 15      | 0            |
| 37  | Z     | 29    | 0        | 0        | 5       | 0            |
| All | All   | 99039 | 0        | 59899    | 2298    | 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 15.

All (2298) 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) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:236:THR:HG22 | 5:C:239:ALA:H    | 1.04                     | 1.11              |
| 20:R:99:ALA:HB1  | 20:R:109:MET:HE1 | 1.29                     | 1.10              |
| 1:0:1160:G:H5'   | 1:0:1161:A:H5'   | 1.26                     | 1.09              |
| 26:X:37:LEU:HD13 | 26:X:85:VAL:HG21 | 1.31                     | 1.09              |
| 1:0:960:G:H4'    | 37:0:6920:HOH:O  | 1.51                     | 1.08              |
| 5:C:5:ILE:HD11   | 5:C:16:VAL:HG23  | 1.36                     | 1.07              |
| 10:H:46:GLN:HB3  | 10:H:167:PRO:HD2 | 1.36                     | 1.06              |
| 10:H:166:SER:HB2 | 10:H:167:PRO:HD3 | 1.37                     | 1.05              |
| 1:0:1242:A:H5'   | 12:J:82:THR:HG23 | 1.38                     | 1.04              |
| 6:D:25:MET:HE2   | 6:D:41:LEU:HG    | 1.41                     | 1.03              |
| 24:V:12:THR:HG22 | 24:V:15:GLU:HG3  | 1.39                     | 1.03              |
| 1:0:156:C:H5''   | 15:M:171:ARG:HD3 | 1.40                     | 1.03              |
| 22:T:71:VAL:HG11 | 22:T:90:PRO:HB3  | 1.40                     | 1.03              |
| 28:Z:10:ARG:HA   | 37:Z:8414:HOH:O  | 1.58                     | 1.01              |
| 1:0:871:G:C8     | 1:0:871:G:H5'    | 1.94                     | 1.01              |
| 2:9:6:C:H5''     | 16:N:37:ARG:NH1  | 1.76                     | 1.00              |
| 2:9:76:G:H3'     | 2:9:77:A:H5''    | 1.44                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:M:164:THR:HG22 | 15:M:167:GLY:H    | 1.22                     | 0.99              |
| 1:O:21:G:H5'      | 20:R:2:ILE:HA     | 1.45                     | 0.99              |
| 6:D:134:LEU:HD11  | 6:D:166:ILE:HD11  | 1.42                     | 0.99              |
| 1:O:1751:G:H2'    | 1:O:1752:G:H5''   | 1.43                     | 0.98              |
| 2:9:56:A:H2'      | 2:9:57:A:H5''     | 1.46                     | 0.98              |
| 4:B:140:LEU:HA    | 37:B:8583:HOH:O   | 1.61                     | 0.98              |
| 18:P:115:SER:H    | 18:P:118:GLN:HE21 | 1.01                     | 0.97              |
| 3:A:191:GLY:HA2   | 3:A:194:MET:HE2   | 1.44                     | 0.97              |
| 13:K:39:GLY:HA2   | 37:K:4183:HOH:O   | 1.62                     | 0.97              |
| 27:Y:200:THR:HG22 | 27:Y:201:GLU:HG3  | 1.46                     | 0.97              |
| 13:K:10:GLN:NE2   | 13:K:10:GLN:H     | 1.61                     | 0.96              |
| 2:9:6:C:H5''      | 16:N:37:ARG:HH12  | 1.30                     | 0.96              |
| 1:O:870:G:H2'     | 1:O:871:G:H5''    | 1.45                     | 0.96              |
| 25:W:137:GLN:HE21 | 25:W:141:HIS:HE1  | 1.12                     | 0.96              |
| 16:N:83:LEU:HD13  | 16:N:175:LEU:HD23 | 1.47                     | 0.95              |
| 25:W:149:LEU:HG   | 25:W:153:MET:HE2  | 1.46                     | 0.95              |
| 6:D:154:LYS:H     | 6:D:154:LYS:HD2   | 1.31                     | 0.94              |
| 25:W:88:THR:HB    | 37:W:6679:HOH:O   | 1.66                     | 0.94              |
| 21:S:57:THR:HG22  | 21:S:59:ASP:H     | 1.32                     | 0.94              |
| 1:O:968:G:H1'     | 10:H:32:LYS:NZ    | 1.80                     | 0.94              |
| 1:O:871:G:H5'     | 1:O:871:G:H8      | 1.29                     | 0.94              |
| 12:J:19:MET:HE3   | 12:J:132:LEU:HD11 | 1.49                     | 0.94              |
| 13:K:29:LEU:HB3   | 13:K:55:VAL:HG11  | 1.48                     | 0.94              |
| 12:J:76:ASP:HA    | 37:J:5907:HOH:O   | 1.68                     | 0.94              |
| 16:N:144:GLY:O    | 16:N:147:ILE:HG22 | 1.68                     | 0.93              |
| 5:C:115:LEU:HD13  | 5:C:223:LEU:HD21  | 1.51                     | 0.93              |
| 5:C:127:ARG:NH2   | 5:C:225:PRO:HG2   | 1.84                     | 0.93              |
| 13:K:81:ARG:HB2   | 13:K:87:ARG:HH11  | 1.28                     | 0.93              |
| 1:O:968:G:H1'     | 10:H:32:LYS:HZ2   | 1.32                     | 0.92              |
| 27:Y:187:VAL:HG23 | 27:Y:192:ASP:HB2  | 1.51                     | 0.92              |
| 4:B:86:ALA:HA     | 37:B:8583:HOH:O   | 1.68                     | 0.92              |
| 25:W:88:THR:HG22  | 25:W:89:ASP:H     | 1.32                     | 0.91              |
| 16:N:47:LEU:HD11  | 16:N:127:LEU:HD21 | 1.52                     | 0.91              |
| 4:B:264:GLU:HG2   | 4:B:267:LYS:HE2   | 1.49                     | 0.90              |
| 5:C:236:THR:HG22  | 5:C:239:ALA:N     | 1.86                     | 0.90              |
| 5:C:2:GLN:HB3     | 37:C:8334:HOH:O   | 1.70                     | 0.90              |
| 10:H:46:GLN:HE21  | 10:H:137:TYR:HE2  | 1.20                     | 0.90              |
| 1:O:1835:U:H5     | 1:O:1840:A:N7     | 1.70                     | 0.90              |
| 1:O:1116:U:H3     | 1:O:1246:A:H62    | 1.19                     | 0.90              |
| 13:K:10:GLN:HE21  | 13:K:10:GLN:N     | 1.69                     | 0.89              |
| 15:M:102:GLU:OE1  | 15:M:164:THR:HG21 | 1.71                     | 0.89              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:I:110:GLU:HA  | 11:I:113:HIS:NE2  | 1.86                     | 0.89              |
| 3:A:199:HIS:HD2  | 3:A:201:PHE:H     | 1.20                     | 0.89              |
| 4:B:62:ARG:HA    | 4:B:65:MET:HE3    | 1.55                     | 0.89              |
| 25:W:6:GLN:HB2   | 25:W:26:ILE:HD12  | 1.53                     | 0.88              |
| 16:N:164:ASP:CG  | 16:N:167:ASP:HA   | 1.98                     | 0.88              |
| 1:O:1701:A:H4'   | 1:O:1702:U:H5''   | 1.53                     | 0.88              |
| 13:K:10:GLN:H    | 13:K:10:GLN:HE21  | 0.89                     | 0.88              |
| 16:N:163:PHE:O   | 16:N:164:ASP:CG   | 2.17                     | 0.88              |
| 1:O:542:A:H5'    | 1:O:542:A:H8      | 1.37                     | 0.88              |
| 25:W:122:ARG:HG2 | 25:W:122:ARG:HH11 | 1.38                     | 0.88              |
| 1:O:645:U:OP2    | 14:L:4:LYS:HE2    | 1.74                     | 0.88              |
| 1:O:214:U:H5'    | 37:O:5641:HOH:O   | 1.73                     | 0.87              |
| 10:H:56:GLN:HE21 | 10:H:126:ARG:HE   | 1.18                     | 0.87              |
| 24:V:42:ASN:HB3  | 37:V:7247:HOH:O   | 1.75                     | 0.87              |
| 1:O:1184:C:H1'   | 37:O:6954:HOH:O   | 1.75                     | 0.87              |
| 3:A:211:LYS:HB3  | 3:A:212:PRO:HD2   | 1.55                     | 0.86              |
| 10:H:166:SER:HB2 | 10:H:167:PRO:CD   | 2.05                     | 0.86              |
| 4:B:7:ARG:HG2    | 4:B:7:ARG:HH11    | 1.39                     | 0.86              |
| 4:B:212:GLN:HB2  | 4:B:257:THR:HG21  | 1.54                     | 0.86              |
| 1:O:2716:G:H5''  | 4:B:206:THR:HG21  | 1.58                     | 0.86              |
| 16:N:7:LYS:HE3   | 19:Q:21:ARG:O     | 1.74                     | 0.86              |
| 6:D:27:ILE:HG22  | 6:D:28:GLY:H      | 1.40                     | 0.85              |
| 7:E:15:GLN:HG3   | 7:E:20:ILE:HG12   | 1.58                     | 0.85              |
| 1:O:856:G:H2'    | 37:O:4928:HOH:O   | 1.75                     | 0.85              |
| 6:D:95:THR:OG1   | 6:D:174:VAL:HG22  | 1.76                     | 0.85              |
| 26:X:30:MET:HE1  | 26:X:58:ALA:HB3   | 1.57                     | 0.85              |
| 1:O:2717:C:H2'   | 1:O:2718:C:H5''   | 1.58                     | 0.85              |
| 4:B:238:ASN:HD22 | 4:B:240:GLY:H     | 1.24                     | 0.85              |
| 5:C:236:THR:CG2  | 5:C:239:ALA:H     | 1.88                     | 0.85              |
| 13:K:81:ARG:HB2  | 13:K:87:ARG:NH1   | 1.91                     | 0.85              |
| 30:2:41:HIS:H    | 30:2:45:ASN:HD22  | 1.25                     | 0.85              |
| 1:O:1116:U:HO2'  | 1:O:1118:A:H2     | 0.87                     | 0.85              |
| 1:O:381:G:H5''   | 37:O:3823:HOH:O   | 1.75                     | 0.85              |
| 16:N:23:ARG:HD3  | 37:N:8545:HOH:O   | 1.77                     | 0.85              |
| 25:W:88:THR:HG23 | 25:W:110:GLN:NE2  | 1.92                     | 0.84              |
| 1:O:1474:C:H6    | 1:O:1474:C:H5'    | 1.43                     | 0.84              |
| 4:B:162:MET:HE1  | 4:B:308:LEU:HD21  | 1.59                     | 0.84              |
| 7:E:97:VAL:HG12  | 37:E:4191:HOH:O   | 1.77                     | 0.84              |
| 13:K:74:VAL:HG11 | 13:K:113:ILE:HG12 | 1.57                     | 0.84              |
| 1:O:560:C:H42    | 1:O:597:A:H61     | 1.24                     | 0.84              |
| 1:O:2717:C:C2'   | 1:O:2718:C:H5''   | 2.08                     | 0.84              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:W:154:ARG:OXT | 37:W:4276:HOH:O   | 1.95                     | 0.84              |
| 10:H:56:GLN:NE2  | 10:H:126:ARG:HE   | 1.74                     | 0.84              |
| 25:W:88:THR:HG23 | 25:W:110:GLN:HE21 | 1.42                     | 0.83              |
| 1:O:2506:A:HO2'  | 1:O:2507:G:H8     | 0.88                     | 0.83              |
| 11:I:118:SER:HB2 | 11:I:123:ASN:HB2  | 1.57                     | 0.83              |
| 1:O:962:C:H1'    | 16:N:5:ARG:NH1    | 1.93                     | 0.83              |
| 10:H:29:ALA:HB3  | 10:H:66:ARG:HH12  | 1.43                     | 0.83              |
| 6:D:54:ALA:HB2   | 6:D:69:ILE:HD12   | 1.58                     | 0.83              |
| 3:A:100:PRO:HG2  | 3:A:103:VAL:HG21  | 1.59                     | 0.82              |
| 4:B:190:MET:HE2  | 4:B:194:PHE:CD1   | 2.13                     | 0.82              |
| 9:G:12:ILE:HA    | 37:G:4499:HOH:O   | 1.77                     | 0.82              |
| 5:C:214:THR:HG21 | 37:C:8402:HOH:O   | 1.79                     | 0.82              |
| 4:B:321:PRO:HA   | 37:B:8664:HOH:O   | 1.79                     | 0.82              |
| 10:H:99:LYS:HD3  | 10:H:119:LYS:HD3  | 1.60                     | 0.82              |
| 16:N:113:SER:HB2 | 37:N:8557:HOH:O   | 1.79                     | 0.82              |
| 14:L:133:VAL:HA  | 37:L:8573:HOH:O   | 1.80                     | 0.82              |
| 1:O:541:C:H2'    | 1:O:542:A:H5''    | 1.61                     | 0.82              |
| 1:O:870:G:C2'    | 1:O:871:G:H5''    | 2.10                     | 0.82              |
| 4:B:162:MET:HE2  | 4:B:310:ARG:HD3   | 1.61                     | 0.81              |
| 17:O:42:GLU:HB2  | 37:O:2176:HOH:O   | 1.78                     | 0.81              |
| 25:W:4:LEU:HD22  | 25:W:52:VAL:HG21  | 1.63                     | 0.81              |
| 3:A:36:ASP:OD2   | 3:A:85:SER:HB2    | 1.81                     | 0.81              |
| 13:K:14:LYS:HB2  | 13:K:45:PRO:HG2   | 1.62                     | 0.81              |
| 7:E:81:GLU:HG2   | 7:E:134:SER:HB3   | 1.63                     | 0.80              |
| 24:V:12:THR:HG22 | 24:V:15:GLU:CG    | 2.11                     | 0.80              |
| 1:O:1667:A:H8    | 1:O:1667:A:H5'    | 1.46                     | 0.80              |
| 1:O:2812:A:H2    | 1:O:2814:A:H62    | 1.23                     | 0.80              |
| 3:A:191:GLY:HA2  | 3:A:194:MET:CE    | 2.11                     | 0.80              |
| 1:O:1372:A:H3'   | 37:O:6680:HOH:O   | 1.80                     | 0.80              |
| 6:D:105:SER:HB2  | 6:D:131:THR:HG23  | 1.63                     | 0.80              |
| 20:R:8:ALA:HB1   | 20:R:13:THR:HG21  | 1.63                     | 0.80              |
| 20:R:18:LEU:HB2  | 20:R:143:VAL:HG12 | 1.62                     | 0.80              |
| 1:O:506:G:H22    | 1:O:509:A:C5'     | 1.94                     | 0.80              |
| 5:C:236:THR:HG21 | 37:C:8373:HOH:O   | 1.81                     | 0.80              |
| 31:3:62:THR:HB   | 37:3:8549:HOH:O   | 1.81                     | 0.80              |
| 37:O:6368:HOH:O  | 15:M:178:LYS:HB2  | 1.81                     | 0.79              |
| 3:A:200:PRO:HG2  | 3:A:225:VAL:HG21  | 1.64                     | 0.79              |
| 5:C:5:ILE:HD11   | 5:C:16:VAL:CG2    | 2.10                     | 0.79              |
| 1:O:1625:U:H4'   | 37:O:4167:HOH:O   | 1.83                     | 0.79              |
| 14:L:79:ASP:HB3  | 37:L:8558:HOH:O   | 1.83                     | 0.79              |
| 8:F:91:VAL:HG12  | 8:F:92:GLY:H      | 1.48                     | 0.79              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2890:A:H1'   | 23:U:56:ARG:NH2   | 1.98                     | 0.79              |
| 3:A:88:ILE:HD13  | 3:A:100:PRO:HD3   | 1.64                     | 0.78              |
| 10:H:27:LYS:H    | 10:H:59:HIS:HD2   | 1.31                     | 0.78              |
| 26:X:78:GLU:HG2  | 26:X:79:GLU:H     | 1.47                     | 0.78              |
| 1:0:871:G:H8     | 1:0:871:G:C5'     | 1.96                     | 0.78              |
| 1:0:1160:G:H5'   | 1:0:1161:A:C5'    | 2.11                     | 0.78              |
| 3:A:192:VAL:HB   | 37:A:8597:HOH:O   | 1.83                     | 0.78              |
| 16:N:163:PHE:O   | 16:N:163:PHE:CG   | 2.35                     | 0.78              |
| 1:0:1162:G:H1'   | 11:I:117:LEU:HD11 | 1.65                     | 0.78              |
| 1:0:1701:A:H5'   | 37:0:5782:HOH:O   | 1.84                     | 0.78              |
| 5:C:78:ARG:HH11  | 5:C:78:ARG:HG3    | 1.48                     | 0.78              |
| 11:I:80:LYS:HD3  | 11:I:86:GLU:O     | 1.84                     | 0.78              |
| 1:0:559:U:H6     | 1:0:559:U:H5'     | 1.49                     | 0.78              |
| 1:0:2710:U:H1'   | 37:0:7113:HOH:O   | 1.84                     | 0.78              |
| 4:B:201:ASP:HB2  | 4:B:312:ARG:HD2   | 1.64                     | 0.78              |
| 25:W:72:PRO:HG2  | 25:W:77:ALA:HB3   | 1.65                     | 0.78              |
| 1:0:545:G:H5'    | 1:0:545:G:H8      | 1.46                     | 0.78              |
| 37:0:6914:HOH:O  | 22:T:9:LYS:HB2    | 1.81                     | 0.78              |
| 37:0:6266:HOH:O  | 16:N:4:PRO:HD2    | 1.83                     | 0.78              |
| 16:N:49:THR:HG22 | 16:N:56:ASP:HB2   | 1.66                     | 0.78              |
| 37:0:5794:HOH:O  | 6:D:99:ASP:HA     | 1.84                     | 0.78              |
| 21:S:51:GLN:HE21 | 21:S:53:ASN:HD21  | 1.32                     | 0.78              |
| 24:V:1:THR:HG23  | 24:V:2:VAL:H      | 1.48                     | 0.78              |
| 1:0:2506:A:O2'   | 1:0:2507:G:H8     | 1.65                     | 0.78              |
| 25:W:21:LEU:HD22 | 25:W:26:ILE:HD11  | 1.66                     | 0.77              |
| 1:0:506:G:H22    | 1:0:509:A:H5'     | 1.48                     | 0.77              |
| 4:B:41:PHE:CD1   | 4:B:79:MET:HE2    | 2.18                     | 0.77              |
| 5:C:132:ASP:HB3  | 37:C:8362:HOH:O   | 1.83                     | 0.77              |
| 2:9:14:G:H5'     | 2:9:14:G:H8       | 1.50                     | 0.77              |
| 5:C:236:THR:HA   | 37:C:8450:HOH:O   | 1.84                     | 0.77              |
| 11:I:110:GLU:HA  | 11:I:113:HIS:CD2  | 2.19                     | 0.77              |
| 1:0:544:G:H2'    | 1:0:545:G:H5''    | 1.65                     | 0.77              |
| 1:0:1119:G:H22   | 1:0:1246:A:H2     | 1.26                     | 0.77              |
| 3:A:35:GLY:O     | 3:A:36:ASP:HB3    | 1.83                     | 0.77              |
| 20:R:17:MET:HE1  | 20:R:19:ARG:NH2   | 1.99                     | 0.77              |
| 25:W:88:THR:HG22 | 25:W:89:ASP:N     | 1.99                     | 0.77              |
| 1:0:346:U:H4'    | 37:0:6338:HOH:O   | 1.84                     | 0.77              |
| 13:K:74:VAL:HG13 | 13:K:113:ILE:HG23 | 1.67                     | 0.77              |
| 1:0:1182:C:H1'   | 1:0:1192:A:H8     | 1.47                     | 0.77              |
| 37:0:9208:HOH:O  | 4:B:254:GLN:HG3   | 1.85                     | 0.77              |
| 31:3:70:ARG:HG2  | 31:3:77:ALA:HB2   | 1.65                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:F:50:VAL:HG13  | 8:F:60:VAL:HG11   | 1.67                     | 0.76              |
| 30:2:39:ARG:HG2  | 37:2:3143:HOH:O   | 1.85                     | 0.76              |
| 1:0:2768:A:H2'   | 1:0:2769:C:O4'    | 1.85                     | 0.76              |
| 11:I:132:CYS:HB3 | 11:I:137:VAL:HB   | 1.67                     | 0.76              |
| 1:0:2291:A:C8    | 1:0:2309:C:H5'    | 2.20                     | 0.76              |
| 11:I:99:ASP:O    | 11:I:100:LEU:HD23 | 1.85                     | 0.76              |
| 1:0:1160:G:C5'   | 1:0:1161:A:H5'    | 2.10                     | 0.76              |
| 2:9:39:U:H1'     | 2:9:44:A:H61      | 1.51                     | 0.76              |
| 3:A:153:ARG:HB2  | 3:A:153:ARG:HH11  | 1.50                     | 0.76              |
| 8:F:96:ALA:HA    | 37:F:3111:HOH:O   | 1.83                     | 0.76              |
| 1:0:541:C:C2'    | 1:0:542:A:H5''    | 2.16                     | 0.76              |
| 37:0:4336:HOH:O  | 12:J:47:THR:HB    | 1.85                     | 0.76              |
| 1:0:1130:U:H5'   | 37:0:7165:HOH:O   | 1.86                     | 0.76              |
| 1:0:1751:G:C2'   | 1:0:1752:G:H5''   | 2.15                     | 0.76              |
| 20:R:9:ASP:O     | 20:R:13:THR:HB    | 1.86                     | 0.76              |
| 16:N:164:ASP:OD2 | 16:N:167:ASP:HA   | 1.87                     | 0.75              |
| 1:0:1166:A:H1'   | 1:0:1192:A:C2     | 2.21                     | 0.75              |
| 1:0:1634:G:H3'   | 37:0:3396:HOH:O   | 1.85                     | 0.75              |
| 7:E:84:MET:HE2   | 7:E:133:VAL:CG2   | 2.16                     | 0.75              |
| 2:9:56:A:C2'     | 2:9:57:A:H5''     | 2.16                     | 0.75              |
| 11:I:75:THR:HA   | 11:I:112:LYS:HZ1  | 1.51                     | 0.75              |
| 10:H:166:SER:CB  | 10:H:167:PRO:HD3  | 2.16                     | 0.75              |
| 17:O:47:ARG:HH11 | 17:O:47:ARG:HG3   | 1.50                     | 0.75              |
| 21:S:57:THR:HG22 | 21:S:59:ASP:N     | 2.01                     | 0.75              |
| 10:H:169:GLY:HA3 | 37:H:8391:HOH:O   | 1.86                     | 0.75              |
| 11:I:78:LEU:HD12 | 11:I:112:LYS:HE3  | 1.68                     | 0.75              |
| 11:I:113:HIS:N   | 11:I:114:PRO:HD2  | 2.01                     | 0.75              |
| 10:H:162:ARG:HD2 | 37:H:8383:HOH:O   | 1.86                     | 0.75              |
| 12:J:93:ARG:HB3  | 12:J:93:ARG:HH11  | 1.49                     | 0.75              |
| 18:P:115:SER:H   | 18:P:118:GLN:NE2  | 1.82                     | 0.75              |
| 37:0:9741:HOH:O  | 11:I:92:PRO:HD2   | 1.87                     | 0.74              |
| 7:E:20:ILE:HD11  | 7:E:40:VAL:HG11   | 1.68                     | 0.74              |
| 8:F:91:VAL:HG12  | 8:F:92:GLY:N      | 2.03                     | 0.74              |
| 12:J:74:ARG:HB3  | 12:J:74:ARG:HH11  | 1.50                     | 0.74              |
| 25:W:68:THR:HG23 | 25:W:69:ARG:HG2   | 1.70                     | 0.74              |
| 1:0:288:A:H61    | 1:0:364:C:H42     | 1.35                     | 0.74              |
| 4:B:320:GLN:HE21 | 4:B:321:PRO:HD2   | 1.52                     | 0.74              |
| 4:B:18:ARG:HG3   | 4:B:256:GLN:HG3   | 1.67                     | 0.74              |
| 27:Y:189:ASN:HA  | 27:Y:217:ILE:HD11 | 1.67                     | 0.74              |
| 1:0:2637:A:H5'   | 37:0:8785:HOH:O   | 1.87                     | 0.74              |
| 4:B:36:PRO:HA    | 4:B:168:GLY:HA3   | 1.70                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:57:THR:HG23   | 6:D:63:ILE:HA     | 1.70                     | 0.74              |
| 14:L:143:THR:HG22 | 14:L:144:ASP:N    | 2.03                     | 0.73              |
| 3:A:179:MET:HA    | 3:A:179:MET:HE3   | 1.68                     | 0.73              |
| 3:A:105:VAL:HG11  | 3:A:154:ALA:HB1   | 1.69                     | 0.73              |
| 3:A:131:HIS:O     | 3:A:132:ASP:HB2   | 1.88                     | 0.73              |
| 31:3:70:ARG:HD3   | 37:3:8538:HOH:O   | 1.86                     | 0.73              |
| 16:N:179:LEU:HD23 | 16:N:184:ILE:CD1  | 2.19                     | 0.73              |
| 1:0:2054:A:N3     | 20:R:128:ARG:NH2  | 2.37                     | 0.73              |
| 16:N:48:VAL:CG1   | 16:N:55:ASP:HB3   | 2.19                     | 0.73              |
| 1:0:1328:A:OP1    | 27:Y:169:ARG:HD2  | 1.88                     | 0.73              |
| 18:P:59:ARG:NH2   | 18:P:66:GLN:HE22  | 1.87                     | 0.73              |
| 25:W:65:VAL:HA    | 25:W:68:THR:HG22  | 1.71                     | 0.73              |
| 1:0:21:G:C5'      | 20:R:2:ILE:HA     | 2.18                     | 0.73              |
| 1:0:289:G:H22     | 1:0:363:A:H2      | 1.37                     | 0.73              |
| 18:P:115:SER:OG   | 18:P:118:GLN:HG3  | 1.88                     | 0.73              |
| 20:R:39:THR:HB    | 20:R:42:GLU:HG3   | 1.69                     | 0.73              |
| 1:0:2586:U:H3     | 1:0:2592:G:H22    | 1.34                     | 0.73              |
| 1:0:1666:C:H2'    | 1:0:1667:A:H5'    | 1.71                     | 0.73              |
| 37:0:5779:HOH:O   | 28:Z:49:ARG:HD2   | 1.87                     | 0.73              |
| 5:C:115:LEU:HD21  | 5:C:243:VAL:HG13  | 1.71                     | 0.73              |
| 27:Y:187:VAL:HG23 | 27:Y:192:ASP:CB   | 2.18                     | 0.73              |
| 4:B:221:GLN:HE22  | 13:K:42:ASN:HD22  | 1.37                     | 0.72              |
| 14:L:136:ALA:HB3  | 37:L:8573:HOH:O   | 1.88                     | 0.72              |
| 18:P:115:SER:N    | 18:P:118:GLN:HE21 | 1.84                     | 0.72              |
| 1:0:1594:C:OP2    | 18:P:120:ARG:HD2  | 1.88                     | 0.72              |
| 30:2:41:HIS:N     | 30:2:45:ASN:HD22  | 1.87                     | 0.72              |
| 1:0:1118:A:C8     | 1:0:1118:A:H3'    | 2.24                     | 0.72              |
| 25:W:137:GLN:HE21 | 25:W:141:HIS:CE1  | 2.02                     | 0.72              |
| 1:0:281:U:H2'     | 1:0:282:C:O4'     | 1.90                     | 0.72              |
| 12:J:19:MET:HE2   | 12:J:79:PHE:HA    | 1.70                     | 0.72              |
| 1:0:272:A:H3'     | 37:0:7018:HOH:O   | 1.88                     | 0.72              |
| 4:B:162:MET:HE2   | 4:B:310:ARG:CD    | 2.19                     | 0.72              |
| 6:D:146:LYS:NZ    | 16:N:107:ASN:HD21 | 1.87                     | 0.72              |
| 1:0:657:G:OP1     | 5:C:27:ARG:NH2    | 2.20                     | 0.72              |
| 3:A:199:HIS:CD2   | 3:A:201:PHE:H     | 2.07                     | 0.72              |
| 14:L:148:GLU:HA   | 37:L:8572:HOH:O   | 1.90                     | 0.72              |
| 22:T:9:LYS:HE3    | 22:T:13:ARG:NH1   | 2.05                     | 0.72              |
| 1:0:1118:A:H3'    | 1:0:1118:A:H8     | 1.54                     | 0.71              |
| 1:0:871:G:C8      | 1:0:871:G:C5'     | 2.70                     | 0.71              |
| 1:0:1351:G:OP1    | 5:C:96:LYS:NZ     | 2.23                     | 0.71              |
| 17:O:14:LEU:HD23  | 17:O:102:ILE:HD11 | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:V:39:ALA:N     | 24:V:40:PRO:HD2   | 2.05                     | 0.71              |
| 1:0:1116:U:O2'    | 1:0:1118:A:H2     | 1.67                     | 0.71              |
| 37:0:6942:HOH:O   | 4:B:211:THR:HG21  | 1.90                     | 0.71              |
| 5:C:242:GLU:HG3   | 37:C:8381:HOH:O   | 1.89                     | 0.71              |
| 15:M:164:THR:HG22 | 15:M:167:GLY:N    | 2.03                     | 0.71              |
| 20:R:39:THR:HG22  | 20:R:42:GLU:H     | 1.56                     | 0.71              |
| 1:0:1450:C:H4'    | 1:0:1451:C:OP2    | 1.89                     | 0.71              |
| 1:0:1559:A:H1'    | 37:0:5365:HOH:O   | 1.91                     | 0.71              |
| 2:9:6:C:OP1       | 16:N:37:ARG:NH1   | 2.24                     | 0.71              |
| 4:B:51:VAL:CG2    | 4:B:327:VAL:HG13  | 2.21                     | 0.71              |
| 22:T:41:ARG:HG2   | 22:T:41:ARG:HH11  | 1.55                     | 0.71              |
| 28:Z:46:ARG:HD2   | 28:Z:59:TYR:HB2   | 1.72                     | 0.71              |
| 10:H:20:ILE:HG23  | 10:H:120:ILE:HD11 | 1.73                     | 0.70              |
| 12:J:45:VAL:HG23  | 12:J:130:VAL:O    | 1.90                     | 0.70              |
| 13:K:62:PRO:HG3   | 13:K:65:ARG:HH21  | 1.56                     | 0.70              |
| 20:R:99:ALA:CB    | 20:R:109:MET:HE1  | 2.16                     | 0.70              |
| 1:0:1119:G:H8     | 12:J:52:GLN:HE22  | 1.38                     | 0.70              |
| 1:0:1163:G:H5'    | 11:I:115:ASP:O    | 1.92                     | 0.70              |
| 5:C:246:ARG:NE    | 37:C:8423:HOH:O   | 2.23                     | 0.70              |
| 6:D:88:LEU:HB2    | 6:D:89:PRO:HD3    | 1.74                     | 0.70              |
| 9:G:12:ILE:N      | 9:G:13:PRO:HD3    | 2.06                     | 0.70              |
| 1:0:236:A:H4'     | 1:0:237:G:H5'     | 1.74                     | 0.70              |
| 25:W:21:LEU:HD22  | 25:W:26:ILE:CD1   | 2.22                     | 0.70              |
| 1:0:282:C:H1'     | 1:0:368:C:N4      | 2.07                     | 0.70              |
| 1:0:2896:A:H5''   | 37:0:5599:HOH:O   | 1.90                     | 0.70              |
| 8:F:50:VAL:CG1    | 8:F:60:VAL:HG11   | 2.21                     | 0.70              |
| 1:0:284:C:H4'     | 1:0:285:A:O5'     | 1.92                     | 0.70              |
| 1:0:877:G:H5'     | 1:0:878:G:OP1     | 1.90                     | 0.70              |
| 1:0:1119:G:N2     | 1:0:1246:A:C2     | 2.57                     | 0.70              |
| 4:B:71:VAL:HG11   | 4:B:296:LEU:HB3   | 1.73                     | 0.70              |
| 11:I:106:LYS:O    | 11:I:110:GLU:HG3  | 1.91                     | 0.70              |
| 11:I:110:GLU:HA   | 11:I:113:HIS:CE1  | 2.26                     | 0.70              |
| 20:R:18:LEU:HD12  | 20:R:143:VAL:HG11 | 1.72                     | 0.70              |
| 10:H:146:VAL:HG13 | 37:H:8379:HOH:O   | 1.92                     | 0.70              |
| 23:U:14:GLU:O     | 23:U:17:THR:HB    | 1.92                     | 0.70              |
| 1:0:2908:A:H2'    | 1:0:2909:G:O4'    | 1.92                     | 0.69              |
| 2:9:49:G:H5''     | 37:9:8464:HOH:O   | 1.92                     | 0.69              |
| 37:C:8357:HOH:O   | 17:O:3:THR:HG21   | 1.91                     | 0.69              |
| 12:J:107:ASN:ND2  | 12:J:109:TYR:H    | 1.89                     | 0.69              |
| 4:B:190:MET:HE2   | 4:B:194:PHE:HD1   | 1.55                     | 0.69              |
| 1:0:2426:G:H1'    | 37:0:5592:HOH:O   | 1.91                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:9:29:C:H2'      | 2:9:30:C:H5'      | 1.75                     | 0.69              |
| 3:A:105:VAL:CG1   | 3:A:154:ALA:HB1   | 2.22                     | 0.69              |
| 15:M:99:ARG:HH21  | 15:M:170:ASN:HD22 | 1.39                     | 0.69              |
| 4:B:103:ASP:HB2   | 37:B:8597:HOH:O   | 1.92                     | 0.69              |
| 30:2:18:ASN:HD21  | 30:2:40:ARG:H     | 1.41                     | 0.69              |
| 1:0:396:U:H1'     | 37:0:7121:HOH:O   | 1.93                     | 0.69              |
| 1:0:1505:U:H6     | 1:0:1505:U:H5'    | 1.57                     | 0.69              |
| 37:9:8464:HOH:O   | 16:N:147:ILE:HB   | 1.92                     | 0.69              |
| 3:A:81:GLN:HB2    | 3:A:92:ASN:ND2    | 2.07                     | 0.69              |
| 5:C:162:VAL:HG12  | 5:C:192:ILE:HD11  | 1.73                     | 0.69              |
| 7:E:68:HIS:O      | 7:E:72:MET:HG3    | 1.93                     | 0.69              |
| 12:J:19:MET:HE1   | 12:J:78:ILE:HG22  | 1.75                     | 0.69              |
| 20:R:111:ILE:HG23 | 20:R:145:LEU:HD11 | 1.74                     | 0.69              |
| 31:3:65:THR:HG23  | 31:3:67:LEU:HG    | 1.74                     | 0.69              |
| 4:B:16:ARG:NH1    | 37:B:8621:HOH:O   | 2.25                     | 0.69              |
| 5:C:1:MET:HG2     | 5:C:2:GLN:H       | 1.56                     | 0.69              |
| 24:V:12:THR:CG2   | 24:V:15:GLU:HG3   | 2.20                     | 0.69              |
| 1:0:182:G:H5'     | 37:0:4653:HOH:O   | 1.93                     | 0.69              |
| 3:A:190:ARG:NH2   | 3:A:207:GLN:OE1   | 2.26                     | 0.69              |
| 13:K:74:VAL:CG1   | 13:K:113:ILE:HG12 | 2.23                     | 0.69              |
| 1:0:2468:A:H61    | 31:3:48:ASN:HD21  | 1.38                     | 0.68              |
| 4:B:264:GLU:HG2   | 4:B:267:LYS:CE    | 2.23                     | 0.68              |
| 1:0:1701:A:H4'    | 1:0:1702:U:C5'    | 2.23                     | 0.68              |
| 5:C:236:THR:H     | 5:C:239:ALA:HB3   | 1.59                     | 0.68              |
| 6:D:64:ARG:HG2    | 6:D:67:ASP:HB3    | 1.76                     | 0.68              |
| 5:C:140:VAL:HB    | 37:C:8450:HOH:O   | 1.93                     | 0.68              |
| 25:W:13:MET:CE    | 25:W:17:ILE:HG22  | 2.23                     | 0.68              |
| 5:C:139:VAL:HG13  | 37:C:8447:HOH:O   | 1.93                     | 0.68              |
| 16:N:80:SER:HB2   | 37:N:8534:HOH:O   | 1.92                     | 0.68              |
| 1:0:542:A:H5'     | 1:0:542:A:C8      | 2.26                     | 0.68              |
| 1:0:1973:A:H5'    | 1:0:1973:A:H8     | 1.59                     | 0.68              |
| 1:0:1165:G:H4'    | 1:0:1174:A:O2'    | 1.93                     | 0.68              |
| 1:0:1474:C:H5'    | 1:0:1474:C:C6     | 2.29                     | 0.68              |
| 1:0:2878:U:H2'    | 1:0:2879:A:O4'    | 1.94                     | 0.68              |
| 3:A:210:GLY:HA3   | 37:A:8589:HOH:O   | 1.93                     | 0.68              |
| 4:B:141:ARG:HD2   | 4:B:163:GLU:OE2   | 1.94                     | 0.68              |
| 6:D:54:ALA:CB     | 6:D:69:ILE:HD12   | 2.23                     | 0.68              |
| 31:3:73:GLU:HB3   | 37:3:8559:HOH:O   | 1.93                     | 0.68              |
| 1:0:2840:A:OP1    | 4:B:211:THR:HG23  | 1.94                     | 0.68              |
| 1:0:20:G:H21      | 20:R:117:HIS:HD2  | 1.43                     | 0.67              |
| 3:A:192:VAL:HG13  | 37:A:8558:HOH:O   | 1.92                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:X:76:ARG:HH11  | 26:X:76:ARG:HG3  | 1.59                     | 0.67              |
| 1:O:962:C:H1'     | 16:N:5:ARG:HH12  | 1.58                     | 0.67              |
| 4:B:185:GLY:HA2   | 37:B:8639:HOH:O  | 1.93                     | 0.67              |
| 10:H:9:ILE:HD12   | 10:H:54:THR:HG22 | 1.77                     | 0.67              |
| 12:J:107:ASN:HD21 | 12:J:109:TYR:HB2 | 1.60                     | 0.67              |
| 14:L:72:ASN:HB2   | 37:L:8583:HOH:O  | 1.93                     | 0.67              |
| 25:W:149:LEU:CG   | 25:W:153:MET:HE2 | 2.23                     | 0.67              |
| 29:1:25:LYS:HE2   | 37:2:7213:HOH:O  | 1.93                     | 0.67              |
| 6:D:135:VAL:HG22  | 6:D:136:ARG:H    | 1.59                     | 0.67              |
| 7:E:100:ASP:HB2   | 37:E:2789:HOH:O  | 1.94                     | 0.67              |
| 5:C:115:LEU:O     | 5:C:118:THR:HB   | 1.95                     | 0.67              |
| 7:E:7:ILE:HD11    | 7:E:11:VAL:C     | 2.19                     | 0.67              |
| 12:J:74:ARG:HH11  | 12:J:74:ARG:CB   | 2.07                     | 0.67              |
| 22:T:47:THR:HB    | 22:T:100:ASP:HB3 | 1.77                     | 0.67              |
| 27:Y:141:THR:HG23 | 37:Y:8589:HOH:O  | 1.93                     | 0.67              |
| 30:2:41:HIS:H     | 30:2:45:ASN:ND2  | 1.92                     | 0.67              |
| 1:O:1329:A:H2     | 37:O:4183:HOH:O  | 1.76                     | 0.67              |
| 2:9:51:A:H5'      | 16:N:160:SER:HB3 | 1.77                     | 0.67              |
| 1:O:541:C:H2'     | 1:O:542:A:C5'    | 2.25                     | 0.67              |
| 1:O:1377:C:H5'    | 1:O:1377:C:H6    | 1.60                     | 0.67              |
| 4:B:62:ARG:HA     | 4:B:65:MET:CE    | 2.24                     | 0.67              |
| 4:B:74:ILE:HD13   | 4:B:309:VAL:HG21 | 1.76                     | 0.67              |
| 13:K:34:VAL:HG22  | 13:K:47:ALA:HB2  | 1.76                     | 0.67              |
| 1:O:1080:C:H4'    | 1:O:1081:A:OP1   | 1.94                     | 0.67              |
| 15:M:169:ARG:HD2  | 37:M:8590:HOH:O  | 1.95                     | 0.67              |
| 30:2:22:PRO:HG2   | 30:2:25:VAL:CG2  | 2.25                     | 0.67              |
| 1:O:1206:U:H5'    | 1:O:1206:U:H6    | 1.58                     | 0.67              |
| 2:9:14:G:H5'      | 2:9:14:G:C8      | 2.28                     | 0.67              |
| 8:F:63:ILE:HB     | 8:F:64:PRO:HD3   | 1.76                     | 0.67              |
| 10:H:3:ALA:HA     | 10:H:58:ARG:NH1  | 2.10                     | 0.66              |
| 1:O:2346:C:O2'    | 6:D:52:THR:HG21  | 1.94                     | 0.66              |
| 25:W:21:LEU:HD21  | 25:W:48:VAL:HG11 | 1.76                     | 0.66              |
| 8:F:39:SER:HB3    | 8:F:45:ALA:HB2   | 1.76                     | 0.66              |
| 8:F:58:GLU:OE1    | 15:M:27:ARG:NH2  | 2.24                     | 0.66              |
| 1:O:2508:C:H2'    | 37:O:6248:HOH:O  | 1.95                     | 0.66              |
| 8:F:99:THR:HA     | 37:F:3461:HOH:O  | 1.95                     | 0.66              |
| 15:M:80:GLY:O     | 15:M:81:ARG:HD3  | 1.95                     | 0.66              |
| 25:W:6:GLN:HB2    | 25:W:26:ILE:CD1  | 2.26                     | 0.66              |
| 22:T:53:GLY:HA3   | 37:T:6384:HOH:O  | 1.94                     | 0.66              |
| 1:O:31:C:H2'      | 37:O:7180:HOH:O  | 1.96                     | 0.66              |
| 1:O:1701:A:H5''   | 1:O:1702:U:H3'   | 1.78                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:307:ARG:HH11  | 4:B:307:ARG:HB2  | 1.61                     | 0.66              |
| 5:C:104:ASP:HA    | 5:C:107:ARG:HH12 | 1.60                     | 0.66              |
| 1:O:1118:A:H62    | 1:O:1244:U:H3    | 1.44                     | 0.66              |
| 1:O:2533:C:H5'    | 1:O:2533:C:H6    | 1.61                     | 0.66              |
| 7:E:69:ILE:HA     | 7:E:72:MET:HE2   | 1.78                     | 0.66              |
| 10:H:59:HIS:HA    | 10:H:62:LEU:HD23 | 1.78                     | 0.66              |
| 22:T:61:GLU:HG3   | 37:T:3851:HOH:O  | 1.93                     | 0.66              |
| 25:W:122:ARG:NH2  | 25:W:154:ARG:OXT | 2.28                     | 0.66              |
| 1:O:299:U:H5'     | 37:O:6826:HOH:O  | 1.96                     | 0.65              |
| 1:O:1603:A:H5'    | 1:O:1605:G:O4'   | 1.96                     | 0.65              |
| 1:O:2635:A:O2'    | 1:O:2636:C:H5'   | 1.97                     | 0.65              |
| 2:9:6:C:C5'       | 16:N:37:ARG:NH1  | 2.57                     | 0.65              |
| 2:9:39:U:H1'      | 2:9:44:A:N6      | 2.11                     | 0.65              |
| 9:G:23:ILE:HD13   | 9:G:67:LEU:HD23  | 1.76                     | 0.65              |
| 10:H:9:ILE:O      | 10:H:9:ILE:HG22  | 1.95                     | 0.65              |
| 24:V:39:ALA:C     | 24:V:41:GLU:H    | 2.04                     | 0.65              |
| 13:K:81:ARG:HD3   | 13:K:87:ARG:NH1  | 2.10                     | 0.65              |
| 14:L:68:GLU:HA    | 37:L:8542:HOH:O  | 1.97                     | 0.65              |
| 23:U:20:MET:HE2   | 23:U:30:HIS:NE2  | 2.11                     | 0.65              |
| 1:O:1058:A:H2'    | 1:O:1060:C:H5''  | 1.77                     | 0.65              |
| 1:O:1766:U:O2     | 1:O:1778:A:H5'   | 1.96                     | 0.65              |
| 14:L:67:ARG:O     | 14:L:71:GLU:HG3  | 1.96                     | 0.65              |
| 1:O:259:G:H21     | 15:M:58:GLN:NE2  | 1.95                     | 0.65              |
| 1:O:1172:G:H1'    | 37:O:4474:HOH:O  | 1.96                     | 0.65              |
| 1:O:1778:A:H2'    | 1:O:1779:A:H5'   | 1.78                     | 0.65              |
| 25:W:4:LEU:O      | 25:W:32:CYS:HA   | 1.97                     | 0.65              |
| 26:X:21:PRO:HG2   | 26:X:24:LYS:HD3  | 1.78                     | 0.65              |
| 1:O:1819:G:H2'    | 1:O:1820:G:H4'   | 1.78                     | 0.65              |
| 1:O:2748:G:H2'    | 37:O:7030:HOH:O  | 1.96                     | 0.65              |
| 1:O:2756:U:H3     | 1:O:2896:A:H2    | 1.39                     | 0.65              |
| 26:X:71:ARG:HB3   | 26:X:88:GLU:OE1  | 1.96                     | 0.65              |
| 5:C:27:ARG:HG3    | 5:C:29:ASP:OD1   | 1.97                     | 0.65              |
| 7:E:3:VAL:HG22    | 7:E:49:ILE:HB    | 1.78                     | 0.65              |
| 17:O:32:ARG:O     | 17:O:32:ARG:HD3  | 1.95                     | 0.65              |
| 27:Y:133:HIS:HD2  | 37:Y:8582:HOH:O  | 1.78                     | 0.65              |
| 1:O:2676:C:H4'    | 12:J:70:PHE:CE1  | 2.32                     | 0.65              |
| 7:E:23:GLU:HG2    | 7:E:28:SER:HB3   | 1.79                     | 0.65              |
| 7:E:132:THR:HB    | 37:E:2227:HOH:O  | 1.97                     | 0.65              |
| 8:F:53:ASP:OD1    | 8:F:80:GLN:HB2   | 1.97                     | 0.65              |
| 25:W:122:ARG:HH11 | 25:W:122:ARG:CG  | 2.09                     | 0.65              |
| 26:X:15:ARG:HB3   | 26:X:15:ARG:HH11 | 1.62                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:2:22:PRO:HG2  | 30:2:25:VAL:HG23  | 1.79                     | 0.65              |
| 1:0:474:C:O3'    | 5:C:73:LEU:HD21   | 1.96                     | 0.65              |
| 1:0:1730:G:H5'   | 1:0:1731:C:C5     | 2.32                     | 0.65              |
| 3:A:55:VAL:HG22  | 3:A:68:ILE:O      | 1.97                     | 0.65              |
| 10:H:47:ILE:HD12 | 37:H:8379:HOH:O   | 1.97                     | 0.65              |
| 1:0:558:C:O2'    | 1:0:559:U:H5''    | 1.97                     | 0.65              |
| 6:D:25:MET:CE    | 6:D:37:ALA:HB1    | 2.27                     | 0.65              |
| 11:I:72:VAL:HG13 | 11:I:73:PRO:HD2   | 1.79                     | 0.65              |
| 4:B:125:GLU:O    | 4:B:129:ARG:HG3   | 1.97                     | 0.64              |
| 1:0:1684:A:H1'   | 30:2:43:ARG:HH22  | 1.62                     | 0.64              |
| 4:B:51:VAL:HG23  | 4:B:329:TYR:O     | 1.96                     | 0.64              |
| 7:E:69:ILE:HA    | 7:E:72:MET:CE     | 2.28                     | 0.64              |
| 13:K:22:ASP:HB2  | 37:K:5264:HOH:O   | 1.96                     | 0.64              |
| 16:N:37:ARG:NE   | 37:N:8532:HOH:O   | 2.30                     | 0.64              |
| 1:0:553:G:P      | 27:Y:204:ARG:HH22 | 2.20                     | 0.64              |
| 18:P:18:LYS:O    | 18:P:21:VAL:HG22  | 1.97                     | 0.64              |
| 1:0:69:A:H5'     | 1:0:69:A:C8       | 2.33                     | 0.64              |
| 1:0:2827:A:H2'   | 1:0:2828:G:O4'    | 1.97                     | 0.64              |
| 7:E:93:MET:HE1   | 7:E:165:GLY:N     | 2.12                     | 0.64              |
| 10:H:9:ILE:HG23  | 10:H:126:ARG:CZ   | 2.28                     | 0.64              |
| 18:P:10:ALA:HA   | 18:P:13:VAL:HG12  | 1.78                     | 0.64              |
| 1:0:1209:C:H2'   | 1:0:1210:G:H8     | 1.61                     | 0.64              |
| 5:C:107:ARG:NE   | 37:C:8457:HOH:O   | 2.22                     | 0.64              |
| 7:E:11:VAL:HG12  | 7:E:12:ASP:N      | 2.11                     | 0.64              |
| 7:E:101:GLU:HB2  | 7:E:116:THR:O     | 1.98                     | 0.64              |
| 7:E:84:MET:HE1   | 7:E:148:ILE:HD12  | 1.80                     | 0.64              |
| 20:R:39:THR:HG23 | 20:R:107:GLU:O    | 1.98                     | 0.64              |
| 25:W:21:LEU:HB3  | 25:W:26:ILE:HG12  | 1.80                     | 0.64              |
| 1:0:603:A:H5''   | 1:0:604:G:OP1     | 1.97                     | 0.64              |
| 1:0:1120:U:H5''  | 1:0:1120:U:C6     | 2.33                     | 0.64              |
| 1:0:1666:C:O2'   | 1:0:1667:A:H5''   | 1.98                     | 0.64              |
| 2:9:13:A:O2'     | 2:9:14:G:H5''     | 1.97                     | 0.64              |
| 26:X:72:VAL:HG22 | 26:X:85:VAL:HG12  | 1.78                     | 0.64              |
| 6:D:65:GLU:HG3   | 37:D:6752:HOH:O   | 1.96                     | 0.64              |
| 22:T:9:LYS:HE3   | 22:T:13:ARG:HH11  | 1.63                     | 0.64              |
| 1:0:544:G:C2'    | 1:0:545:G:H5''    | 2.27                     | 0.64              |
| 1:0:2505:G:O2'   | 1:0:2506:A:H5'    | 1.98                     | 0.64              |
| 1:0:558:C:C2'    | 1:0:559:U:H5''    | 2.28                     | 0.63              |
| 3:A:33:GLU:O     | 3:A:34:ASP:HB2    | 1.97                     | 0.63              |
| 4:B:36:PRO:HA    | 4:B:168:GLY:CA    | 2.28                     | 0.63              |
| 6:D:64:ARG:CD    | 6:D:67:ASP:HB3    | 2.28                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:99:ASP:HB3    | 6:D:103:ASN:H     | 1.63                     | 0.63              |
| 16:N:73:ALA:HB2   | 16:N:163:PHE:CZ   | 2.33                     | 0.63              |
| 17:O:14:LEU:CD2   | 17:O:102:ILE:HD11 | 2.27                     | 0.63              |
| 4:B:62:ARG:CA     | 4:B:65:MET:HE3    | 2.26                     | 0.63              |
| 4:B:248:ARG:O     | 4:B:251:VAL:HG13  | 1.98                     | 0.63              |
| 1:O:902:G:N7      | 14:L:18:HIS:HD2   | 1.97                     | 0.63              |
| 1:O:2783:A:H3'    | 37:O:4728:HOH:O   | 1.97                     | 0.63              |
| 2:9:69:U:OP1      | 16:N:4:PRO:HG3    | 1.99                     | 0.63              |
| 6:D:44:ILE:HG23   | 6:D:45:THR:HG23   | 1.81                     | 0.63              |
| 24:V:64:GLY:O     | 24:V:65:ASP:HB2   | 1.97                     | 0.63              |
| 25:W:21:LEU:HD21  | 25:W:48:VAL:CG1   | 2.28                     | 0.63              |
| 37:O:6896:HOH:O   | 22:T:2:LYS:HE2    | 1.99                     | 0.63              |
| 4:B:175:LEU:C     | 4:B:175:LEU:HD23  | 2.24                     | 0.63              |
| 4:B:307:ARG:HH11  | 4:B:307:ARG:CG    | 2.11                     | 0.63              |
| 1:O:1008:C:H5''   | 10:H:16:ARG:HH12  | 1.63                     | 0.63              |
| 37:O:3483:HOH:O   | 31:3:57:GLY:HA2   | 1.98                     | 0.63              |
| 1:O:2414:A:H2'    | 1:O:2415:A:C8     | 2.33                     | 0.63              |
| 17:O:87:THR:O     | 17:O:91:GLN:HG3   | 1.99                     | 0.63              |
| 25:W:38:THR:HG22  | 37:W:3580:HOH:O   | 1.99                     | 0.63              |
| 6:D:55:LYS:O      | 6:D:56:ARG:HB2    | 1.98                     | 0.63              |
| 27:Y:235:GLU:CD   | 27:Y:235:GLU:H    | 2.06                     | 0.63              |
| 7:E:15:GLN:HG2    | 7:E:19:ASP:O      | 1.97                     | 0.62              |
| 23:U:46:ALA:HB1   | 23:U:52:THR:HG21  | 1.81                     | 0.62              |
| 27:Y:220:GLU:HG2  | 37:Y:8549:HOH:O   | 1.98                     | 0.62              |
| 4:B:55:ASN:HB3    | 4:B:63:GLU:HA     | 1.80                     | 0.62              |
| 11:I:78:LEU:HD12  | 11:I:112:LYS:CE   | 2.29                     | 0.62              |
| 20:R:111:ILE:HG23 | 20:R:145:LEU:CD1  | 2.29                     | 0.62              |
| 37:9:8438:HOH:O   | 16:N:41:LYS:HD3   | 1.99                     | 0.62              |
| 5:C:162:VAL:HG13  | 5:C:232:LEU:HD21  | 1.81                     | 0.62              |
| 1:O:2694:A:H4'    | 7:E:91:PHE:CE1    | 2.33                     | 0.62              |
| 9:G:23:ILE:O      | 9:G:27:ILE:HG13   | 2.00                     | 0.62              |
| 16:N:86:LEU:HD12  | 16:N:125:ALA:HB2  | 1.81                     | 0.62              |
| 20:R:44:VAL:O     | 20:R:48:GLU:HG3   | 1.99                     | 0.62              |
| 24:V:44:GLY:O     | 24:V:48:GLU:HG2   | 2.00                     | 0.62              |
| 3:A:153:ARG:HH11  | 3:A:153:ARG:CB    | 2.11                     | 0.62              |
| 10:H:3:ALA:HA     | 10:H:58:ARG:HH12  | 1.64                     | 0.62              |
| 10:H:170:ASN:HD22 | 10:H:170:ASN:N    | 1.96                     | 0.62              |
| 11:I:108:ILE:HG21 | 11:I:128:VAL:HG11 | 1.82                     | 0.62              |
| 1:O:417:G:P       | 37:O:6908:HOH:O   | 2.57                     | 0.62              |
| 1:O:1835:U:C5     | 1:O:1840:A:N7     | 2.61                     | 0.62              |
| 1:O:2547:C:OP2    | 4:B:5:ARG:NH1     | 2.33                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2570:G:H5''   | 37:0:4412:HOH:O   | 2.00                     | 0.62              |
| 37:0:6519:HOH:O   | 3:A:211:LYS:HG2   | 1.99                     | 0.62              |
| 4:B:7:ARG:HH11    | 4:B:7:ARG:CG      | 2.10                     | 0.62              |
| 4:B:162:MET:HG3   | 4:B:310:ARG:CZ    | 2.30                     | 0.62              |
| 14:L:143:THR:HG22 | 14:L:144:ASP:H    | 1.65                     | 0.62              |
| 27:Y:144:ARG:NH1  | 37:Y:8576:HOH:O   | 2.33                     | 0.62              |
| 29:1:17:THR:HG22  | 30:2:49:GLU:OXT   | 1.99                     | 0.62              |
| 3:A:194:MET:HE3   | 3:A:199:HIS:CB    | 2.30                     | 0.62              |
| 5:C:78:ARG:HG3    | 5:C:78:ARG:NH1    | 2.14                     | 0.62              |
| 20:R:39:THR:HB    | 20:R:42:GLU:CG    | 2.29                     | 0.62              |
| 23:U:9:CYS:HA     | 23:U:52:THR:HG23  | 1.80                     | 0.62              |
| 8:F:117:GLU:C     | 8:F:119:ARG:H     | 2.08                     | 0.62              |
| 1:0:1189:A:H3'    | 37:0:7173:HOH:O   | 1.99                     | 0.62              |
| 1:0:2769:C:H2'    | 1:0:2770:G:O4'    | 2.00                     | 0.62              |
| 4:B:238:ASN:HD22  | 4:B:240:GLY:N     | 1.97                     | 0.62              |
| 13:K:55:VAL:HG12  | 13:K:56:SER:N     | 2.15                     | 0.62              |
| 21:S:43:GLU:HB3   | 37:S:8342:HOH:O   | 1.99                     | 0.62              |
| 1:0:2830:U:H3'    | 37:0:4724:HOH:O   | 2.00                     | 0.62              |
| 8:F:101:ALA:HB3   | 8:F:105:ASP:OD1   | 2.00                     | 0.62              |
| 16:N:23:ARG:NH1   | 37:N:8545:HOH:O   | 2.33                     | 0.62              |
| 3:A:96:LEU:HD22   | 3:A:128:LEU:HD13  | 1.80                     | 0.61              |
| 1:0:282:C:O2'     | 1:0:283:U:H5'     | 2.00                     | 0.61              |
| 7:E:84:MET:HE1    | 7:E:148:ILE:CD1   | 2.29                     | 0.61              |
| 13:K:62:PRO:HG3   | 13:K:65:ARG:NH2   | 2.15                     | 0.61              |
| 20:R:18:LEU:HB2   | 20:R:143:VAL:CG1  | 2.30                     | 0.61              |
| 3:A:125:ASN:HB3   | 3:A:158:VAL:HG12  | 1.81                     | 0.61              |
| 5:C:237:GLU:HB2   | 37:C:8429:HOH:O   | 2.00                     | 0.61              |
| 10:H:27:LYS:N     | 10:H:59:HIS:HD2   | 1.98                     | 0.61              |
| 25:W:5:VAL:HG11   | 25:W:153:MET:HE1  | 1.83                     | 0.61              |
| 28:Z:11:SER:HB3   | 28:Z:23:ARG:HB2   | 1.81                     | 0.61              |
| 1:0:69:A:H5'      | 1:0:69:A:H8       | 1.65                     | 0.61              |
| 3:A:69:LEU:HD21   | 3:A:120:ARG:HB3   | 1.82                     | 0.61              |
| 7:E:6:GLU:HA      | 7:E:46:THR:HG22   | 1.83                     | 0.61              |
| 15:M:99:ARG:HH21  | 15:M:170:ASN:ND2  | 1.98                     | 0.61              |
| 22:T:32:ARG:NH1   | 22:T:38:ARG:HH12  | 1.98                     | 0.61              |
| 1:0:2346:C:H6     | 1:0:2346:C:O5'    | 1.83                     | 0.61              |
| 6:D:23:VAL:HG23   | 6:D:23:VAL:O      | 2.01                     | 0.61              |
| 7:E:20:ILE:CD1    | 7:E:40:VAL:HG11   | 2.30                     | 0.61              |
| 11:I:134:SER:O    | 11:I:135:LEU:HD23 | 2.01                     | 0.61              |
| 16:N:12:ARG:HD3   | 16:N:18:THR:OG1   | 2.00                     | 0.61              |
| 20:R:99:ALA:HB1   | 20:R:109:MET:CE   | 2.19                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:Y:144:ARG:CZ   | 37:Y:8612:HOH:O   | 2.47                     | 0.61              |
| 1:O:1189:A:O2'    | 1:O:1208:C:H2'    | 2.01                     | 0.61              |
| 12:J:131:THR:HG22 | 12:J:134:GLU:H    | 1.64                     | 0.61              |
| 16:N:64:SER:C     | 16:N:66:LEU:H     | 2.09                     | 0.61              |
| 24:V:8:ILE:HA     | 24:V:11:MET:HE3   | 1.83                     | 0.61              |
| 31:3:25:VAL:HG22  | 31:3:68:LYS:HG3   | 1.82                     | 0.61              |
| 1:O:470:U:O2'     | 29:1:16:HIS:HD2   | 1.82                     | 0.61              |
| 1:O:2851:G:O2'    | 1:O:2852:A:H5'    | 2.00                     | 0.61              |
| 5:C:76:ARG:HD3    | 37:C:8366:HOH:O   | 1.99                     | 0.61              |
| 27:Y:186:ARG:HG2  | 27:Y:186:ARG:HH11 | 1.66                     | 0.61              |
| 1:O:545:G:H5'     | 1:O:545:G:C8      | 2.32                     | 0.61              |
| 5:C:16:VAL:HG12   | 5:C:17:ASP:N      | 2.16                     | 0.61              |
| 12:J:103:VAL:HG12 | 37:J:5907:HOH:O   | 2.00                     | 0.61              |
| 28:Z:30:GLU:HA    | 28:Z:33:MET:HE3   | 1.81                     | 0.61              |
| 1:O:1189:A:H1'    | 1:O:1209:C:O4'    | 2.00                     | 0.61              |
| 6:D:146:LYS:HZ3   | 16:N:107:ASN:HD21 | 1.48                     | 0.61              |
| 2:9:48:C:H4'      | 16:N:141:ARG:HH21 | 1.66                     | 0.61              |
| 6:D:99:ASP:CB     | 6:D:103:ASN:H     | 2.14                     | 0.61              |
| 7:E:81:GLU:HG2    | 7:E:134:SER:CB    | 2.31                     | 0.61              |
| 13:K:75:ARG:CZ    | 37:K:4172:HOH:O   | 2.48                     | 0.61              |
| 26:X:75:ALA:O     | 26:X:83:ALA:HA    | 2.00                     | 0.61              |
| 1:O:1159:G:H21    | 1:O:1189:A:H8     | 1.48                     | 0.60              |
| 8:F:107:ASP:O     | 8:F:111:ILE:HG13  | 2.00                     | 0.60              |
| 1:O:338:C:H4'     | 5:C:174:ILE:CD1   | 2.31                     | 0.60              |
| 6:D:166:ILE:HD12  | 37:D:6326:HOH:O   | 2.01                     | 0.60              |
| 8:F:58:GLU:HG3    | 8:F:61:MET:HE2    | 1.83                     | 0.60              |
| 11:I:105:VAL:HG11 | 11:I:129:VAL:HG23 | 1.83                     | 0.60              |
| 16:N:179:LEU:HD23 | 16:N:184:ILE:HD12 | 1.84                     | 0.60              |
| 1:O:1528:A:H2'    | 1:O:1529:G:O4'    | 2.01                     | 0.60              |
| 1:O:1667:A:H5'    | 1:O:1667:A:C8     | 2.34                     | 0.60              |
| 1:O:1862:C:H1'    | 37:O:6711:HOH:O   | 2.00                     | 0.60              |
| 1:O:2638:G:H5'    | 37:O:4429:HOH:O   | 2.00                     | 0.60              |
| 6:D:149:ARG:NH1   | 37:D:3066:HOH:O   | 2.24                     | 0.60              |
| 16:N:47:LEU:HD12  | 16:N:92:ALA:HB1   | 1.84                     | 0.60              |
| 27:Y:185:VAL:HG12 | 37:Y:8570:HOH:O   | 2.01                     | 0.60              |
| 27:Y:187:VAL:HB   | 37:Y:8570:HOH:O   | 2.01                     | 0.60              |
| 1:O:1741:U:H5'    | 1:O:1742:A:OP1    | 2.02                     | 0.60              |
| 3:A:194:MET:HE3   | 3:A:199:HIS:HB2   | 1.83                     | 0.60              |
| 12:J:75:PRO:HG2   | 12:J:105:LEU:CD2  | 2.31                     | 0.60              |
| 25:W:4:LEU:HD22   | 25:W:52:VAL:CG2   | 2.29                     | 0.60              |
| 26:X:74:ALA:CB    | 26:X:85:VAL:HG22  | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1120:U:H5''   | 1:0:1120:U:H6     | 1.67                     | 0.60              |
| 4:B:307:ARG:HH11  | 4:B:307:ARG:CB    | 2.15                     | 0.60              |
| 1:0:2548:C:OP2    | 4:B:5:ARG:NH2     | 2.35                     | 0.60              |
| 1:0:2676:C:H4'    | 12:J:70:PHE:HE1   | 1.67                     | 0.60              |
| 6:D:23:VAL:HG22   | 6:D:73:VAL:HB     | 1.84                     | 0.60              |
| 18:P:80:ARG:HG2   | 18:P:87:ARG:CZ    | 2.31                     | 0.60              |
| 1:0:1244:U:OP1    | 12:J:18:ILE:HD13  | 2.01                     | 0.60              |
| 1:0:1641:A:H2'    | 1:0:1642:A:H5'    | 1.82                     | 0.60              |
| 37:0:3349:HOH:O   | 10:H:11:LYS:HE2   | 2.01                     | 0.60              |
| 37:0:3491:HOH:O   | 22:T:82:THR:HA    | 2.01                     | 0.60              |
| 5:C:98:ARG:NH1    | 37:C:8355:HOH:O   | 2.33                     | 0.60              |
| 1:0:1679:C:H5'    | 37:0:8834:HOH:O   | 2.02                     | 0.60              |
| 1:0:2721:U:H4'    | 13:K:87:ARG:HG3   | 1.83                     | 0.60              |
| 4:B:314:ALA:HB3   | 4:B:317:PRO:HG3   | 1.84                     | 0.60              |
| 6:D:41:LEU:HA     | 6:D:44:ILE:HG22   | 1.83                     | 0.60              |
| 14:L:73:VAL:HG23  | 14:L:74:THR:H     | 1.66                     | 0.60              |
| 21:S:51:GLN:HE21  | 21:S:53:ASN:ND2   | 1.99                     | 0.60              |
| 25:W:13:MET:HE3   | 25:W:17:ILE:HG22  | 1.84                     | 0.60              |
| 29:1:21:ARG:HD2   | 29:1:37:CYS:SG    | 2.41                     | 0.60              |
| 4:B:179:LEU:O     | 4:B:183:GLU:HG2   | 2.01                     | 0.60              |
| 6:D:37:ALA:O      | 6:D:40:ILE:HG12   | 2.02                     | 0.60              |
| 7:E:31:ARG:NH1    | 7:E:68:HIS:CG     | 2.70                     | 0.60              |
| 10:H:46:GLN:HG3   | 10:H:137:TYR:CE2  | 2.37                     | 0.60              |
| 25:W:88:THR:CG2   | 25:W:89:ASP:H     | 2.10                     | 0.60              |
| 8:F:26:THR:HG21   | 8:F:103:GLU:CG    | 2.32                     | 0.59              |
| 13:K:82:ARG:NH2   | 13:K:115:ARG:HG2  | 2.17                     | 0.59              |
| 16:N:164:ASP:OD1  | 16:N:167:ASP:HA   | 2.02                     | 0.59              |
| 1:0:1187:U:O2'    | 1:0:1189:A:H2     | 1.85                     | 0.59              |
| 16:N:43:VAL:HG11  | 16:N:81:ALA:HA    | 1.84                     | 0.59              |
| 27:Y:112:GLU:CD   | 27:Y:115:ARG:NH1  | 2.60                     | 0.59              |
| 7:E:84:MET:HE2    | 7:E:133:VAL:HG21  | 1.83                     | 0.59              |
| 26:X:25:ARG:HG2   | 37:X:5356:HOH:O   | 2.01                     | 0.59              |
| 1:0:2438:G:H5'    | 37:0:5671:HOH:O   | 2.01                     | 0.59              |
| 14:L:114:VAL:HG11 | 37:L:8573:HOH:O   | 2.02                     | 0.59              |
| 21:S:81:ILE:HG23  | 37:S:8335:HOH:O   | 2.02                     | 0.59              |
| 1:0:191:A:OP1     | 15:M:176:LYS:HE3  | 2.03                     | 0.59              |
| 1:0:2779:G:H21    | 7:E:143:GLN:NE2   | 2.00                     | 0.59              |
| 3:A:121:ALA:O     | 3:A:124:VAL:HG22  | 2.02                     | 0.59              |
| 4:B:7:ARG:CD      | 4:B:9:GLY:O       | 2.50                     | 0.59              |
| 5:C:12:THR:HB     | 37:C:8440:HOH:O   | 2.01                     | 0.59              |
| 10:H:21:THR:O     | 10:H:120:ILE:HD12 | 2.01                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:K:408:HOH:O    | 23:U:37:GLU:HB3   | 2.01                     | 0.59              |
| 15:M:64:ARG:HD2   | 37:M:8585:HOH:O   | 2.02                     | 0.59              |
| 1:O:2630:G:O6     | 3:A:206:ARG:NH2   | 2.36                     | 0.59              |
| 4:B:204:GLY:HA3   | 37:B:8660:HOH:O   | 2.03                     | 0.59              |
| 25:W:13:MET:HE2   | 25:W:18:GLN:HA    | 1.84                     | 0.59              |
| 27:Y:126:PRO:HG2  | 27:Y:128:PHE:CE1  | 2.38                     | 0.59              |
| 1:O:289:G:N2      | 1:O:363:A:H2      | 2.01                     | 0.59              |
| 1:O:2241:C:O2'    | 1:O:2242:U:H5'    | 2.02                     | 0.59              |
| 2:9:41:C:O4'      | 6:D:50:VAL:HG23   | 2.03                     | 0.59              |
| 6:D:44:ILE:HG12   | 6:D:83:PHE:HE1    | 1.66                     | 0.59              |
| 6:D:136:ARG:HD2   | 6:D:155:HIS:O     | 2.02                     | 0.59              |
| 9:G:63:ARG:O      | 9:G:67:LEU:HG     | 2.02                     | 0.59              |
| 12:J:131:THR:HG22 | 12:J:133:GLY:N    | 2.18                     | 0.59              |
| 14:L:149:ARG:O    | 14:L:150:GLN:HB2  | 2.03                     | 0.59              |
| 1:O:558:C:H2'     | 1:O:559:U:C5'     | 2.32                     | 0.59              |
| 1:O:2578:G:H5'    | 1:O:2578:G:H8     | 1.67                     | 0.59              |
| 37:O:4451:HOH:O   | 2:9:103:A:H4'     | 2.01                     | 0.59              |
| 3:A:223:ARG:HG3   | 37:A:8605:HOH:O   | 2.02                     | 0.59              |
| 4:B:51:VAL:HG21   | 4:B:327:VAL:HG13  | 1.83                     | 0.59              |
| 7:E:172:PRO:HB3   | 37:E:6931:HOH:O   | 2.02                     | 0.59              |
| 8:F:26:THR:HG21   | 8:F:103:GLU:HG3   | 1.84                     | 0.59              |
| 12:J:75:PRO:HG2   | 12:J:105:LEU:HD21 | 1.82                     | 0.59              |
| 15:M:60:VAL:C     | 15:M:61:ILE:HD12  | 2.27                     | 0.59              |
| 21:S:81:ILE:HG12  | 37:S:8335:HOH:O   | 2.02                     | 0.59              |
| 25:W:80:ASP:O     | 25:W:84:VAL:HG23  | 2.02                     | 0.59              |
| 1:O:328:U:O4'     | 5:C:202:THR:HG22  | 2.02                     | 0.59              |
| 1:O:710:G:OP1     | 17:O:24:ALA:HB3   | 2.03                     | 0.59              |
| 1:O:1162:G:H1'    | 11:I:117:LEU:CD1  | 2.32                     | 0.59              |
| 2:9:76:G:C3'      | 2:9:77:A:H5''     | 2.27                     | 0.59              |
| 1:O:1299:G:O6     | 14:L:6:ARG:HD3    | 2.03                     | 0.59              |
| 4:B:145:HIS:HD2   | 4:B:146:THR:O     | 1.86                     | 0.59              |
| 22:T:80:GLU:OE2   | 22:T:84:GLY:HA2   | 2.03                     | 0.59              |
| 25:W:106:THR:OG1  | 25:W:109:GLU:HG3  | 2.02                     | 0.59              |
| 27:Y:189:ASN:C    | 27:Y:189:ASN:HD22 | 2.10                     | 0.59              |
| 1:O:2502:C:C2'    | 1:O:2503:A:H5'    | 2.33                     | 0.58              |
| 7:E:31:ARG:HH12   | 7:E:68:HIS:CD2    | 2.21                     | 0.58              |
| 23:U:13:ILE:HG12  | 23:U:32:CYS:HB3   | 1.84                     | 0.58              |
| 23:U:31:PHE:CG    | 23:U:37:GLU:HG2   | 2.38                     | 0.58              |
| 1:O:567:U:H5''    | 37:W:5817:HOH:O   | 2.03                     | 0.58              |
| 3:A:211:LYS:NZ    | 37:A:8623:HOH:O   | 2.36                     | 0.58              |
| 16:N:47:LEU:HD13  | 16:N:97:VAL:HG11  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:Q:11:ARG:HD3   | 37:Q:5620:HOH:O   | 2.01                     | 0.58              |
| 23:U:14:GLU:OE1   | 23:U:15:PRO:HD2   | 2.03                     | 0.58              |
| 4:B:162:MET:HG3   | 4:B:310:ARG:NH1   | 2.18                     | 0.58              |
| 5:C:79:ARG:O      | 5:C:87:ARG:HG2    | 2.03                     | 0.58              |
| 7:E:31:ARG:NH1    | 37:E:5919:HOH:O   | 2.36                     | 0.58              |
| 11:I:129:VAL:HG13 | 11:I:139:ILE:HD11 | 1.85                     | 0.58              |
| 24:V:39:ALA:N     | 24:V:40:PRO:CD    | 2.66                     | 0.58              |
| 1:O:558:C:H5'     | 37:O:4756:HOH:O   | 2.01                     | 0.58              |
| 1:O:1086:A:C6     | 25:W:11:VAL:HG11  | 2.38                     | 0.58              |
| 1:O:1182:C:H1'    | 1:O:1192:A:C8     | 2.34                     | 0.58              |
| 1:O:2270:G:H4'    | 3:A:223:ARG:HH12  | 1.67                     | 0.58              |
| 1:O:2694:A:H4'    | 7:E:91:PHE:HE1    | 1.68                     | 0.58              |
| 3:A:101:GLU:OE2   | 3:A:131:HIS:HB2   | 2.04                     | 0.58              |
| 6:D:69:ILE:HG22   | 6:D:69:ILE:O      | 2.02                     | 0.58              |
| 9:G:64:ASN:HD22   | 9:G:64:ASN:N      | 2.00                     | 0.58              |
| 11:I:98:ALA:O     | 11:I:137:VAL:HA   | 2.03                     | 0.58              |
| 13:K:32:ILE:HD11  | 13:K:56:SER:HB3   | 1.84                     | 0.58              |
| 5:C:142:ASP:OD1   | 5:C:237:GLU:HB3   | 2.04                     | 0.58              |
| 12:J:107:ASN:C    | 12:J:107:ASN:HD22 | 2.11                     | 0.58              |
| 15:M:61:ILE:HG13  | 37:M:8618:HOH:O   | 2.02                     | 0.58              |
| 16:N:71:TRP:CE3   | 16:N:175:LEU:HD22 | 2.38                     | 0.58              |
| 1:O:1525:G:H5'    | 1:O:1526:A:OP2    | 2.04                     | 0.58              |
| 3:A:164:ARG:NE    | 37:A:8590:HOH:O   | 2.36                     | 0.58              |
| 10:H:148:GLU:OE1  | 10:H:148:GLU:HA   | 2.04                     | 0.58              |
| 23:U:52:THR:HG22  | 23:U:54:THR:N     | 2.17                     | 0.58              |
| 1:O:485:A:N3      | 1:O:487:G:H5''    | 2.18                     | 0.58              |
| 1:O:1119:G:N2     | 1:O:1246:A:H2     | 1.99                     | 0.58              |
| 1:O:2781:U:H1'    | 7:E:139:GLU:OE2   | 2.03                     | 0.58              |
| 4:B:42:ALA:HB1    | 4:B:308:LEU:HD11  | 1.85                     | 0.58              |
| 4:B:212:GLN:HB2   | 4:B:257:THR:CG2   | 2.30                     | 0.58              |
| 6:D:23:VAL:HG21   | 6:D:45:THR:HG21   | 1.85                     | 0.58              |
| 12:J:130:VAL:HG12 | 12:J:131:THR:N    | 2.18                     | 0.58              |
| 1:O:1441:G:O2'    | 1:O:1442:A:H5'    | 2.04                     | 0.58              |
| 1:O:2004:U:H4'    | 37:O:4805:HOH:O   | 2.03                     | 0.58              |
| 1:O:2587:OMU:H2'  | 1:O:2589:U:H5''   | 1.85                     | 0.58              |
| 3:A:88:ILE:O      | 3:A:88:ILE:HG22   | 2.02                     | 0.58              |
| 10:H:147:LYS:HG3  | 37:H:8379:HOH:O   | 2.02                     | 0.58              |
| 13:K:30:LYS:O     | 13:K:55:VAL:HG13  | 2.03                     | 0.58              |
| 14:L:104:ASP:HB3  | 37:L:8563:HOH:O   | 2.04                     | 0.58              |
| 22:T:9:LYS:CE     | 22:T:13:ARG:NH1   | 2.67                     | 0.58              |
| 28:Z:53:GLY:HA2   | 28:Z:67:GLY:O     | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1130:U:H2'    | 1:0:1131:G:O4'    | 2.04                     | 0.58              |
| 25:W:81:ASP:OD1   | 25:W:92:ASP:HB2   | 2.03                     | 0.58              |
| 1:0:2064:U:H5'    | 1:0:2652:U:O3'    | 2.04                     | 0.58              |
| 5:C:76:ARG:HG2    | 5:C:78:ARG:NH1    | 2.18                     | 0.58              |
| 10:H:99:LYS:CD    | 10:H:119:LYS:HD3  | 2.33                     | 0.58              |
| 26:X:9:VAL:HG22   | 26:X:88:GLU:OE2   | 2.03                     | 0.58              |
| 31:3:18:GLN:OE1   | 31:3:73:GLU:HB3   | 2.04                     | 0.58              |
| 14:L:145:LEU:O    | 14:L:148:GLU:HG3  | 2.04                     | 0.57              |
| 24:V:38:GLY:C     | 24:V:40:PRO:HD2   | 2.29                     | 0.57              |
| 24:V:55:ARG:O     | 24:V:59:ILE:HG12  | 2.04                     | 0.57              |
| 26:X:25:ARG:HD2   | 37:X:3861:HOH:O   | 2.04                     | 0.57              |
| 26:X:31:ILE:O     | 26:X:35:GLU:HG3   | 2.04                     | 0.57              |
| 1:0:31:C:H4'      | 37:0:6914:HOH:O   | 2.03                     | 0.57              |
| 5:C:118:THR:O     | 5:C:136:VAL:HG13  | 2.04                     | 0.57              |
| 7:E:23:GLU:HG2    | 7:E:28:SER:CB     | 2.34                     | 0.57              |
| 10:H:73:LEU:HD21  | 10:H:146:VAL:HA   | 1.85                     | 0.57              |
| 16:N:34:LEU:HA    | 16:N:47:LEU:HD23  | 1.87                     | 0.57              |
| 16:N:78:MET:HB2   | 16:N:79:PRO:HD3   | 1.86                     | 0.57              |
| 16:N:154:LEU:O    | 16:N:155:GLU:HB3  | 2.05                     | 0.57              |
| 6:D:62:ASP:HA     | 37:D:4233:HOH:O   | 2.04                     | 0.57              |
| 4:B:267:LYS:HD3   | 37:B:8528:HOH:O   | 2.04                     | 0.57              |
| 6:D:35:ALA:N      | 37:D:5576:HOH:O   | 2.37                     | 0.57              |
| 6:D:50:VAL:O      | 6:D:71:ALA:HA     | 2.04                     | 0.57              |
| 6:D:64:ARG:CG     | 6:D:67:ASP:HB3    | 2.33                     | 0.57              |
| 21:S:51:GLN:NE2   | 21:S:53:ASN:HD21  | 1.99                     | 0.57              |
| 2:9:44:A:O4'      | 6:D:76:ARG:NE     | 2.38                     | 0.57              |
| 30:2:35:ARG:HB2   | 37:2:2691:HOH:O   | 2.04                     | 0.57              |
| 1:0:285:A:H2'     | 1:0:286:U:O4'     | 2.05                     | 0.57              |
| 1:0:536:A:H3'     | 37:0:4546:HOH:O   | 2.03                     | 0.57              |
| 7:E:7:ILE:HG22    | 7:E:45:ASP:O      | 2.04                     | 0.57              |
| 8:F:37:THR:O      | 8:F:41:GLU:HG3    | 2.04                     | 0.57              |
| 15:M:99:ARG:HD2   | 15:M:167:GLY:HA2  | 1.86                     | 0.57              |
| 20:R:106:GLY:HA2  | 20:R:109:MET:HE3  | 1.87                     | 0.57              |
| 1:0:1053:G:OP1    | 10:H:12:PRO:HG3   | 2.04                     | 0.57              |
| 11:I:129:VAL:HG13 | 11:I:139:ILE:CD1  | 2.35                     | 0.57              |
| 14:L:90:ARG:NH2   | 14:L:121:ILE:HD11 | 2.20                     | 0.57              |
| 16:N:155:GLU:O    | 16:N:156:GLU:HG3  | 2.05                     | 0.57              |
| 1:0:57:C:H5''     | 37:0:6253:HOH:O   | 2.05                     | 0.57              |
| 1:0:2420:G:O2'    | 1:0:2421:G:H5'    | 2.04                     | 0.57              |
| 6:D:170:TYR:O     | 6:D:171:ASP:HB3   | 2.05                     | 0.57              |
| 10:H:27:LYS:H     | 10:H:59:HIS:CD2   | 2.17                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 27:Y:212:ARG:HD2 | 37:Y:8602:HOH:O  | 2.05                     | 0.57              |
| 27:Y:216:ARG:HD3 | 37:Y:8569:HOH:O  | 2.04                     | 0.57              |
| 1:0:111:C:O2'    | 29:1:20:ARG:HG2  | 2.04                     | 0.57              |
| 1:0:506:G:H22    | 1:0:509:A:H5''   | 1.67                     | 0.57              |
| 1:0:2533:C:H5'   | 1:0:2533:C:C6    | 2.39                     | 0.57              |
| 1:0:2780:C:H1'   | 7:E:143:GLN:HE21 | 1.69                     | 0.57              |
| 30:2:31:ARG:CZ   | 37:2:7177:HOH:O  | 2.52                     | 0.57              |
| 1:0:797:A:C4'    | 28:Z:10:ARG:N    | 2.68                     | 0.57              |
| 6:D:25:MET:HE3   | 6:D:37:ALA:HB1   | 1.87                     | 0.57              |
| 10:H:9:ILE:HG23  | 10:H:126:ARG:NE  | 2.20                     | 0.57              |
| 11:I:75:THR:HA   | 11:I:112:LYS:NZ  | 2.18                     | 0.57              |
| 22:T:111:ARG:HB3 | 22:T:119:ALA:HB2 | 1.87                     | 0.56              |
| 26:X:78:GLU:CG   | 26:X:79:GLU:H    | 2.17                     | 0.56              |
| 27:Y:155:ARG:NH1 | 37:Y:8557:HOH:O  | 2.38                     | 0.56              |
| 1:0:2456:A:H5'   | 37:0:5194:HOH:O  | 2.05                     | 0.56              |
| 25:W:149:LEU:HG  | 25:W:153:MET:CE  | 2.27                     | 0.56              |
| 29:1:8:GLN:HE22  | 29:1:11:LYS:NZ   | 2.03                     | 0.56              |
| 1:0:316:A:H5'    | 22:T:54:ASP:OD2  | 2.04                     | 0.56              |
| 1:0:500:G:H21    | 20:R:98:ASN:HD21 | 1.53                     | 0.56              |
| 1:0:1189:A:H1'   | 1:0:1209:C:C1'   | 2.35                     | 0.56              |
| 1:0:1377:C:H5'   | 1:0:1377:C:C6    | 2.40                     | 0.56              |
| 1:0:1878:G:H1'   | 37:0:5621:HOH:O  | 2.04                     | 0.56              |
| 1:0:2769:C:C2'   | 1:0:2770:G:H5'   | 2.35                     | 0.56              |
| 3:A:153:ARG:HB2  | 3:A:153:ARG:NH1  | 2.20                     | 0.56              |
| 12:J:93:ARG:HB3  | 12:J:93:ARG:NH1  | 2.19                     | 0.56              |
| 16:N:110:THR:HB  | 16:N:113:SER:OG  | 2.04                     | 0.56              |
| 20:R:39:THR:HB   | 20:R:42:GLU:CD   | 2.31                     | 0.56              |
| 25:W:13:MET:HE2  | 25:W:18:GLN:CA   | 2.34                     | 0.56              |
| 25:W:139:GLY:O   | 25:W:141:HIS:HD2 | 1.88                     | 0.56              |
| 4:B:85:ARG:NH1   | 37:B:8640:HOH:O  | 2.39                     | 0.56              |
| 14:L:143:THR:CG2 | 14:L:144:ASP:N   | 2.68                     | 0.56              |
| 18:P:59:ARG:HH22 | 18:P:66:GLN:HE22 | 1.52                     | 0.56              |
| 1:0:449:A:N7     | 5:C:43:LYS:HG2   | 2.20                     | 0.56              |
| 1:0:2815:G:OP2   | 12:J:99:GLU:HG2  | 2.06                     | 0.56              |
| 10:H:170:ASN:N   | 10:H:170:ASN:ND2 | 2.53                     | 0.56              |
| 20:R:132:ARG:NH1 | 37:R:8582:HOH:O  | 2.38                     | 0.56              |
| 37:0:7046:HOH:O  | 31:3:60:LYS:HG3  | 2.05                     | 0.56              |
| 16:N:151:ASP:O   | 16:N:154:LEU:HB2 | 2.06                     | 0.56              |
| 23:U:11:THR:HG22 | 23:U:53:ASP:OD2  | 2.06                     | 0.56              |
| 23:U:52:THR:CG2  | 23:U:54:THR:HB   | 2.36                     | 0.56              |
| 28:Z:60:CYS:O    | 28:Z:61:ASP:HB2  | 2.05                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:558:C:H2'     | 1:0:559:U:H5'    | 1.88                     | 0.56              |
| 1:0:738:G:H3'     | 37:0:6540:HOH:O  | 2.06                     | 0.56              |
| 1:0:1119:G:H2'    | 12:J:52:GLN:NE2  | 2.21                     | 0.56              |
| 1:0:1667:A:H2'    | 1:0:1668:U:C6    | 2.40                     | 0.56              |
| 25:W:21:LEU:HD13  | 25:W:26:ILE:HD11 | 1.88                     | 0.56              |
| 1:0:1119:G:H8     | 12:J:52:GLN:NE2  | 2.03                     | 0.56              |
| 1:0:2690:U:O2'    | 7:E:111:LYS:HE3  | 2.06                     | 0.56              |
| 12:J:107:ASN:HD22 | 12:J:109:TYR:H   | 1.52                     | 0.56              |
| 26:X:74:ALA:HB2   | 26:X:85:VAL:HG13 | 1.86                     | 0.56              |
| 1:0:1116:U:O2'    | 1:0:1118:A:C2    | 2.50                     | 0.56              |
| 1:0:1268:C:O2'    | 27:Y:169:ARG:HB2 | 2.06                     | 0.56              |
| 3:A:95:PRO:HG2    | 3:A:98:GLU:HG2   | 1.88                     | 0.56              |
| 4:B:154:VAL:HG12  | 4:B:156:LYS:HG2  | 1.87                     | 0.56              |
| 10:H:38:LYS:HE2   | 10:H:42:ASP:CB   | 2.36                     | 0.56              |
| 14:L:53:ARG:NH2   | 14:L:57:VAL:HG12 | 2.20                     | 0.56              |
| 26:X:12:ILE:HD12  | 26:X:36:HIS:ND1  | 2.21                     | 0.56              |
| 1:0:1919:A:H4'    | 37:0:4350:HOH:O  | 2.06                     | 0.56              |
| 2:9:49:G:H2'      | 2:9:50:G:O4'     | 2.06                     | 0.56              |
| 3:A:105:VAL:HG12  | 3:A:106:CYS:N    | 2.21                     | 0.56              |
| 3:A:179:MET:HG2   | 3:A:186:TRP:CB   | 2.36                     | 0.56              |
| 4:B:195:ARG:HG2   | 4:B:323:LEU:HD22 | 1.86                     | 0.56              |
| 13:K:34:VAL:CG2   | 13:K:47:ALA:HB2  | 2.34                     | 0.56              |
| 18:P:121:ASP:HB2  | 37:P:195:HOH:O   | 2.05                     | 0.56              |
| 21:S:23:LYS:HE2   | 37:S:8330:HOH:O  | 2.04                     | 0.56              |
| 1:0:711:G:H1'     | 37:0:6586:HOH:O  | 2.05                     | 0.55              |
| 1:0:1615:A:H5'    | 37:0:3687:HOH:O  | 2.06                     | 0.55              |
| 2:9:54:A:O2'      | 2:9:55:U:H5'     | 2.06                     | 0.55              |
| 4:B:14:GLY:HA2    | 4:B:15:PRO:C     | 2.31                     | 0.55              |
| 6:D:99:ASP:HB2    | 6:D:103:ASN:HB2  | 1.87                     | 0.55              |
| 8:F:46:GLU:OE1    | 8:F:100:ASP:HA   | 2.05                     | 0.55              |
| 1:0:244:C:OP2     | 8:F:38:LYS:HE3   | 2.07                     | 0.55              |
| 1:0:1118:A:H8     | 1:0:1119:G:H5''  | 1.69                     | 0.55              |
| 1:0:2862:G:H4'    | 4:B:336:GLN:O    | 2.05                     | 0.55              |
| 4:B:82:VAL:O      | 4:B:82:VAL:HG12  | 2.06                     | 0.55              |
| 7:E:15:GLN:NE2    | 7:E:40:VAL:O     | 2.38                     | 0.55              |
| 14:L:77:ALA:HB3   | 37:L:8529:HOH:O  | 2.04                     | 0.55              |
| 16:N:61:ALA:HB3   | 16:N:88:ALA:HB2  | 1.88                     | 0.55              |
| 19:Q:64:GLU:HG3   | 19:Q:74:ASP:OD2  | 2.06                     | 0.55              |
| 1:0:1299:G:N2     | 37:0:4183:HOH:O  | 2.38                     | 0.55              |
| 1:0:2837:U:H2'    | 37:0:6334:HOH:O  | 2.05                     | 0.55              |
| 3:A:100:PRO:HG2   | 3:A:103:VAL:CG2  | 2.33                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:104:ASP:HA   | 5:C:107:ARG:NH1   | 2.21                     | 0.55              |
| 10:H:63:GLU:HA   | 37:H:8382:HOH:O   | 2.06                     | 0.55              |
| 10:H:147:LYS:N   | 37:H:8379:HOH:O   | 2.40                     | 0.55              |
| 16:N:157:PRO:HA  | 37:N:8525:HOH:O   | 2.05                     | 0.55              |
| 1:O:280:C:H2'    | 1:O:281:U:O4'     | 2.07                     | 0.55              |
| 37:O:9044:HOH:O  | 18:P:81:LYS:HG2   | 2.05                     | 0.55              |
| 5:C:235:PHE:HE2  | 5:C:243:VAL:HG21  | 1.72                     | 0.55              |
| 16:N:48:VAL:HG11 | 16:N:55:ASP:HB3   | 1.87                     | 0.55              |
| 20:R:29:LYS:HB3  | 37:R:8532:HOH:O   | 2.06                     | 0.55              |
| 21:S:38:ALA:O    | 21:S:42:GLU:HG3   | 2.06                     | 0.55              |
| 24:V:4:HIS:HB3   | 37:V:6622:HOH:O   | 2.07                     | 0.55              |
| 1:O:1044:C:H5''  | 37:O:8542:HOH:O   | 2.06                     | 0.55              |
| 11:I:72:VAL:CG1  | 11:I:73:PRO:HD2   | 2.36                     | 0.55              |
| 1:O:282:C:H1'    | 1:O:368:C:H42     | 1.72                     | 0.55              |
| 1:O:1123:A:C6    | 1:O:1238:C:H5'    | 2.42                     | 0.55              |
| 1:O:1306:U:OP1   | 5:C:184:ARG:HD2   | 2.07                     | 0.55              |
| 1:O:1878:G:O2'   | 1:O:1879:U:C6     | 2.57                     | 0.55              |
| 1:O:2604:A:H5'   | 37:O:5291:HOH:O   | 2.07                     | 0.55              |
| 3:A:53:ALA:HB3   | 37:A:8609:HOH:O   | 2.06                     | 0.55              |
| 4:B:119:HIS:O    | 4:B:121:PRO:HD3   | 2.07                     | 0.55              |
| 4:B:140:LEU:HD23 | 37:B:8583:HOH:O   | 2.06                     | 0.55              |
| 4:B:258:GLY:H    | 4:B:260:HIS:CE1   | 2.25                     | 0.55              |
| 7:E:93:MET:HE1   | 7:E:165:GLY:H     | 1.70                     | 0.55              |
| 13:K:115:ARG:HG3 | 13:K:116:GLU:N    | 2.21                     | 0.55              |
| 16:N:179:LEU:HA  | 16:N:184:ILE:HD12 | 1.89                     | 0.55              |
| 27:Y:144:ARG:NE  | 37:Y:8612:HOH:O   | 2.39                     | 0.55              |
| 29:1:28:HIS:CD2  | 29:1:30:LYS:HB2   | 2.41                     | 0.55              |
| 3:A:34:ASP:OD1   | 3:A:35:GLY:N      | 2.35                     | 0.55              |
| 3:A:212:PRO:HB2  | 37:A:8562:HOH:O   | 2.06                     | 0.55              |
| 4:B:141:ARG:HG2  | 4:B:165:ARG:HA    | 1.88                     | 0.55              |
| 20:R:33:ARG:NH1  | 37:R:8543:HOH:O   | 2.37                     | 0.55              |
| 22:T:63:ILE:HD11 | 22:T:75:GLU:HB2   | 1.88                     | 0.55              |
| 1:O:263:U:O4'    | 8:F:59:ILE:HD13   | 2.06                     | 0.55              |
| 1:O:2717:C:O2'   | 1:O:2718:C:H5''   | 2.06                     | 0.55              |
| 3:A:37:VAL:HG22  | 37:A:8600:HOH:O   | 2.06                     | 0.55              |
| 3:A:175:LYS:HE2  | 37:A:8578:HOH:O   | 2.07                     | 0.55              |
| 4:B:297:VAL:HB   | 37:B:8610:HOH:O   | 2.07                     | 0.55              |
| 14:L:133:VAL:HB  | 37:L:8557:HOH:O   | 2.06                     | 0.55              |
| 20:R:18:LEU:HD12 | 20:R:143:VAL:CG1  | 2.37                     | 0.55              |
| 1:O:775:G:OP1    | 29:1:16:HIS:HE1   | 1.90                     | 0.55              |
| 1:O:2081:A:H4'   | 12:J:69:TYR:CE1   | 2.42                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2718:C:H6     | 1:0:2718:C:H5'    | 1.72                     | 0.55              |
| 1:0:2815:G:N7     | 12:J:80:LYS:NZ    | 2.54                     | 0.55              |
| 1:0:2866:U:H4'    | 1:0:2867:G:H5'    | 1.88                     | 0.55              |
| 1:0:2898:G:H4'    | 4:B:288:GLY:HA2   | 1.88                     | 0.55              |
| 6:D:93:LEU:O      | 6:D:174:VAL:O     | 2.25                     | 0.55              |
| 13:K:109:LEU:HD13 | 13:K:113:ILE:HD11 | 1.89                     | 0.55              |
| 15:M:61:ILE:HA    | 37:M:8618:HOH:O   | 2.07                     | 0.55              |
| 25:W:21:LEU:HB3   | 25:W:26:ILE:CG1   | 2.36                     | 0.55              |
| 30:2:19:SER:HB3   | 37:2:4479:HOH:O   | 2.07                     | 0.55              |
| 31:3:60:LYS:HG3   | 31:3:61:PRO:HD2   | 1.88                     | 0.55              |
| 1:0:1299:G:H5'    | 37:0:3576:HOH:O   | 2.07                     | 0.55              |
| 4:B:16:ARG:NE     | 37:B:8557:HOH:O   | 2.26                     | 0.55              |
| 6:D:94:ALA:HB3    | 6:D:97:GLN:HG3    | 1.89                     | 0.55              |
| 14:L:73:VAL:HG23  | 14:L:74:THR:N     | 2.22                     | 0.55              |
| 16:N:38:LYS:HD2   | 16:N:114:LYS:HE3  | 1.89                     | 0.55              |
| 16:N:154:LEU:HG   | 16:N:155:GLU:H    | 1.71                     | 0.55              |
| 1:0:1506:U:H6     | 1:0:1506:U:H5'    | 1.72                     | 0.54              |
| 1:0:2064:U:H5'    | 1:0:2652:U:H4'    | 1.89                     | 0.54              |
| 6:D:36:ASN:HA     | 37:D:7500:HOH:O   | 2.06                     | 0.54              |
| 22:T:92:ASP:OD1   | 22:T:94:SER:HB3   | 2.07                     | 0.54              |
| 25:W:38:THR:HG22  | 25:W:39:ASP:H     | 1.73                     | 0.54              |
| 26:X:78:GLU:HG2   | 26:X:79:GLU:N     | 2.21                     | 0.54              |
| 7:E:11:VAL:HG13   | 7:E:23:GLU:O      | 2.06                     | 0.54              |
| 10:H:28:ILE:HA    | 10:H:63:GLU:OE1   | 2.07                     | 0.54              |
| 21:S:33:SER:OG    | 21:S:36:GLU:HG3   | 2.07                     | 0.54              |
| 1:0:1209:C:H4'    | 37:0:4778:HOH:O   | 2.06                     | 0.54              |
| 1:0:2502:C:H2'    | 1:0:2503:A:H5'    | 1.88                     | 0.54              |
| 8:F:101:ALA:HA    | 37:F:5413:HOH:O   | 2.07                     | 0.54              |
| 16:N:11:ARG:NH2   | 37:N:8519:HOH:O   | 2.40                     | 0.54              |
| 27:Y:178:HIS:CG   | 27:Y:179:PRO:HD2  | 2.43                     | 0.54              |
| 1:0:138:U:H5''    | 1:0:139:C:OP2     | 2.08                     | 0.54              |
| 1:0:1477:C:H5'    | 1:0:1868:G:C5'    | 2.37                     | 0.54              |
| 1:0:1669:A:H2'    | 1:0:1670:G:C8     | 2.42                     | 0.54              |
| 6:D:51:ARG:HD3    | 37:D:7636:HOH:O   | 2.06                     | 0.54              |
| 6:D:154:LYS:H     | 6:D:154:LYS:CD    | 2.09                     | 0.54              |
| 28:Z:13:ARG:NH1   | 37:Z:8419:HOH:O   | 2.39                     | 0.54              |
| 1:0:602:A:O2'     | 1:0:605:C:H4'     | 2.08                     | 0.54              |
| 1:0:951:A:C2'     | 1:0:952:G:H5'     | 2.37                     | 0.54              |
| 1:0:1118:A:C8     | 1:0:1118:A:C3'    | 2.87                     | 0.54              |
| 1:0:1191:A:H3'    | 1:0:1192:A:H5''   | 1.88                     | 0.54              |
| 1:0:2795:C:O2'    | 1:0:2796:U:H5'    | 2.06                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:I:79:ILE:HA   | 11:I:108:ILE:HD11 | 1.88                     | 0.54              |
| 24:V:58:THR:O    | 24:V:62:GLU:HG3   | 2.08                     | 0.54              |
| 25:W:125:HIS:CD2 | 25:W:127:GLY:H    | 2.25                     | 0.54              |
| 1:0:272:A:H5'    | 1:0:273:G:OP2     | 2.06                     | 0.54              |
| 1:0:899:C:H5'    | 37:0:9708:HOH:O   | 2.07                     | 0.54              |
| 1:0:1181:A:H2'   | 1:0:1182:C:O4'    | 2.08                     | 0.54              |
| 1:0:1441:G:H1'   | 37:0:7256:HOH:O   | 2.05                     | 0.54              |
| 1:0:2289:G:H21   | 1:0:2291:A:H2     | 1.54                     | 0.54              |
| 1:0:2361:A:H5''  | 37:0:8523:HOH:O   | 2.08                     | 0.54              |
| 1:0:2717:C:H2'   | 1:0:2718:C:C5'    | 2.34                     | 0.54              |
| 37:0:8593:HOH:O  | 4:B:214:PRO:HD2   | 2.07                     | 0.54              |
| 4:B:7:ARG:HG2    | 4:B:7:ARG:NH1     | 2.16                     | 0.54              |
| 5:C:214:THR:HG23 | 37:C:8436:HOH:O   | 2.07                     | 0.54              |
| 8:F:99:THR:O     | 8:F:100:ASP:HB2   | 2.07                     | 0.54              |
| 11:I:118:SER:CB  | 11:I:123:ASN:HB2  | 2.35                     | 0.54              |
| 15:M:30:GLU:O    | 15:M:34:GLU:HG3   | 2.07                     | 0.54              |
| 31:3:17:HIS:O    | 31:3:18:GLN:HG3   | 2.08                     | 0.54              |
| 1:0:21:G:H5''    | 20:R:1:GLY:O      | 2.07                     | 0.54              |
| 6:D:91:ALA:HB1   | 37:D:5198:HOH:O   | 2.08                     | 0.54              |
| 15:M:57:LYS:HE2  | 15:M:140:ALA:O    | 2.08                     | 0.54              |
| 27:Y:187:VAL:CG2 | 27:Y:192:ASP:HB2  | 2.33                     | 0.54              |
| 1:0:200:U:H2'    | 37:0:9953:HOH:O   | 2.06                     | 0.54              |
| 37:9:8515:HOH:O  | 16:N:107:ASN:HB3  | 2.08                     | 0.54              |
| 16:N:152:GLU:C   | 16:N:154:LEU:H    | 2.14                     | 0.54              |
| 23:U:52:THR:HG22 | 23:U:54:THR:H     | 1.73                     | 0.54              |
| 4:B:41:PHE:HB3   | 4:B:190:MET:HE1   | 1.89                     | 0.54              |
| 16:N:163:PHE:O   | 16:N:163:PHE:CD2  | 2.61                     | 0.54              |
| 23:U:39:ASN:ND2  | 23:U:44:ARG:HH11  | 2.06                     | 0.54              |
| 24:V:49:LEU:O    | 24:V:53:ILE:HG13  | 2.08                     | 0.54              |
| 1:0:703:G:O2'    | 1:0:704:C:H5'     | 2.08                     | 0.54              |
| 2:9:1:U:H5'      | 2:9:121:C:O2      | 2.08                     | 0.54              |
| 3:A:105:VAL:HG11 | 3:A:154:ALA:CB    | 2.36                     | 0.54              |
| 7:E:49:ILE:HD11  | 7:E:69:ILE:HD12   | 1.89                     | 0.54              |
| 11:I:113:HIS:N   | 11:I:114:PRO:CD   | 2.69                     | 0.54              |
| 25:W:84:VAL:HG12 | 37:W:6679:HOH:O   | 2.08                     | 0.54              |
| 1:0:2787:C:H5    | 37:0:4133:HOH:O   | 1.91                     | 0.53              |
| 3:A:192:VAL:CG1  | 3:A:207:GLN:HB3   | 2.38                     | 0.53              |
| 6:D:57:THR:HG23  | 6:D:63:ILE:CA     | 2.37                     | 0.53              |
| 9:G:12:ILE:O     | 9:G:12:ILE:HG22   | 2.08                     | 0.53              |
| 10:H:45:VAL:HA   | 10:H:167:PRO:O    | 2.07                     | 0.53              |
| 14:L:143:THR:CG2 | 14:L:144:ASP:H    | 2.20                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 20:R:119:VAL:HG12 | 20:R:119:VAL:O   | 2.07                     | 0.53              |
| 37:O:9459:HOH:O   | 26:X:23:HIS:HD2  | 1.91                     | 0.53              |
| 5:C:127:ARG:CZ    | 5:C:225:PRO:HG2  | 2.36                     | 0.53              |
| 17:O:38:ARG:NH1   | 37:O:7674:HOH:O  | 2.41                     | 0.53              |
| 1:O:1333:U:H2'    | 1:O:1334:C:C6    | 2.44                     | 0.53              |
| 1:O:2591:C:H2'    | 1:O:2592:G:O4'   | 2.09                     | 0.53              |
| 4:B:329:TYR:CE2   | 23:U:15:PRO:HG2  | 2.43                     | 0.53              |
| 1:O:542:A:H2'     | 1:O:543:G:O4'    | 2.08                     | 0.53              |
| 1:O:949:U:O2'     | 19:Q:40:HIS:HE1  | 1.92                     | 0.53              |
| 1:O:2756:U:N3     | 1:O:2896:A:H2    | 2.06                     | 0.53              |
| 1:O:2821:C:H4'    | 4:B:116:PRO:HB3  | 1.91                     | 0.53              |
| 12:J:133:GLY:O    | 12:J:137:GLU:HG3 | 2.09                     | 0.53              |
| 18:P:91:LYS:O     | 18:P:95:GLU:HG3  | 2.07                     | 0.53              |
| 1:O:317:A:H5''    | 22:T:52:ARG:HD2  | 1.91                     | 0.53              |
| 1:O:371:U:H2'     | 1:O:372:A:H8     | 1.74                     | 0.53              |
| 1:O:1151:G:OP1    | 9:G:63:ARG:NH1   | 2.42                     | 0.53              |
| 4:B:75:GLU:C      | 4:B:77:PRO:HD3   | 2.34                     | 0.53              |
| 14:L:61:ALA:HA    | 37:L:8563:HOH:O  | 2.09                     | 0.53              |
| 25:W:122:ARG:HG2  | 25:W:122:ARG:NH1 | 2.18                     | 0.53              |
| 25:W:122:ARG:CZ   | 37:W:5817:HOH:O  | 2.55                     | 0.53              |
| 2:9:42:C:O2       | 6:D:76:ARG:NH1   | 2.41                     | 0.53              |
| 5:C:47:GLY:HA2    | 5:C:92:PRO:HB2   | 1.90                     | 0.53              |
| 11:I:88:GLY:C     | 37:I:5128:HOH:O  | 2.50                     | 0.53              |
| 16:N:62:HIS:HB3   | 16:N:65:ASP:OD1  | 2.09                     | 0.53              |
| 17:O:39:THR:O     | 17:O:115:ARG:NH2 | 2.42                     | 0.53              |
| 25:W:38:THR:HG22  | 25:W:39:ASP:N    | 2.24                     | 0.53              |
| 1:O:65:C:O2'      | 1:O:66:G:H5'     | 2.09                     | 0.53              |
| 1:O:681:G:N3      | 1:O:681:G:H5'    | 2.24                     | 0.53              |
| 3:A:211:LYS:HB3   | 3:A:212:PRO:CD   | 2.33                     | 0.53              |
| 4:B:168:GLY:O     | 4:B:169:GLY:O    | 2.27                     | 0.53              |
| 5:C:1:MET:HG2     | 5:C:2:GLN:N      | 2.22                     | 0.53              |
| 6:D:23:VAL:HG21   | 6:D:45:THR:CG2   | 2.38                     | 0.53              |
| 6:D:27:ILE:HG22   | 6:D:28:GLY:N     | 2.17                     | 0.53              |
| 9:G:12:ILE:N      | 9:G:13:PRO:CD    | 2.71                     | 0.53              |
| 13:K:125:ALA:C    | 13:K:127:ALA:H   | 2.17                     | 0.53              |
| 22:T:24:ARG:HH21  | 22:T:39:ASN:HD22 | 1.55                     | 0.53              |
| 25:W:122:ARG:HH21 | 25:W:154:ARG:HD2 | 1.73                     | 0.53              |
| 27:Y:106:THR:HG23 | 27:Y:107:PRO:HD2 | 1.91                     | 0.53              |
| 1:O:1209:C:H2'    | 1:O:1210:G:C8    | 2.42                     | 0.53              |
| 1:O:2094:G:H4'    | 4:B:245:SER:HB3  | 1.90                     | 0.53              |
| 1:O:2419:U:H5''   | 1:O:2420:G:H5'   | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:9:24:U:H3'     | 2:9:25:G:H5'      | 1.90                     | 0.53              |
| 4:B:305:ASP:O    | 4:B:306:LYS:HB2   | 2.09                     | 0.53              |
| 4:B:310:ARG:NH2  | 37:B:8560:HOH:O   | 2.41                     | 0.53              |
| 6:D:163:VAL:HA   | 37:D:6326:HOH:O   | 2.09                     | 0.53              |
| 22:T:41:ARG:NH1  | 22:T:42:VAL:O     | 2.42                     | 0.53              |
| 25:W:106:THR:HG1 | 25:W:109:GLU:HG3  | 1.72                     | 0.53              |
| 1:0:1044:C:H3'   | 1:0:1045:G:H5''   | 1.91                     | 0.53              |
| 1:0:1353:C:P     | 37:0:4179:HOH:O   | 2.67                     | 0.53              |
| 11:I:108:ILE:CG2 | 11:I:128:VAL:HG11 | 2.39                     | 0.53              |
| 12:J:19:MET:HE3  | 12:J:132:LEU:CD1  | 2.31                     | 0.53              |
| 20:R:29:LYS:HD3  | 37:R:8532:HOH:O   | 2.08                     | 0.53              |
| 29:1:28:HIS:CD2  | 29:1:31:LYS:HG3   | 2.44                     | 0.53              |
| 1:0:338:C:H5''   | 37:C:8420:HOH:O   | 2.09                     | 0.53              |
| 3:A:164:ARG:CZ   | 37:A:8590:HOH:O   | 2.57                     | 0.53              |
| 13:K:58:THR:HG22 | 13:K:59:LYS:HG3   | 1.91                     | 0.53              |
| 16:N:49:THR:CG2  | 16:N:56:ASP:HB2   | 2.37                     | 0.53              |
| 23:U:33:SER:O    | 23:U:37:GLU:HG3   | 2.09                     | 0.53              |
| 24:V:39:ALA:O    | 24:V:41:GLU:N     | 2.42                     | 0.53              |
| 1:0:1500:U:P     | 18:P:41:ARG:HH22  | 2.32                     | 0.52              |
| 1:0:1972:U:H2'   | 1:0:1973:A:C5'    | 2.40                     | 0.52              |
| 1:0:2812:A:C2    | 1:0:2814:A:N6     | 2.69                     | 0.52              |
| 4:B:2:GLN:HA     | 37:B:8626:HOH:O   | 2.08                     | 0.52              |
| 5:C:76:ARG:HG2   | 5:C:78:ARG:HH12   | 1.73                     | 0.52              |
| 5:C:246:ARG:NH2  | 37:C:8423:HOH:O   | 2.41                     | 0.52              |
| 12:J:45:VAL:HG21 | 12:J:129:PHE:CD1  | 2.45                     | 0.52              |
| 17:O:47:ARG:HG3  | 17:O:47:ARG:NH1   | 2.23                     | 0.52              |
| 1:0:1205:U:H2'   | 1:0:1206:U:C5'    | 2.39                     | 0.52              |
| 1:0:1527:A:H1'   | 1:0:1528:A:C8     | 2.44                     | 0.52              |
| 1:0:1834:C:H2'   | 1:0:1840:A:N6     | 2.24                     | 0.52              |
| 2:9:6:C:C5'      | 16:N:37:ARG:HH12  | 2.12                     | 0.52              |
| 2:9:55:U:H4'     | 2:9:56:A:C8       | 2.43                     | 0.52              |
| 4:B:7:ARG:NH1    | 4:B:11:LEU:HD22   | 2.24                     | 0.52              |
| 6:D:135:VAL:HG21 | 6:D:139:TYR:CD1   | 2.45                     | 0.52              |
| 11:I:128:VAL:HA  | 37:I:5331:HOH:O   | 2.09                     | 0.52              |
| 17:O:96:VAL:HG13 | 17:O:100:GLN:HB2  | 1.91                     | 0.52              |
| 1:0:1972:U:H2'   | 1:0:1973:A:H5'    | 1.92                     | 0.52              |
| 4:B:307:ARG:HH11 | 4:B:307:ARG:HG3   | 1.74                     | 0.52              |
| 6:D:135:VAL:HG22 | 6:D:136:ARG:N     | 2.24                     | 0.52              |
| 23:U:47:ARG:HG3  | 37:U:4381:HOH:O   | 2.08                     | 0.52              |
| 25:W:122:ARG:NH2 | 25:W:154:ARG:HD2  | 2.25                     | 0.52              |
| 1:0:920:C:H5''   | 1:0:921:G:O5'     | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:2812:A:N7    | 37:0:7006:HOH:O  | 2.34                     | 0.52              |
| 7:E:7:ILE:HD11   | 7:E:11:VAL:O     | 2.08                     | 0.52              |
| 8:F:2:VAL:HG22   | 8:F:57:GLU:OE1   | 2.08                     | 0.52              |
| 12:J:99:GLU:HA   | 37:J:7377:HOH:O  | 2.09                     | 0.52              |
| 13:K:87:ARG:CZ   | 37:K:4854:HOH:O  | 2.57                     | 0.52              |
| 18:P:10:ALA:HA   | 18:P:13:VAL:CG1  | 2.39                     | 0.52              |
| 22:T:41:ARG:HG2  | 22:T:41:ARG:NH1  | 2.24                     | 0.52              |
| 25:W:41:TYR:HA   | 25:W:44:MET:HE3  | 1.91                     | 0.52              |
| 26:X:43:VAL:HG12 | 26:X:44:ASP:N    | 2.24                     | 0.52              |
| 1:0:281:U:H3'    | 37:0:6698:HOH:O  | 2.09                     | 0.52              |
| 1:0:2265:U:H2'   | 1:0:2266:A:C8    | 2.45                     | 0.52              |
| 3:A:153:ARG:HD3  | 37:A:8531:HOH:O  | 2.09                     | 0.52              |
| 25:W:13:MET:HE3  | 25:W:17:ILE:CG2  | 2.40                     | 0.52              |
| 1:0:396:U:O2'    | 1:0:418:C:H4'    | 2.10                     | 0.52              |
| 1:0:1137:G:H1'   | 37:0:3380:HOH:O  | 2.09                     | 0.52              |
| 1:0:2301:A:H5''  | 1:0:2302:A:H5'   | 1.91                     | 0.52              |
| 10:H:58:ARG:O    | 10:H:62:LEU:HD22 | 2.10                     | 0.52              |
| 11:I:75:THR:N    | 11:I:112:LYS:HE2 | 2.24                     | 0.52              |
| 25:W:122:ARG:NH2 | 37:W:5817:HOH:O  | 2.43                     | 0.52              |
| 26:X:41:PHE:O    | 26:X:43:VAL:HG23 | 2.08                     | 0.52              |
| 1:0:2768:A:O2'   | 1:0:2769:C:H5'   | 2.09                     | 0.52              |
| 2:9:29:C:C2'     | 2:9:30:C:H5'     | 2.39                     | 0.52              |
| 4:B:156:LYS:HE3  | 37:B:8636:HOH:O  | 2.09                     | 0.52              |
| 4:B:333:GLU:HB2  | 23:U:14:GLU:OE2  | 2.09                     | 0.52              |
| 8:F:117:GLU:C    | 8:F:119:ARG:N    | 2.67                     | 0.52              |
| 11:I:130:GLY:C   | 37:I:5371:HOH:O  | 2.52                     | 0.52              |
| 1:0:2256:G:H2'   | 1:0:2257:G:C5'   | 2.40                     | 0.52              |
| 1:0:2256:G:H2'   | 1:0:2257:G:H5'   | 1.92                     | 0.52              |
| 1:0:2506:A:O2'   | 1:0:2507:G:O5'   | 2.27                     | 0.52              |
| 2:9:64:C:H2'     | 2:9:65:A:H5'     | 1.92                     | 0.52              |
| 4:B:79:MET:HE3   | 4:B:144:THR:HG21 | 1.92                     | 0.52              |
| 4:B:215:VAL:HB   | 4:B:234:ARG:HH12 | 1.75                     | 0.52              |
| 4:B:307:ARG:HD3  | 37:B:8524:HOH:O  | 2.10                     | 0.52              |
| 5:C:233:THR:HG22 | 5:C:234:VAL:N    | 2.24                     | 0.52              |
| 6:D:86:THR:O     | 6:D:90:LEU:HG    | 2.10                     | 0.52              |
| 8:F:50:VAL:HG21  | 8:F:63:ILE:HG21  | 1.92                     | 0.52              |
| 16:N:11:ARG:HG3  | 16:N:14:ARG:NH1  | 2.25                     | 0.52              |
| 16:N:77:ASN:OD1  | 16:N:80:SER:HB2  | 2.10                     | 0.52              |
| 21:S:56:ASN:O    | 30:2:8:LYS:HE2   | 2.10                     | 0.52              |
| 25:W:119:HIS:HD2 | 25:W:120:PRO:O   | 1.93                     | 0.52              |
| 28:Z:11:SER:CB   | 28:Z:23:ARG:HB2  | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2004:U:H2'    | 1:0:2004:U:O2     | 2.08                     | 0.52              |
| 1:0:2526:C:O2'    | 1:0:2527:U:H5'    | 2.10                     | 0.52              |
| 1:0:2638:G:H1'    | 37:0:7250:HOH:O   | 2.09                     | 0.52              |
| 1:0:2768:A:H5''   | 37:0:3931:HOH:O   | 2.09                     | 0.52              |
| 2:9:49:G:O2'      | 2:9:50:G:H5'      | 2.10                     | 0.52              |
| 13:K:74:VAL:HG12  | 13:K:75:ARG:HG3   | 1.91                     | 0.52              |
| 25:W:141:HIS:HB2  | 25:W:146:ILE:HG12 | 1.90                     | 0.52              |
| 1:0:1384:C:H5'    | 26:X:30:MET:HG2   | 1.92                     | 0.52              |
| 1:0:2072:G:C6     | 1:0:2533:C:H1'    | 2.45                     | 0.52              |
| 1:0:2090:G:H2'    | 1:0:2091:G:C8     | 2.44                     | 0.52              |
| 1:0:2300:A:H4'    | 1:0:2301:A:O5'    | 2.11                     | 0.52              |
| 1:0:2316:G:H4'    | 37:0:5592:HOH:O   | 2.09                     | 0.52              |
| 37:0:5631:HOH:O   | 30:2:20:ARG:HB3   | 2.10                     | 0.52              |
| 2:9:35:C:H5''     | 37:9:8453:HOH:O   | 2.10                     | 0.52              |
| 4:B:30:PRO:HB2    | 4:B:39:GLN:NE2    | 2.25                     | 0.52              |
| 8:F:19:ALA:O      | 8:F:22:VAL:HG22   | 2.10                     | 0.52              |
| 11:I:134:SER:N    | 37:I:7330:HOH:O   | 2.43                     | 0.52              |
| 18:P:38:GLU:HA    | 18:P:41:ARG:NH1   | 2.25                     | 0.52              |
| 25:W:108:ARG:HE   | 25:W:114:PRO:HG3  | 1.75                     | 0.52              |
| 1:0:644:G:H5'     | 1:0:644:G:N3      | 2.24                     | 0.51              |
| 1:0:1170:U:O2'    | 1:0:1172:G:N7     | 2.35                     | 0.51              |
| 1:0:1185:U:OP1    | 11:I:126:LYS:HD3  | 2.10                     | 0.51              |
| 3:A:125:ASN:CB    | 3:A:158:VAL:HG12  | 2.40                     | 0.51              |
| 4:B:7:ARG:CG      | 4:B:7:ARG:NH1     | 2.71                     | 0.51              |
| 10:H:56:GLN:HE21  | 10:H:126:ARG:NE   | 1.98                     | 0.51              |
| 11:I:74:PRO:HG2   | 11:I:77:GLU:CD    | 2.34                     | 0.51              |
| 14:L:57:VAL:HG12  | 14:L:57:VAL:O     | 2.10                     | 0.51              |
| 20:R:68:HIS:CD2   | 20:R:76:ASP:HB2   | 2.45                     | 0.51              |
| 24:V:56:ILE:O     | 24:V:60:GLN:HG3   | 2.09                     | 0.51              |
| 27:Y:189:ASN:ND2  | 27:Y:192:ASP:H    | 2.08                     | 0.51              |
| 1:0:1266:U:H4'    | 27:Y:115:ARG:HH21 | 1.74                     | 0.51              |
| 1:0:1450:C:C4'    | 1:0:1451:C:OP2    | 2.57                     | 0.51              |
| 1:0:1730:G:H5'    | 1:0:1731:C:C6     | 2.45                     | 0.51              |
| 15:M:24:GLN:NE2   | 15:M:27:ARG:HH11  | 2.08                     | 0.51              |
| 25:W:65:VAL:HA    | 25:W:68:THR:CG2   | 2.39                     | 0.51              |
| 27:Y:144:ARG:NH2  | 37:Y:8612:HOH:O   | 2.44                     | 0.51              |
| 7:E:36:PRO:HD3    | 12:J:127:ILE:HD12 | 1.91                     | 0.51              |
| 11:I:82:GLU:OE1   | 11:I:108:ILE:HG13 | 2.10                     | 0.51              |
| 16:N:154:LEU:HG   | 16:N:155:GLU:N    | 2.24                     | 0.51              |
| 26:X:74:ALA:HB1   | 26:X:85:VAL:HG22  | 1.91                     | 0.51              |
| 27:Y:200:THR:HG22 | 27:Y:201:GLU:CG   | 2.31                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:2488:A:H61   | 1:O:2534:C:H42   | 1.58                     | 0.51              |
| 10:H:162:ARG:HD3 | 37:H:8384:HOH:O  | 2.10                     | 0.51              |
| 13:K:87:ARG:NE   | 37:K:4854:HOH:O  | 2.43                     | 0.51              |
| 1:O:2363:G:O3'   | 19:Q:11:ARG:NH1  | 2.44                     | 0.51              |
| 1:O:2434:A:O3'   | 31:3:28:GLY:HA3  | 2.11                     | 0.51              |
| 6:D:10:PHE:CE1   | 6:D:11:HIS:HB3   | 2.45                     | 0.51              |
| 6:D:58:VAL:HG12  | 6:D:59:GLY:N     | 2.25                     | 0.51              |
| 7:E:31:ARG:HH12  | 7:E:68:HIS:CE1   | 2.29                     | 0.51              |
| 8:F:16:ALA:HA    | 8:F:111:ILE:HD13 | 1.92                     | 0.51              |
| 8:F:46:GLU:N     | 37:F:3461:HOH:O  | 2.43                     | 0.51              |
| 13:K:98:VAL:HG22 | 13:K:102:GLU:C   | 2.35                     | 0.51              |
| 17:O:96:VAL:HA   | 37:O:4258:HOH:O  | 2.10                     | 0.51              |
| 1:O:1173:A:H2'   | 37:O:3853:HOH:O  | 2.09                     | 0.51              |
| 1:O:1878:G:H4'   | 37:O:3621:HOH:O  | 2.11                     | 0.51              |
| 2:9:20:G:H3'     | 37:9:8433:HOH:O  | 2.10                     | 0.51              |
| 3:A:129:LEU:CD1  | 3:A:145:MET:HE1  | 2.41                     | 0.51              |
| 6:D:65:GLU:HA    | 37:D:6752:HOH:O  | 2.10                     | 0.51              |
| 6:D:146:LYS:NZ   | 16:N:107:ASN:ND2 | 2.57                     | 0.51              |
| 8:F:99:THR:O     | 8:F:99:THR:HG23  | 2.10                     | 0.51              |
| 10:H:38:LYS:HE2  | 10:H:42:ASP:HB2  | 1.93                     | 0.51              |
| 16:N:169:PRO:O   | 16:N:172:PHE:HB3 | 2.11                     | 0.51              |
| 16:N:171:HIS:CE1 | 37:N:8565:HOH:O  | 2.64                     | 0.51              |
| 18:P:13:VAL:HG21 | 18:P:41:ARG:HG2  | 1.92                     | 0.51              |
| 20:R:25:PHE:CE2  | 20:R:29:LYS:HE2  | 2.45                     | 0.51              |
| 20:R:132:ARG:CZ  | 37:R:8582:HOH:O  | 2.58                     | 0.51              |
| 1:O:1562:C:H42   | 1:O:2738:G:H1    | 1.58                     | 0.51              |
| 1:O:2769:C:O2'   | 1:O:2770:G:H5'   | 2.10                     | 0.51              |
| 14:L:62:ALA:HB2  | 14:L:103:ALA:CB  | 2.41                     | 0.51              |
| 16:N:37:ARG:NH2  | 37:N:8532:HOH:O  | 2.44                     | 0.51              |
| 22:T:49:GLU:HB3  | 22:T:59:GLU:CG   | 2.40                     | 0.51              |
| 1:O:818:A:O2'    | 28:Z:13:ARG:HD3  | 2.10                     | 0.51              |
| 1:O:1497:G:H4'   | 1:O:1627:G:O2'   | 2.11                     | 0.51              |
| 1:O:2251:G:H2'   | 1:O:2252:A:C8    | 2.46                     | 0.51              |
| 4:B:138:GLY:O    | 4:B:139:ASP:O    | 2.28                     | 0.51              |
| 5:C:27:ARG:HG2   | 5:C:30:LEU:HG    | 1.92                     | 0.51              |
| 6:D:81:GLU:O     | 6:D:85:GLN:HG3   | 2.11                     | 0.51              |
| 22:T:52:ARG:HB2  | 22:T:95:ASN:HB3  | 1.93                     | 0.51              |
| 29:1:10:LYS:HG3  | 37:1:8429:HOH:O  | 2.10                     | 0.51              |
| 31:3:56:PRO:N    | 37:3:8548:HOH:O  | 2.43                     | 0.51              |
| 1:O:2896:A:OP1   | 26:X:15:ARG:NH1  | 2.44                     | 0.51              |
| 37:O:4070:HOH:O  | 5:C:50:GLU:HG2   | 2.09                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:9:91:C:H2'      | 2:9:92:G:O4'      | 2.10                     | 0.51              |
| 3:A:66:ARG:HH11   | 3:A:66:ARG:HB2    | 1.74                     | 0.51              |
| 3:A:94:LEU:HG     | 3:A:99:ILE:HD11   | 1.93                     | 0.51              |
| 5:C:246:ARG:HB3   | 5:C:246:ARG:NH1   | 2.26                     | 0.51              |
| 6:D:64:ARG:HB3    | 6:D:67:ASP:OD2    | 2.10                     | 0.51              |
| 6:D:153:THR:HG22  | 37:D:5234:HOH:O   | 2.11                     | 0.51              |
| 7:E:31:ARG:HH12   | 7:E:68:HIS:CG     | 2.29                     | 0.51              |
| 7:E:43:ASP:HA     | 37:E:5864:HOH:O   | 2.11                     | 0.51              |
| 11:I:82:GLU:CD    | 11:I:108:ILE:HG13 | 2.36                     | 0.51              |
| 1:0:88:G:H8       | 1:0:88:G:H5'      | 1.76                     | 0.51              |
| 1:0:656:G:OP2     | 17:O:37:ARG:HD2   | 2.11                     | 0.51              |
| 1:0:1503:U:H2'    | 1:0:1504:A:O4'    | 2.11                     | 0.51              |
| 1:0:1592:G:O2'    | 1:0:1593:C:O4'    | 2.27                     | 0.51              |
| 1:0:2415:A:C2     | 16:N:25:ARG:HB3   | 2.46                     | 0.51              |
| 3:A:128:LEU:HD21  | 3:A:131:HIS:HE1   | 1.76                     | 0.51              |
| 5:C:129:HIS:CE1   | 5:C:231:ARG:HA    | 2.46                     | 0.51              |
| 5:C:246:ARG:CZ    | 37:C:8423:HOH:O   | 2.56                     | 0.51              |
| 6:D:99:ASP:O      | 6:D:159:PRO:HG3   | 2.10                     | 0.51              |
| 6:D:128:LEU:N     | 37:D:6007:HOH:O   | 2.44                     | 0.51              |
| 10:H:167:PRO:O    | 10:H:168:ALA:HB2  | 2.11                     | 0.51              |
| 13:K:28:GLU:HB3   | 13:K:59:LYS:HB2   | 1.93                     | 0.51              |
| 14:L:101:ASP:C    | 14:L:103:ALA:H    | 2.18                     | 0.51              |
| 15:M:15:PRO:HA    | 15:M:20:LEU:HD23  | 1.92                     | 0.51              |
| 19:Q:75:ILE:CD1   | 19:Q:84:ILE:HD11  | 2.41                     | 0.51              |
| 25:W:31:HIS:HB3   | 37:W:5420:HOH:O   | 2.10                     | 0.51              |
| 26:X:43:VAL:CG1   | 26:X:47:ALA:HB3   | 2.41                     | 0.51              |
| 27:Y:107:PRO:HB3  | 27:Y:182:PHE:CE2  | 2.46                     | 0.51              |
| 1:0:538:C:H5''    | 1:0:539:G:C8      | 2.45                     | 0.50              |
| 1:0:558:C:C2'     | 1:0:559:U:C5'     | 2.89                     | 0.50              |
| 1:0:1236:A:H2'    | 1:0:1237:U:O4'    | 2.11                     | 0.50              |
| 2:9:2:U:H4'       | 2:9:2:U:OP2       | 2.11                     | 0.50              |
| 8:F:58:GLU:CD     | 15:M:27:ARG:HH22  | 2.15                     | 0.50              |
| 18:P:103:THR:O    | 18:P:107:GLU:HG3  | 2.11                     | 0.50              |
| 25:W:122:ARG:CG   | 25:W:122:ARG:NH1  | 2.73                     | 0.50              |
| 1:0:2507:G:H2'    | 1:0:2510:C:H42    | 1.76                     | 0.50              |
| 37:O:6954:HOH:O   | 11:I:127:GLU:HG2  | 2.11                     | 0.50              |
| 14:L:120:LEU:HD12 | 14:L:133:VAL:HG21 | 1.94                     | 0.50              |
| 19:Q:40:HIS:CE1   | 19:Q:94:GLN:HA    | 2.47                     | 0.50              |
| 20:R:18:LEU:HG    | 20:R:91:LEU:HD13  | 1.92                     | 0.50              |
| 25:W:5:VAL:O      | 25:W:52:VAL:HG22  | 2.11                     | 0.50              |
| 27:Y:184:GLU:OE1  | 27:Y:204:ARG:NH1  | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:9:20:G:O2'      | 2:9:21:G:H5'      | 2.11                     | 0.50              |
| 3:A:132:ASP:OD1   | 3:A:133:ARG:N     | 2.44                     | 0.50              |
| 4:B:17:LYS:O      | 4:B:260:HIS:HD2   | 1.94                     | 0.50              |
| 8:F:91:VAL:CG1    | 8:F:92:GLY:H      | 2.21                     | 0.50              |
| 14:L:125:PHE:CZ   | 14:L:140:VAL:HG13 | 2.46                     | 0.50              |
| 21:S:57:THR:CG2   | 21:S:58:MET:N     | 2.74                     | 0.50              |
| 25:W:137:GLN:NE2  | 25:W:141:HIS:HE1  | 1.95                     | 0.50              |
| 1:0:447:A:OP1     | 22:T:2:LYS:HG2    | 2.12                     | 0.50              |
| 1:0:797:A:H4'     | 28:Z:10:ARG:N     | 2.26                     | 0.50              |
| 1:0:960:G:N3      | 1:0:960:G:H2'     | 2.26                     | 0.50              |
| 1:0:1234:U:N3     | 4:B:244:PRO:HB3   | 2.27                     | 0.50              |
| 1:0:2270:G:H4'    | 3:A:223:ARG:NH1   | 2.26                     | 0.50              |
| 4:B:162:MET:CE    | 4:B:308:LEU:HD21  | 2.38                     | 0.50              |
| 5:C:129:HIS:HD2   | 5:C:165:ASP:OD2   | 1.95                     | 0.50              |
| 7:E:22:VAL:O      | 7:E:28:SER:HA     | 2.12                     | 0.50              |
| 18:P:16:VAL:HG12  | 18:P:17:GLY:N     | 2.26                     | 0.50              |
| 28:Z:19:GLY:O     | 28:Z:23:ARG:HG2   | 2.10                     | 0.50              |
| 1:0:710:G:P       | 17:O:24:ALA:HB3   | 2.52                     | 0.50              |
| 1:0:941:G:O2'     | 1:0:942:U:H5'     | 2.11                     | 0.50              |
| 2:9:41:C:C6       | 6:D:50:VAL:HG21   | 2.46                     | 0.50              |
| 3:A:130:THR:HG22  | 3:A:131:HIS:O     | 2.10                     | 0.50              |
| 5:C:16:VAL:HG12   | 5:C:17:ASP:H      | 1.74                     | 0.50              |
| 5:C:107:ARG:NH1   | 5:C:107:ARG:HB3   | 2.26                     | 0.50              |
| 11:I:92:PRO:HG3   | 11:I:134:SER:O    | 2.10                     | 0.50              |
| 11:I:100:LEU:HD22 | 11:I:104:GLN:OE1  | 2.12                     | 0.50              |
| 1:0:256:C:H2'     | 1:0:257:G:O4'     | 2.12                     | 0.50              |
| 1:0:1205:U:C2'    | 1:0:1206:U:H5''   | 2.42                     | 0.50              |
| 1:0:2842:G:H2'    | 1:0:2843:A:H5'    | 1.92                     | 0.50              |
| 5:C:166:ILE:CD1   | 5:C:207:LEU:HD13  | 2.42                     | 0.50              |
| 11:I:132:CYS:N    | 37:I:5371:HOH:O   | 2.43                     | 0.50              |
| 12:J:88:PRO:O     | 12:J:94:GLY:HA3   | 2.11                     | 0.50              |
| 23:U:52:THR:HG22  | 23:U:54:THR:HB    | 1.94                     | 0.50              |
| 28:Z:44:GLU:HG3   | 28:Z:46:ARG:HG3   | 1.94                     | 0.50              |
| 31:3:87:ARG:NH1   | 37:3:8525:HOH:O   | 2.45                     | 0.50              |
| 1:0:1717:A:H5''   | 18:P:54:LYS:HB2   | 1.94                     | 0.50              |
| 1:0:2320:U:H4'    | 1:0:2321:A:O4'    | 2.12                     | 0.50              |
| 3:A:36:ASP:O      | 3:A:38:ILE:N      | 2.44                     | 0.50              |
| 4:B:102:THR:HG21  | 4:B:182:VAL:O     | 2.11                     | 0.50              |
| 5:C:77:ALA:O      | 5:C:78:ARG:HG3    | 2.11                     | 0.50              |
| 5:C:150:THR:HA    | 5:C:203:ALA:O     | 2.12                     | 0.50              |
| 6:D:10:PHE:CD1    | 6:D:11:HIS:N      | 2.80                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:22:VAL:HG22  | 6:D:74:THR:HG22  | 1.94                     | 0.50              |
| 28:Z:26:VAL:O    | 28:Z:30:GLU:HG3  | 2.12                     | 0.50              |
| 1:0:1595:G:O2'   | 1:0:1596:U:H5'   | 2.11                     | 0.50              |
| 5:C:219:ASN:O    | 5:C:222:ASP:OD1  | 2.30                     | 0.50              |
| 7:E:11:VAL:CG1   | 7:E:12:ASP:N     | 2.74                     | 0.50              |
| 12:J:45:VAL:HG22 | 12:J:46:ILE:N    | 2.26                     | 0.50              |
| 25:W:41:TYR:O    | 25:W:45:VAL:HG13 | 2.11                     | 0.50              |
| 1:0:1185:U:H5'   | 37:0:6954:HOH:O  | 2.12                     | 0.50              |
| 1:0:2524:G:H21   | 1:0:2526:C:N4    | 2.10                     | 0.50              |
| 2:9:55:U:H4'     | 2:9:56:A:H8      | 1.74                     | 0.50              |
| 3:A:192:VAL:HG12 | 3:A:207:GLN:HB3  | 1.94                     | 0.50              |
| 7:E:21:THR:HG23  | 7:E:30:THR:OG1   | 2.12                     | 0.50              |
| 25:W:19:ASP:O    | 25:W:23:MET:HG3  | 2.12                     | 0.50              |
| 1:0:281:U:O2'    | 1:0:282:C:H5'    | 2.12                     | 0.49              |
| 1:0:1462:C:H2'   | 1:0:1463:A:C8    | 2.47                     | 0.49              |
| 1:0:2329:C:O2'   | 1:0:2330:U:H5'   | 2.12                     | 0.49              |
| 5:C:162:VAL:CG1  | 5:C:192:ILE:HD11 | 2.42                     | 0.49              |
| 8:F:91:VAL:CG1   | 8:F:92:GLY:N     | 2.73                     | 0.49              |
| 12:J:46:ILE:HA   | 37:J:1123:HOH:O  | 2.11                     | 0.49              |
| 13:K:106:GLY:HA3 | 37:K:5264:HOH:O  | 2.12                     | 0.49              |
| 16:N:7:LYS:HE2   | 37:N:8513:HOH:O  | 2.10                     | 0.49              |
| 17:O:7:LEU:HD22  | 37:O:5650:HOH:O  | 2.12                     | 0.49              |
| 18:P:143:ALA:HA  | 37:P:190:HOH:O   | 2.11                     | 0.49              |
| 22:T:38:ARG:NH1  | 37:T:6217:HOH:O  | 2.44                     | 0.49              |
| 1:0:797:A:O4'    | 28:Z:10:ARG:N    | 2.45                     | 0.49              |
| 1:0:1787:C:OP1   | 18:P:68:LYS:HE2  | 2.12                     | 0.49              |
| 3:A:94:LEU:HD23  | 3:A:94:LEU:N     | 2.26                     | 0.49              |
| 6:D:10:PHE:CG    | 6:D:11:HIS:N     | 2.80                     | 0.49              |
| 11:I:112:LYS:C   | 11:I:114:PRO:HD2 | 2.36                     | 0.49              |
| 26:X:76:ARG:O    | 26:X:77:PHE:HB3  | 2.12                     | 0.49              |
| 1:0:656:G:H5'    | 17:O:3:THR:CG2   | 2.42                     | 0.49              |
| 1:0:1060:C:H6    | 1:0:1060:C:H5'   | 1.78                     | 0.49              |
| 1:0:1183:C:N4    | 1:0:1184:C:H41   | 2.10                     | 0.49              |
| 1:0:1699:C:H4'   | 37:0:5939:HOH:O  | 2.13                     | 0.49              |
| 4:B:108:GLU:HB3  | 4:B:111:ARG:HD2  | 1.93                     | 0.49              |
| 16:N:143:ARG:HA  | 16:N:172:PHE:CD2 | 2.47                     | 0.49              |
| 25:W:126:ASP:HB3 | 25:W:135:GLY:O   | 2.12                     | 0.49              |
| 1:0:291:C:H2'    | 1:0:292:G:O4'    | 2.12                     | 0.49              |
| 1:0:470:U:O2'    | 29:1:16:HIS:CD2  | 2.64                     | 0.49              |
| 1:0:2403:C:H3'   | 37:0:4708:HOH:O  | 2.12                     | 0.49              |
| 1:0:2756:U:N3    | 1:0:2896:A:C2    | 2.70                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:O:3568:HOH:O   | 4:B:27:ASN:HB2    | 2.11                     | 0.49              |
| 4:B:27:ASN:HD22   | 4:B:27:ASN:H      | 1.60                     | 0.49              |
| 5:C:236:THR:O     | 5:C:237:GLU:C     | 2.55                     | 0.49              |
| 12:J:74:ARG:O     | 12:J:78:ILE:HG12  | 2.12                     | 0.49              |
| 14:L:143:THR:HG22 | 14:L:145:LEU:H    | 1.77                     | 0.49              |
| 18:P:105:LEU:HD21 | 18:P:137:LEU:HD21 | 1.95                     | 0.49              |
| 23:U:44:ARG:HB3   | 37:U:3805:HOH:O   | 2.11                     | 0.49              |
| 27:Y:107:PRO:HB3  | 27:Y:182:PHE:CD2  | 2.48                     | 0.49              |
| 1:O:189:A:OP1     | 15:M:171:ARG:NH2  | 2.44                     | 0.49              |
| 1:O:1164:U:H4'    | 1:O:1165:G:OP1    | 2.12                     | 0.49              |
| 1:O:1940:C:H4'    | 37:O:6837:HOH:O   | 2.11                     | 0.49              |
| 5:C:180:SER:HB2   | 37:C:8444:HOH:O   | 2.11                     | 0.49              |
| 6:D:56:ARG:N      | 37:D:6752:HOH:O   | 2.43                     | 0.49              |
| 7:E:10:ASP:HA     | 37:E:3707:HOH:O   | 2.11                     | 0.49              |
| 7:E:166:VAL:HG12  | 37:E:3134:HOH:O   | 2.12                     | 0.49              |
| 11:I:110:GLU:HG2  | 11:I:113:HIS:NE2  | 2.28                     | 0.49              |
| 24:V:64:GLY:O     | 24:V:65:ASP:CB    | 2.59                     | 0.49              |
| 27:Y:186:ARG:HG2  | 27:Y:186:ARG:NH1  | 2.27                     | 0.49              |
| 1:O:1118:A:C8     | 1:O:1119:G:H5''   | 2.47                     | 0.49              |
| 1:O:1197:G:N2     | 37:O:5734:HOH:O   | 2.45                     | 0.49              |
| 1:O:1996:U:O2'    | 1:O:1997:A:H5'    | 2.13                     | 0.49              |
| 1:O:2563:U:H2'    | 1:O:2565:C:O5'    | 2.12                     | 0.49              |
| 2:9:31:C:H2'      | 2:9:32:G:O4'      | 2.13                     | 0.49              |
| 4:B:56:ASP:OD1    | 4:B:322:ARG:HB3   | 2.12                     | 0.49              |
| 4:B:241:PRO:HD2   | 37:B:8662:HOH:O   | 2.11                     | 0.49              |
| 5:C:151:GLN:O     | 5:C:154:VAL:HB    | 2.13                     | 0.49              |
| 14:L:97:VAL:HG12  | 14:L:98:GLU:O     | 2.13                     | 0.49              |
| 16:N:143:ARG:HH12 | 16:N:173:ASP:CG   | 2.21                     | 0.49              |
| 22:T:71:VAL:HG11  | 22:T:90:PRO:CB    | 2.29                     | 0.49              |
| 1:O:1168:C:C5'    | 37:I:5128:HOH:O   | 2.61                     | 0.49              |
| 3:A:123:GLY:HA3   | 3:A:162:GLY:HA2   | 1.95                     | 0.49              |
| 5:C:236:THR:HG22  | 5:C:239:ALA:CB    | 2.43                     | 0.49              |
| 6:D:86:THR:C      | 6:D:89:PRO:HD2    | 2.37                     | 0.49              |
| 1:O:2672:C:O2'    | 1:O:2673:U:H5'    | 2.13                     | 0.49              |
| 4:B:60:SER:C      | 4:B:62:ARG:H      | 2.20                     | 0.49              |
| 16:N:58:LEU:N     | 16:N:58:LEU:HD12  | 2.28                     | 0.49              |
| 19:Q:30:VAL:HG12  | 19:Q:30:VAL:O     | 2.13                     | 0.49              |
| 25:W:130:HIS:O    | 25:W:136:GLY:HA3  | 2.13                     | 0.49              |
| 1:O:380:A:OP2     | 15:M:9:ARG:HD2    | 2.12                     | 0.49              |
| 1:O:2912:C:H2'    | 1:O:2913:A:O4'    | 2.13                     | 0.49              |
| 4:B:63:GLU:HG3    | 4:B:63:GLU:O      | 2.12                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:314:ALA:CB    | 4:B:317:PRO:HG3  | 2.43                     | 0.49              |
| 7:E:84:MET:HE2    | 7:E:133:VAL:HG23 | 1.92                     | 0.49              |
| 13:K:79:PRO:HB2   | 37:K:782:HOH:O   | 2.12                     | 0.49              |
| 15:M:34:GLU:HB3   | 15:M:38:GLU:HG3  | 1.94                     | 0.49              |
| 20:R:17:MET:HE1   | 20:R:19:ARG:CZ   | 2.43                     | 0.49              |
| 23:U:49:LEU:HD11  | 37:U:3805:HOH:O  | 2.13                     | 0.49              |
| 25:W:13:MET:HE2   | 25:W:18:GLN:N    | 2.28                     | 0.49              |
| 27:Y:122:ARG:NH2  | 37:Y:8535:HOH:O  | 2.46                     | 0.49              |
| 27:Y:126:PRO:HG2  | 27:Y:128:PHE:CZ  | 2.47                     | 0.49              |
| 1:O:407:A:H5'     | 37:O:5526:HOH:O  | 2.12                     | 0.49              |
| 1:O:2044:G:OP1    | 26:X:23:HIS:HE1  | 1.96                     | 0.49              |
| 4:B:248:ARG:HG2   | 37:B:8578:HOH:O  | 2.12                     | 0.49              |
| 14:L:65:ASP:CG    | 14:L:111:ALA:HB3 | 2.38                     | 0.49              |
| 15:M:43:PRO:HG3   | 15:M:62:VAL:HG21 | 1.95                     | 0.49              |
| 22:T:18:GLU:O     | 22:T:21:LYS:HG2  | 2.13                     | 0.49              |
| 1:O:95:A:H5''     | 1:O:97:G:O4'     | 2.12                     | 0.48              |
| 1:O:447:A:O2'     | 1:O:448:G:H5'    | 2.14                     | 0.48              |
| 1:O:1010:C:H4'    | 16:N:4:PRO:HB2   | 1.95                     | 0.48              |
| 1:O:1789:G:O6     | 18:P:73:HIS:HE1  | 1.96                     | 0.48              |
| 4:B:16:ARG:NH2    | 37:B:8557:HOH:O  | 2.40                     | 0.48              |
| 4:B:41:PHE:CZ     | 4:B:79:MET:HG3   | 2.47                     | 0.48              |
| 4:B:80:ARG:HD3    | 37:B:8611:HOH:O  | 2.13                     | 0.48              |
| 4:B:156:LYS:HZ1   | 4:B:160:ASP:CG   | 2.21                     | 0.48              |
| 7:E:107:PHE:CE2   | 7:E:108:LEU:HD13 | 2.48                     | 0.48              |
| 11:I:108:ILE:HG21 | 11:I:128:VAL:CG1 | 2.43                     | 0.48              |
| 13:K:29:LEU:HB3   | 13:K:55:VAL:CG1  | 2.33                     | 0.48              |
| 16:N:37:ARG:CZ    | 37:N:8532:HOH:O  | 2.61                     | 0.48              |
| 20:R:119:VAL:HG21 | 20:R:142:ASP:CG  | 2.38                     | 0.48              |
| 21:S:73:ASP:OD1   | 21:S:75:GLN:HB2  | 2.13                     | 0.48              |
| 27:Y:115:ARG:NE   | 37:Y:8555:HOH:O  | 2.45                     | 0.48              |
| 31:3:48:ASN:ND2   | 31:3:50:GLY:H    | 2.11                     | 0.48              |
| 1:O:538:C:OP2     | 27:Y:134:HIS:HE1 | 1.96                     | 0.48              |
| 1:O:584:U:H3'     | 37:O:5595:HOH:O  | 2.12                     | 0.48              |
| 1:O:654:A:OP2     | 17:O:38:ARG:HD3  | 2.13                     | 0.48              |
| 1:O:1500:U:OP2    | 18:P:41:ARG:NH2  | 2.46                     | 0.48              |
| 5:C:19:PRO:HG2    | 5:C:22:PHE:CD1   | 2.48                     | 0.48              |
| 6:D:41:LEU:HA     | 6:D:44:ILE:CG2   | 2.42                     | 0.48              |
| 8:F:58:GLU:HA     | 8:F:61:MET:HE2   | 1.95                     | 0.48              |
| 1:O:1056:U:H2'    | 1:O:1057:A:O4'   | 2.14                     | 0.48              |
| 1:O:1484:G:H2'    | 37:O:8618:HOH:O  | 2.13                     | 0.48              |
| 6:D:23:VAL:HG12   | 6:D:130:VAL:HG22 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:H:3:ALA:CA     | 10:H:58:ARG:HH12  | 2.25                     | 0.48              |
| 15:M:99:ARG:NH2   | 15:M:170:ASN:HD22 | 2.09                     | 0.48              |
| 23:U:17:THR:HG22  | 23:U:18:GLY:N     | 2.28                     | 0.48              |
| 1:O:474:C:O3'     | 5:C:73:LEU:CD2    | 2.62                     | 0.48              |
| 1:O:475:G:OP1     | 5:C:73:LEU:HD22   | 2.13                     | 0.48              |
| 1:O:2521:A:OP2    | 10:H:3:ALA:HB3    | 2.13                     | 0.48              |
| 7:E:77:THR:OG1    | 7:E:78:GLU:N      | 2.45                     | 0.48              |
| 7:E:145:ALA:HB1   | 7:E:168:ILE:CD1   | 2.43                     | 0.48              |
| 16:N:86:LEU:O     | 16:N:90:LEU:HG    | 2.13                     | 0.48              |
| 27:Y:112:GLU:OE2  | 27:Y:115:ARG:NH1  | 2.47                     | 0.48              |
| 1:O:450:C:OP1     | 5:C:184:ARG:NH2   | 2.29                     | 0.48              |
| 37:O:6914:HOH:O   | 22:T:9:LYS:HD2    | 2.12                     | 0.48              |
| 3:A:36:ASP:HA     | 3:A:83:GLY:HA3    | 1.95                     | 0.48              |
| 3:A:194:MET:CE    | 3:A:199:HIS:HB2   | 2.43                     | 0.48              |
| 10:H:111:ASP:HB2  | 37:H:8349:HOH:O   | 2.13                     | 0.48              |
| 15:M:134:ILE:HG23 | 15:M:141:ILE:HD13 | 1.94                     | 0.48              |
| 18:P:98:ILE:HD12  | 18:P:102:ARG:NE   | 2.28                     | 0.48              |
| 1:O:1163:G:H5''   | 11:I:115:ASP:HB3  | 1.95                     | 0.48              |
| 1:O:1878:G:O2'    | 1:O:1879:U:P      | 2.72                     | 0.48              |
| 1:O:1909:A:N1     | 1:O:2128:G:H1'    | 2.28                     | 0.48              |
| 2:9:92:G:H2'      | 2:9:93:A:C8       | 2.49                     | 0.48              |
| 4:B:217:ARG:HG3   | 4:B:257:THR:HG22  | 1.95                     | 0.48              |
| 6:D:84:LEU:C      | 6:D:86:THR:H      | 2.21                     | 0.48              |
| 6:D:84:LEU:HA     | 6:D:87:ALA:HB3    | 1.96                     | 0.48              |
| 8:F:22:VAL:HG21   | 8:F:104:ALA:HB2   | 1.96                     | 0.48              |
| 8:F:28:ALA:CB     | 8:F:99:THR:HG23   | 2.43                     | 0.48              |
| 10:H:146:VAL:HG22 | 37:H:8379:HOH:O   | 2.12                     | 0.48              |
| 15:M:84:LYS:HE2   | 37:M:8574:HOH:O   | 2.13                     | 0.48              |
| 15:M:164:THR:HB   | 37:M:8519:HOH:O   | 2.13                     | 0.48              |
| 16:N:67:ALA:C     | 16:N:69:TYR:H     | 2.21                     | 0.48              |
| 16:N:71:TRP:HE3   | 16:N:175:LEU:HD22 | 1.78                     | 0.48              |
| 23:U:9:CYS:CA     | 23:U:52:THR:HG23  | 2.43                     | 0.48              |
| 26:X:76:ARG:HG3   | 26:X:76:ARG:NH1   | 2.27                     | 0.48              |
| 31:3:3:MET:O      | 31:3:90:PHE:HA    | 2.13                     | 0.48              |
| 1:O:920:C:H5'     | 1:O:921:G:C4      | 2.49                     | 0.48              |
| 1:O:1730:G:C5'    | 1:O:1731:C:C6     | 2.96                     | 0.48              |
| 16:N:79:PRO:HG3   | 16:N:142:THR:O    | 2.14                     | 0.48              |
| 24:V:57:LYS:HA    | 24:V:60:GLN:HE21  | 1.78                     | 0.48              |
| 27:Y:172:THR:HG22 | 27:Y:173:ALA:N    | 2.29                     | 0.48              |
| 28:Z:37:HIS:HB2   | 28:Z:47:VAL:HB    | 1.95                     | 0.48              |
| 28:Z:59:TYR:HA    | 37:Z:8432:HOH:O   | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:396:U:OP2     | 31:3:38:ARG:NH1   | 2.45                     | 0.48              |
| 1:0:1014:A:H2'    | 1:0:1015:C:H5'    | 1.95                     | 0.48              |
| 9:G:12:ILE:HD12   | 37:G:692:HOH:O    | 2.14                     | 0.48              |
| 9:G:19:GLU:O      | 9:G:23:ILE:HG13   | 2.14                     | 0.48              |
| 22:T:49:GLU:HB3   | 22:T:59:GLU:HG3   | 1.96                     | 0.48              |
| 11:I:105:VAL:HG11 | 11:I:129:VAL:CG2  | 2.44                     | 0.48              |
| 12:J:42:GLU:O     | 12:J:131:THR:HG23 | 2.13                     | 0.48              |
| 13:K:75:ARG:HE    | 13:K:94:ALA:HB3   | 1.78                     | 0.48              |
| 20:R:106:GLY:HA2  | 20:R:109:MET:CE   | 2.44                     | 0.48              |
| 20:R:132:ARG:HG2  | 20:R:133:ALA:N    | 2.26                     | 0.48              |
| 27:Y:165:GLU:HB3  | 37:Y:8594:HOH:O   | 2.13                     | 0.48              |
| 1:0:1470:A:OP1    | 15:M:93:ARG:HD2   | 2.14                     | 0.48              |
| 1:0:2837:U:H1'    | 4:B:307:ARG:HH12  | 1.79                     | 0.48              |
| 37:0:5031:HOH:O   | 15:M:58:GLN:HG3   | 2.14                     | 0.48              |
| 4:B:205:VAL:O     | 4:B:307:ARG:NE    | 2.46                     | 0.48              |
| 8:F:2:VAL:HG11    | 15:M:23:LEU:HD23  | 1.94                     | 0.48              |
| 11:I:80:LYS:HB3   | 11:I:85:PHE:O     | 2.12                     | 0.48              |
| 25:W:6:GLN:CB     | 25:W:26:ILE:HD12  | 2.36                     | 0.48              |
| 30:2:48:ASP:O     | 30:2:49:GLU:HB2   | 2.14                     | 0.48              |
| 1:0:121:U:OP2     | 30:2:10:ARG:NH2   | 2.39                     | 0.47              |
| 1:0:344:C:H2'     | 1:0:345:G:O4'     | 2.13                     | 0.47              |
| 1:0:432:G:O2'     | 1:0:433:C:H5'     | 2.14                     | 0.47              |
| 1:0:1741:U:O2'    | 1:0:2723:G:H4'    | 2.14                     | 0.47              |
| 15:M:47:ASP:CG    | 15:M:48:LYS:N     | 2.72                     | 0.47              |
| 16:N:170:GLU:O    | 16:N:174:GLU:HG3  | 2.14                     | 0.47              |
| 1:0:564:G:H1'     | 37:0:5809:HOH:O   | 2.14                     | 0.47              |
| 1:0:2083:A:N6     | 12:J:90:LYS:HE2   | 2.28                     | 0.47              |
| 1:0:2791:U:H1'    | 1:0:2792:A:H5''   | 1.95                     | 0.47              |
| 3:A:1:GLY:HA2     | 3:A:197:VAL:HG23  | 1.97                     | 0.47              |
| 3:A:93:THR:HG23   | 3:A:154:ALA:O     | 2.14                     | 0.47              |
| 4:B:175:LEU:HD23  | 4:B:175:LEU:O     | 2.14                     | 0.47              |
| 4:B:243:ASN:HA    | 4:B:244:PRO:C     | 2.38                     | 0.47              |
| 5:C:13:ASP:OD1    | 5:C:13:ASP:O      | 2.32                     | 0.47              |
| 6:D:101:THR:HG22  | 37:D:7400:HOH:O   | 2.13                     | 0.47              |
| 12:J:52:GLN:HG3   | 12:J:53:ILE:N     | 2.29                     | 0.47              |
| 19:Q:31:GLU:CD    | 19:Q:93:ARG:HH12  | 2.21                     | 0.47              |
| 25:W:3:ALA:O      | 25:W:54:PHE:HA    | 2.14                     | 0.47              |
| 1:0:1505:U:H5'    | 1:0:1505:U:C6     | 2.46                     | 0.47              |
| 1:0:2472:C:O2'    | 1:0:2634:G:H4'    | 2.14                     | 0.47              |
| 8:F:13:GLU:OE2    | 8:F:78:GLU:HG2    | 2.13                     | 0.47              |
| 8:F:38:LYS:NZ     | 15:M:3:SER:HA     | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:U:47:ARG:CG   | 37:U:4381:HOH:O  | 2.61                     | 0.47              |
| 25:W:108:ARG:HE  | 25:W:114:PRO:CG  | 2.27                     | 0.47              |
| 1:0:420:U:H2'    | 1:0:421:C:C6     | 2.50                     | 0.47              |
| 1:0:1289:C:O2'   | 1:0:1290:G:H5'   | 2.14                     | 0.47              |
| 1:0:1439:C:OP1   | 30:2:41:HIS:HE1  | 1.97                     | 0.47              |
| 1:0:1666:C:C2'   | 1:0:1667:A:C5'   | 2.92                     | 0.47              |
| 1:0:1878:G:O2'   | 1:0:1879:U:OP2   | 2.33                     | 0.47              |
| 1:0:2326:U:H4'   | 1:0:2412:G:H4'   | 1.96                     | 0.47              |
| 1:0:2748:G:H5'   | 37:0:7030:HOH:O  | 2.14                     | 0.47              |
| 3:A:211:LYS:HD3  | 37:A:8614:HOH:O  | 2.13                     | 0.47              |
| 4:B:51:VAL:HG22  | 4:B:53:LEU:HD13  | 1.97                     | 0.47              |
| 13:K:4:LEU:HD22  | 13:K:116:GLU:HB3 | 1.97                     | 0.47              |
| 14:L:21:ARG:N    | 37:L:8530:HOH:O  | 2.47                     | 0.47              |
| 1:0:820:G:C5     | 3:A:171:LYS:HB2  | 2.50                     | 0.47              |
| 1:0:1667:A:H2'   | 1:0:1668:U:H6    | 1.78                     | 0.47              |
| 1:0:1733:A:H4'   | 4:B:212:GLN:HA   | 1.95                     | 0.47              |
| 1:0:2728:C:H4'   | 1:0:2894:C:HO2'  | 1.79                     | 0.47              |
| 3:A:33:GLU:H     | 3:A:33:GLU:CD    | 2.22                     | 0.47              |
| 4:B:36:PRO:CA    | 4:B:168:GLY:HA3  | 2.42                     | 0.47              |
| 4:B:207:LYS:HG2  | 4:B:304:PRO:HB3  | 1.95                     | 0.47              |
| 7:E:37:ASP:OD1   | 12:J:125:SER:HB3 | 2.15                     | 0.47              |
| 10:H:9:ILE:HG12  | 10:H:56:GLN:HG2  | 1.96                     | 0.47              |
| 16:N:181:ASP:OD1 | 16:N:182:GLY:N   | 2.47                     | 0.47              |
| 31:3:55:VAL:HB   | 31:3:56:PRO:HD2  | 1.96                     | 0.47              |
| 1:0:119:A:H2'    | 1:0:120:A:H5''   | 1.95                     | 0.47              |
| 1:0:2415:A:H2'   | 1:0:2416:G:H5'   | 1.96                     | 0.47              |
| 37:0:8728:HOH:O  | 3:A:11:ARG:HD3   | 2.15                     | 0.47              |
| 5:C:140:VAL:HG12 | 5:C:141:SER:N    | 2.29                     | 0.47              |
| 8:F:60:VAL:O     | 8:F:60:VAL:HG12  | 2.15                     | 0.47              |
| 8:F:100:ASP:HB3  | 37:F:5691:HOH:O  | 2.15                     | 0.47              |
| 10:H:20:ILE:HG23 | 10:H:120:ILE:CD1 | 2.43                     | 0.47              |
| 12:J:93:ARG:HH11 | 12:J:93:ARG:CB   | 2.22                     | 0.47              |
| 15:M:24:GLN:HE21 | 15:M:27:ARG:HH11 | 1.62                     | 0.47              |
| 16:N:67:ALA:C    | 16:N:69:TYR:N    | 2.73                     | 0.47              |
| 1:0:482:G:H4'    | 1:0:508:A:N1     | 2.30                     | 0.47              |
| 1:0:621:C:H5'    | 27:Y:132:ASP:OD2 | 2.15                     | 0.47              |
| 1:0:1164:U:H3    | 1:0:1192:A:H2    | 1.63                     | 0.47              |
| 1:0:1205:U:H2'   | 1:0:1206:U:H5''  | 1.97                     | 0.47              |
| 1:0:1250:C:O2'   | 1:0:1251:C:H5'   | 2.14                     | 0.47              |
| 1:0:1409:G:H5'   | 37:0:3232:HOH:O  | 2.14                     | 0.47              |
| 1:0:2073:G:OP2   | 1:0:2490:A:H5'   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:2724:U:H2'   | 1:0:2725:G:O4'   | 2.14                     | 0.47              |
| 1:0:2768:A:H3'   | 37:0:3931:HOH:O  | 2.13                     | 0.47              |
| 1:0:2769:C:H2'   | 1:0:2770:G:C5'   | 2.44                     | 0.47              |
| 37:0:8627:HOH:O  | 5:C:103:ASN:HB3  | 2.13                     | 0.47              |
| 3:A:128:LEU:HG   | 37:A:8576:HOH:O  | 2.13                     | 0.47              |
| 4:B:268:ARG:NH2  | 4:B:325:PRO:HG3  | 2.30                     | 0.47              |
| 4:B:275:GLY:O    | 4:B:291:ASP:HA   | 2.15                     | 0.47              |
| 4:B:312:ARG:HD3  | 4:B:315:VAL:HG13 | 1.96                     | 0.47              |
| 5:C:246:ARG:NH1  | 37:C:8369:HOH:O  | 2.47                     | 0.47              |
| 6:D:11:HIS:O     | 6:D:14:ARG:N     | 2.46                     | 0.47              |
| 12:J:47:THR:HG22 | 12:J:48:GLY:N    | 2.30                     | 0.47              |
| 12:J:74:ARG:NH1  | 12:J:76:ASP:HB2  | 2.30                     | 0.47              |
| 13:K:66:ARG:HG2  | 13:K:66:ARG:HH11 | 1.80                     | 0.47              |
| 15:M:99:ARG:CD   | 15:M:167:GLY:HA2 | 2.44                     | 0.47              |
| 16:N:163:PHE:O   | 16:N:164:ASP:CB  | 2.62                     | 0.47              |
| 25:W:4:LEU:HD23  | 25:W:54:PHE:HB3  | 1.96                     | 0.47              |
| 25:W:76:ASP:O    | 25:W:77:ALA:C    | 2.57                     | 0.47              |
| 28:Z:46:ARG:NH1  | 37:Z:8432:HOH:O  | 2.47                     | 0.47              |
| 30:2:18:ASN:ND2  | 30:2:40:ARG:H    | 2.08                     | 0.47              |
| 1:0:926:A:O2'    | 14:L:41:HIS:HD2  | 1.98                     | 0.47              |
| 1:0:1119:G:C8    | 12:J:52:GLN:NE2  | 2.83                     | 0.47              |
| 1:0:2670:G:O2'   | 1:0:2671:U:H5'   | 2.15                     | 0.47              |
| 3:A:105:VAL:HG13 | 3:A:155:THR:O    | 2.15                     | 0.47              |
| 3:A:135:VAL:HG21 | 3:A:147:ARG:NH1  | 2.30                     | 0.47              |
| 4:B:320:GLN:HE21 | 4:B:321:PRO:CD   | 2.26                     | 0.47              |
| 6:D:38:GLU:HB3   | 6:D:49:PRO:HG2   | 1.97                     | 0.47              |
| 10:H:66:ARG:HD3  | 37:H:8382:HOH:O  | 2.14                     | 0.47              |
| 24:V:39:ALA:C    | 24:V:41:GLU:N    | 2.73                     | 0.47              |
| 25:W:21:LEU:CD2  | 25:W:48:VAL:HG11 | 2.42                     | 0.47              |
| 25:W:65:VAL:CA   | 25:W:68:THR:HG22 | 2.44                     | 0.47              |
| 1:0:327:A:OP1    | 5:C:149:LYS:NZ   | 2.42                     | 0.47              |
| 1:0:776:A:OP1    | 29:1:28:HIS:HE1  | 1.98                     | 0.47              |
| 1:0:1477:C:H5'   | 1:0:1868:G:H5''  | 1.96                     | 0.47              |
| 1:0:1819:G:H2'   | 1:0:1820:G:C4'   | 2.45                     | 0.47              |
| 7:E:108:LEU:HB3  | 37:E:1306:HOH:O  | 2.15                     | 0.47              |
| 8:F:28:ALA:HB3   | 8:F:99:THR:HG23  | 1.96                     | 0.47              |
| 14:L:53:ARG:HH22 | 14:L:57:VAL:HG12 | 1.80                     | 0.47              |
| 15:M:5:TYR:HE2   | 15:M:46:LEU:HD13 | 1.80                     | 0.47              |
| 22:T:74:VAL:HB   | 22:T:77:VAL:HG21 | 1.97                     | 0.47              |
| 25:W:125:HIS:HD2 | 25:W:127:GLY:H   | 1.62                     | 0.47              |
| 2:9:64:C:C2'     | 2:9:65:A:H5'     | 2.45                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:10:PHE:N     | 37:D:1492:HOH:O   | 2.48                     | 0.47              |
| 6:D:11:HIS:CG    | 6:D:12:GLU:N      | 2.83                     | 0.47              |
| 6:D:59:GLY:C     | 6:D:61:PHE:H      | 2.23                     | 0.47              |
| 6:D:99:ASP:CB    | 6:D:103:ASN:HB2   | 2.45                     | 0.47              |
| 14:L:70:ASP:OD1  | 14:L:116:HIS:HD2  | 1.97                     | 0.47              |
| 14:L:145:LEU:O   | 14:L:145:LEU:HD23 | 2.15                     | 0.47              |
| 1:O:558:C:H2'    | 1:O:559:U:H5''    | 1.95                     | 0.46              |
| 1:O:1666:C:C2'   | 1:O:1667:A:H5'    | 2.42                     | 0.46              |
| 7:E:92:PRO:HB2   | 37:E:4917:HOH:O   | 2.14                     | 0.46              |
| 9:G:20:VAL:O     | 9:G:24:VAL:HG23   | 2.15                     | 0.46              |
| 13:K:10:GLN:NE2  | 13:K:10:GLN:N     | 2.43                     | 0.46              |
| 21:S:29:ASP:OD1  | 21:S:31:ARG:HG3   | 2.15                     | 0.46              |
| 31:3:73:GLU:HB2  | 37:3:8526:HOH:O   | 2.15                     | 0.46              |
| 1:O:1192:A:H3'   | 1:O:1193:A:H5'    | 1.98                     | 0.46              |
| 37:O:5819:HOH:O  | 6:D:55:LYS:HB2    | 2.16                     | 0.46              |
| 4:B:139:ASP:HB2  | 4:B:165:ARG:HE    | 1.80                     | 0.46              |
| 5:C:65:ARG:HG3   | 5:C:67:GLN:HB2    | 1.97                     | 0.46              |
| 5:C:107:ARG:NH2  | 37:C:8457:HOH:O   | 2.40                     | 0.46              |
| 8:F:48:VAL:CG2   | 8:F:74:PHE:HB3    | 2.44                     | 0.46              |
| 8:F:50:VAL:CG2   | 8:F:63:ILE:HG21   | 2.44                     | 0.46              |
| 16:N:73:ALA:HB1  | 16:N:74:PRO:CD    | 2.45                     | 0.46              |
| 1:O:371:U:H2'    | 1:O:372:A:C8      | 2.49                     | 0.46              |
| 1:O:816:G:C6     | 1:O:817:G:N1      | 2.83                     | 0.46              |
| 1:O:1086:A:N6    | 25:W:11:VAL:HG11  | 2.31                     | 0.46              |
| 13:K:45:PRO:HB2  | 37:K:7169:HOH:O   | 2.15                     | 0.46              |
| 1:O:204:A:C2'    | 1:O:205:U:H5'     | 2.45                     | 0.46              |
| 1:O:1189:A:H1'   | 1:O:1209:C:H1'    | 1.97                     | 0.46              |
| 3:A:88:ILE:HD13  | 3:A:100:PRO:CD    | 2.40                     | 0.46              |
| 8:F:39:SER:CB    | 8:F:45:ALA:HB2    | 2.41                     | 0.46              |
| 15:M:59:GLY:C    | 15:M:141:ILE:HD11 | 2.41                     | 0.46              |
| 17:O:25:VAL:HG23 | 17:O:26:TRP:H     | 1.81                     | 0.46              |
| 22:T:41:ARG:O    | 22:T:43:ASN:ND2   | 2.48                     | 0.46              |
| 1:O:1684:A:O2'   | 1:O:1685:A:H5''   | 2.15                     | 0.46              |
| 1:O:2601:A:N1    | 13:K:38:SER:HB2   | 2.31                     | 0.46              |
| 3:A:223:ARG:NH1  | 37:A:8518:HOH:O   | 2.48                     | 0.46              |
| 7:E:32:ARG:O     | 7:E:33:LEU:HD23   | 2.15                     | 0.46              |
| 12:J:90:LYS:HB2  | 35:J:8502:CL:CL   | 2.52                     | 0.46              |
| 29:1:28:HIS:HD2  | 29:1:30:LYS:H     | 1.62                     | 0.46              |
| 1:O:737:A:H2'    | 1:O:738:G:O4'     | 2.15                     | 0.46              |
| 1:O:951:A:O2'    | 1:O:952:G:H5'     | 2.16                     | 0.46              |
| 1:O:2642:G:H2'   | 1:O:2643:G:O4'    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:F:22:VAL:CG2    | 8:F:104:ALA:HB2   | 2.45                     | 0.46              |
| 25:W:38:THR:O     | 25:W:42:ARG:HB2   | 2.15                     | 0.46              |
| 1:0:1735:C:O2'    | 1:0:1736:A:H5'    | 2.15                     | 0.46              |
| 1:0:2010:A:H2'    | 37:0:5460:HOH:O   | 2.16                     | 0.46              |
| 1:0:2383:G:H1'    | 37:0:6198:HOH:O   | 2.15                     | 0.46              |
| 1:0:2781:U:H2'    | 1:0:2782:G:H5'    | 1.98                     | 0.46              |
| 5:C:33:LYS:HD2    | 37:C:8459:HOH:O   | 2.15                     | 0.46              |
| 8:F:34:ASN:HA     | 15:M:4:ALA:HB2    | 1.98                     | 0.46              |
| 8:F:58:GLU:HA     | 8:F:61:MET:HG3    | 1.98                     | 0.46              |
| 15:M:81:ARG:HG3   | 15:M:85:ARG:HB2   | 1.96                     | 0.46              |
| 20:R:25:PHE:CE2   | 20:R:29:LYS:CE    | 2.98                     | 0.46              |
| 1:0:656:G:H5'     | 17:O:3:THR:HG22   | 1.98                     | 0.46              |
| 1:0:1218:U:H2'    | 1:0:1219:U:C6     | 2.50                     | 0.46              |
| 1:0:1657:A:H2'    | 1:0:1658:A:C8     | 2.51                     | 0.46              |
| 1:0:1853:C:OP1    | 3:A:231:LYS:HG3   | 2.16                     | 0.46              |
| 1:0:1878:G:O2'    | 1:0:1879:U:H6     | 1.99                     | 0.46              |
| 3:A:36:ASP:HB2    | 3:A:83:GLY:HA3    | 1.98                     | 0.46              |
| 14:L:125:PHE:CE1  | 14:L:140:VAL:HG13 | 2.51                     | 0.46              |
| 16:N:42:HIS:CG    | 16:N:62:HIS:HE1   | 2.34                     | 0.46              |
| 16:N:71:TRP:N     | 37:N:8537:HOH:O   | 2.48                     | 0.46              |
| 18:P:16:VAL:CG1   | 18:P:17:GLY:N     | 2.79                     | 0.46              |
| 25:W:22:GLU:HG2   | 25:W:27:HIS:CD2   | 2.51                     | 0.46              |
| 1:0:1249:U:H2'    | 1:0:1250:C:C6     | 2.51                     | 0.46              |
| 1:0:2353:A:H4'    | 1:0:2354:A:O5'    | 2.14                     | 0.46              |
| 4:B:144:THR:HG22  | 4:B:145:HIS:N     | 2.30                     | 0.46              |
| 6:D:173:GLU:HG3   | 6:D:174:VAL:N     | 2.31                     | 0.46              |
| 11:I:102:VAL:HG23 | 11:I:140:GLU:O    | 2.16                     | 0.46              |
| 31:3:7:PHE:HE2    | 31:3:22:VAL:HG21  | 1.81                     | 0.46              |
| 1:0:185:G:H4'     | 1:0:186:A:H4'     | 1.98                     | 0.46              |
| 1:0:514:G:OP1     | 1:0:514:G:H2'     | 2.15                     | 0.46              |
| 1:0:1603:A:H5''   | 1:0:1605:G:H5'    | 1.98                     | 0.46              |
| 1:0:2361:A:H5'    | 1:0:2361:A:H8     | 1.81                     | 0.46              |
| 4:B:66:GLU:OE1    | 4:B:328:ARG:HD2   | 2.15                     | 0.46              |
| 7:E:3:VAL:CG2     | 7:E:49:ILE:HB     | 2.46                     | 0.46              |
| 10:H:83:TYR:CD1   | 10:H:83:TYR:C     | 2.94                     | 0.46              |
| 17:O:23:GLY:C     | 37:O:3062:HOH:O   | 2.59                     | 0.46              |
| 22:T:49:GLU:OE2   | 22:T:97:ARG:HD2   | 2.16                     | 0.46              |
| 25:W:26:ILE:O     | 25:W:26:ILE:HG13  | 2.15                     | 0.46              |
| 26:X:66:THR:HG23  | 26:X:67:PRO:HD2   | 1.98                     | 0.46              |
| 1:0:278:A:H2'     | 1:0:279:C:O4'     | 2.16                     | 0.45              |
| 1:0:559:U:H5'     | 1:0:559:U:C6      | 2.40                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:960:G:N3     | 1:0:960:G:C2'    | 2.79                     | 0.45              |
| 1:0:1132:A:N6    | 1:0:1229:C:H2'   | 2.32                     | 0.45              |
| 1:0:2467:A:O2'   | 1:0:2468:A:H2'   | 2.16                     | 0.45              |
| 37:0:4472:HOH:O  | 10:H:58:ARG:HG3  | 2.16                     | 0.45              |
| 3:A:81:GLN:CB    | 3:A:92:ASN:ND2   | 2.78                     | 0.45              |
| 4:B:23:THR:HG23  | 4:B:162:MET:HE3  | 1.98                     | 0.45              |
| 6:D:23:VAL:CG2   | 6:D:73:VAL:HB    | 2.44                     | 0.45              |
| 11:I:97:VAL:O    | 11:I:97:VAL:HG12 | 2.15                     | 0.45              |
| 22:T:45:GLY:C    | 37:T:3851:HOH:O  | 2.59                     | 0.45              |
| 1:0:820:G:C6     | 3:A:171:LYS:HB2  | 2.51                     | 0.45              |
| 1:0:2388:C:H5'   | 19:Q:83:THR:O    | 2.16                     | 0.45              |
| 1:0:2453:G:H5''  | 37:L:8540:HOH:O  | 2.15                     | 0.45              |
| 1:0:2456:A:H2'   | 1:0:2457:U:C6    | 2.51                     | 0.45              |
| 1:0:2781:U:C2'   | 1:0:2782:G:H5'   | 2.46                     | 0.45              |
| 1:0:2883:A:H2'   | 1:0:2884:G:O4'   | 2.17                     | 0.45              |
| 1:0:2896:A:N3    | 1:0:2896:A:H2'   | 2.31                     | 0.45              |
| 3:A:223:ARG:NE   | 37:A:8575:HOH:O  | 2.50                     | 0.45              |
| 4:B:7:ARG:HD2    | 4:B:9:GLY:O      | 2.16                     | 0.45              |
| 4:B:162:MET:HE2  | 4:B:310:ARG:CG   | 2.47                     | 0.45              |
| 14:L:146:GLY:C   | 14:L:148:GLU:H   | 2.25                     | 0.45              |
| 16:N:143:ARG:NH1 | 16:N:173:ASP:OD2 | 2.46                     | 0.45              |
| 17:O:21:SER:OG   | 17:O:106:PRO:HB2 | 2.17                     | 0.45              |
| 22:T:73:HIS:CD2  | 22:T:88:PRO:HG3  | 2.51                     | 0.45              |
| 1:0:671:A:O2'    | 1:0:672:G:H2'    | 2.16                     | 0.45              |
| 1:0:1333:U:H2'   | 1:0:1334:C:H6    | 1.81                     | 0.45              |
| 1:0:2720:C:O2    | 13:K:87:ARG:NH2  | 2.50                     | 0.45              |
| 6:D:103:ASN:ND2  | 6:D:134:LEU:H    | 2.14                     | 0.45              |
| 7:E:102:VAL:HG11 | 7:E:148:ILE:HD11 | 1.97                     | 0.45              |
| 8:F:46:GLU:O     | 8:F:73:PRO:HD2   | 2.16                     | 0.45              |
| 15:M:94:ARG:NH2  | 37:M:8581:HOH:O  | 2.35                     | 0.45              |
| 15:M:114:VAL:O   | 15:M:158:ARG:HD3 | 2.15                     | 0.45              |
| 16:N:159:TYR:CD2 | 16:N:163:PHE:HD2 | 2.35                     | 0.45              |
| 26:X:70:ILE:HG23 | 26:X:70:ILE:O    | 2.16                     | 0.45              |
| 1:0:2064:U:H4'   | 1:0:2653:A:OP1   | 2.17                     | 0.45              |
| 4:B:275:GLY:C    | 37:B:8657:HOH:O  | 2.60                     | 0.45              |
| 11:I:128:VAL:C   | 11:I:130:GLY:N   | 2.74                     | 0.45              |
| 21:S:6:LYS:HB2   | 21:S:27:ALA:O    | 2.15                     | 0.45              |
| 24:V:55:ARG:NH2  | 37:V:4428:HOH:O  | 2.42                     | 0.45              |
| 1:0:475:G:C5'    | 5:C:73:LEU:HD23  | 2.46                     | 0.45              |
| 3:A:165:THR:HG22 | 37:A:8621:HOH:O  | 2.15                     | 0.45              |
| 7:E:108:LEU:HD11 | 7:E:164:ASP:HB2  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:I:75:THR:OG1   | 11:I:112:LYS:HE2  | 2.16                     | 0.45              |
| 15:M:107:ARG:NH1  | 37:M:8576:HOH:O   | 2.47                     | 0.45              |
| 16:N:164:ASP:OD1  | 16:N:164:ASP:C    | 2.59                     | 0.45              |
| 1:O:314:G:N2      | 1:O:316:A:H3'     | 2.32                     | 0.45              |
| 1:O:338:C:H4'     | 5:C:174:ILE:HD12  | 1.98                     | 0.45              |
| 2:9:56:A:C3'      | 2:9:57:A:H5''     | 2.46                     | 0.45              |
| 5:C:164:ALA:O     | 5:C:167:ASP:HB2   | 2.16                     | 0.45              |
| 6:D:49:PRO:HG3    | 37:D:5828:HOH:O   | 2.15                     | 0.45              |
| 6:D:92:GLU:HB2    | 37:D:3862:HOH:O   | 2.16                     | 0.45              |
| 6:D:169:THR:O     | 6:D:170:TYR:HB2   | 2.16                     | 0.45              |
| 13:K:75:ARG:HH21  | 13:K:94:ALA:CB    | 2.30                     | 0.45              |
| 37:K:7438:HOH:O   | 23:U:20:MET:HE1   | 2.16                     | 0.45              |
| 14:L:130:ARG:HA   | 37:L:8557:HOH:O   | 2.17                     | 0.45              |
| 27:Y:117:LEU:HD12 | 27:Y:174:VAL:HG11 | 1.99                     | 0.45              |
| 1:O:136:C:H2'     | 1:O:137:U:O4'     | 2.16                     | 0.45              |
| 1:O:1314:U:H2'    | 37:O:5374:HOH:O   | 2.16                     | 0.45              |
| 1:O:1613:C:H2'    | 1:O:1614:G:O4'    | 2.16                     | 0.45              |
| 1:O:2488:A:H2     | 37:O:6767:HOH:O   | 1.99                     | 0.45              |
| 4:B:146:THR:O     | 4:B:159:PRO:HB3   | 2.16                     | 0.45              |
| 4:B:280:VAL:HG13  | 4:B:333:GLU:O     | 2.17                     | 0.45              |
| 7:E:80:TRP:O      | 7:E:134:SER:HA    | 2.17                     | 0.45              |
| 7:E:132:THR:HG23  | 7:E:132:THR:O     | 2.16                     | 0.45              |
| 15:M:164:THR:HG23 | 15:M:165:GLY:N    | 2.30                     | 0.45              |
| 26:X:18:ARG:NH1   | 37:X:4132:HOH:O   | 2.46                     | 0.45              |
| 29:1:25:LYS:HD2   | 30:2:49:GLU:H     | 1.82                     | 0.45              |
| 1:O:484:A:N1      | 1:O:506:G:H4'     | 2.31                     | 0.45              |
| 1:O:1681:G:H5''   | 1:O:1682:A:H5'    | 1.98                     | 0.45              |
| 1:O:2515:C:H2'    | 1:O:2516:G:O4'    | 2.17                     | 0.45              |
| 2:9:88:G:OP1      | 25:W:130:HIS:NE2  | 2.47                     | 0.45              |
| 10:H:1:LYS:HA     | 10:H:2:PRO:HD3    | 1.84                     | 0.45              |
| 10:H:38:LYS:HE2   | 10:H:42:ASP:HB3   | 1.98                     | 0.45              |
| 12:J:6:PHE:O      | 12:J:8:ALA:N      | 2.50                     | 0.45              |
| 16:N:5:ARG:HG3    | 19:Q:18:PRO:CB    | 2.47                     | 0.45              |
| 18:P:38:GLU:HA    | 18:P:41:ARG:HH11  | 1.81                     | 0.45              |
| 25:W:110:GLN:NE2  | 25:W:110:GLN:HA   | 2.32                     | 0.45              |
| 26:X:30:MET:HE3   | 26:X:55:ASN:OD1   | 2.17                     | 0.45              |
| 27:Y:154:ARG:NH1  | 27:Y:155:ARG:HG3  | 2.32                     | 0.45              |
| 1:O:585:C:H6      | 37:O:5595:HOH:O   | 1.99                     | 0.45              |
| 1:O:1028:U:H1'    | 37:O:3152:HOH:O   | 2.17                     | 0.45              |
| 1:O:1419:U:H2'    | 1:O:1685:A:C2     | 2.52                     | 0.45              |
| 6:D:55:LYS:HA     | 37:D:6752:HOH:O   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:I:103:ASP:HA   | 11:I:106:LYS:HD2  | 1.98                     | 0.45              |
| 15:M:182:LYS:HD2  | 15:M:193:LYS:HB2  | 1.98                     | 0.45              |
| 1:O:283:U:H5''    | 1:O:284:C:P       | 2.57                     | 0.45              |
| 1:O:1006:A:N1     | 1:O:2311:A:H1'    | 2.32                     | 0.45              |
| 1:O:1902:G:H2'    | 1:O:1903:U:O4'    | 2.17                     | 0.45              |
| 1:O:2890:A:H1'    | 23:U:56:ARG:HH21  | 1.79                     | 0.45              |
| 4:B:72:THR:HB     | 37:B:8610:HOH:O   | 2.16                     | 0.45              |
| 6:D:81:GLU:C      | 6:D:83:PHE:N      | 2.75                     | 0.45              |
| 10:H:58:ARG:HG3   | 10:H:58:ARG:HH11  | 1.81                     | 0.45              |
| 20:R:14:ALA:HB3   | 20:R:147:LEU:HB2  | 1.99                     | 0.45              |
| 1:O:1328:A:C8     | 27:Y:169:ARG:HD3  | 2.52                     | 0.44              |
| 1:O:1342:C:O2'    | 1:O:1343:C:H5'    | 2.16                     | 0.44              |
| 37:9:8464:HOH:O   | 16:N:147:ILE:HD12 | 2.17                     | 0.44              |
| 3:A:81:GLN:HB2    | 3:A:92:ASN:HD22   | 1.82                     | 0.44              |
| 4:B:74:ILE:HG13   | 37:B:8610:HOH:O   | 2.16                     | 0.44              |
| 4:B:307:ARG:HG3   | 4:B:307:ARG:NH1   | 2.32                     | 0.44              |
| 5:C:118:THR:CG2   | 5:C:137:PRO:HB3   | 2.47                     | 0.44              |
| 6:D:167:GLU:OE2   | 6:D:173:GLU:HG2   | 2.16                     | 0.44              |
| 7:E:34:TRP:O      | 12:J:127:ILE:HD11 | 2.17                     | 0.44              |
| 7:E:101:GLU:OE2   | 7:E:115:ARG:HD3   | 2.18                     | 0.44              |
| 11:I:131:THR:HG23 | 37:I:7439:HOH:O   | 2.18                     | 0.44              |
| 25:W:90:TYR:CE2   | 25:W:99:ALA:HB2   | 2.52                     | 0.44              |
| 30:2:18:ASN:HD22  | 30:2:18:ASN:HA    | 1.59                     | 0.44              |
| 1:O:141:C:P       | 37:O:3368:HOH:O   | 2.76                     | 0.44              |
| 1:O:581:G:H5'     | 37:O:7175:HOH:O   | 2.16                     | 0.44              |
| 4:B:41:PHE:CE1    | 4:B:79:MET:HG3    | 2.51                     | 0.44              |
| 4:B:279:THR:OG1   | 4:B:290:VAL:HB    | 2.17                     | 0.44              |
| 5:C:196:THR:HG23  | 37:C:8399:HOH:O   | 2.18                     | 0.44              |
| 7:E:154:ILE:HG13  | 7:E:156:ASP:OD1   | 2.18                     | 0.44              |
| 8:F:28:ALA:HB3    | 8:F:99:THR:O      | 2.16                     | 0.44              |
| 9:G:64:ASN:N      | 9:G:64:ASN:ND2    | 2.64                     | 0.44              |
| 10:H:36:LYS:HD3   | 37:H:8380:HOH:O   | 2.18                     | 0.44              |
| 16:N:108:SER:HA   | 16:N:109:PRO:HD3  | 1.79                     | 0.44              |
| 23:U:13:ILE:HG12  | 23:U:32:CYS:CB    | 2.47                     | 0.44              |
| 27:Y:213:LYS:HE3  | 27:Y:213:LYS:HB2  | 1.87                     | 0.44              |
| 28:Z:23:ARG:NH1   | 37:Z:8404:HOH:O   | 2.45                     | 0.44              |
| 1:O:790:A:H2'     | 1:O:791:A:O4'     | 2.18                     | 0.44              |
| 1:O:2769:C:H2'    | 1:O:2770:G:H5'    | 2.00                     | 0.44              |
| 5:C:170:ASP:O     | 5:C:171:GLU:HG3   | 2.17                     | 0.44              |
| 6:D:57:THR:HG23   | 6:D:63:ILE:CB     | 2.47                     | 0.44              |
| 13:K:118:ALA:C    | 13:K:120:ARG:H    | 2.25                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:P:59:ARG:HD3  | 37:P:192:HOH:O    | 2.16                     | 0.44              |
| 18:P:105:LEU:CD2 | 18:P:137:LEU:HD21 | 2.47                     | 0.44              |
| 25:W:11:VAL:O    | 25:W:12:ASN:HB2   | 2.16                     | 0.44              |
| 26:X:26:ALA:HB1  | 26:X:59:TRP:CE2   | 2.52                     | 0.44              |
| 28:Z:13:ARG:NH1  | 28:Z:14:PHE:CE2   | 2.86                     | 0.44              |
| 1:0:2001:G:O2'   | 1:0:2002:C:H5'    | 2.17                     | 0.44              |
| 1:0:2005:G:H3'   | 1:0:2005:G:OP2    | 2.18                     | 0.44              |
| 1:0:2326:U:H4'   | 1:0:2412:G:C4'    | 2.48                     | 0.44              |
| 1:0:2667:G:H1'   | 1:0:2914:A:N3     | 2.32                     | 0.44              |
| 1:0:2668:G:H2'   | 1:0:2669:U:C6     | 2.52                     | 0.44              |
| 4:B:82:VAL:HG12  | 4:B:101:TRP:CE3   | 2.53                     | 0.44              |
| 6:D:27:ILE:HD11  | 6:D:37:ALA:CB     | 2.46                     | 0.44              |
| 10:H:154:TYR:CD1 | 10:H:154:TYR:C    | 2.95                     | 0.44              |
| 11:I:112:LYS:O   | 11:I:116:LEU:HG   | 2.18                     | 0.44              |
| 16:N:47:LEU:CD1  | 16:N:97:VAL:HG11  | 2.47                     | 0.44              |
| 25:W:139:GLY:O   | 25:W:141:HIS:CD2  | 2.69                     | 0.44              |
| 29:1:25:LYS:O    | 29:1:25:LYS:HG2   | 2.18                     | 0.44              |
| 1:0:426:G:H2'    | 1:0:427:C:O4'     | 2.18                     | 0.44              |
| 1:0:821:U:H5''   | 37:0:9556:HOH:O   | 2.15                     | 0.44              |
| 1:0:2112:A:H2'   | 1:0:2113:G:C8     | 2.53                     | 0.44              |
| 1:0:2807:U:P     | 4:B:27:ASN:HD21   | 2.40                     | 0.44              |
| 2:9:39:U:H3'     | 2:9:40:C:H5''     | 1.99                     | 0.44              |
| 4:B:217:ARG:HG3  | 4:B:257:THR:CG2   | 2.47                     | 0.44              |
| 5:C:39:GLN:O     | 5:C:43:LYS:HD3    | 2.17                     | 0.44              |
| 11:I:87:THR:HG22 | 11:I:88:GLY:N     | 2.33                     | 0.44              |
| 12:J:70:PHE:CD2  | 12:J:70:PHE:O     | 2.70                     | 0.44              |
| 15:M:49:ALA:C    | 15:M:54:TYR:HB3   | 2.42                     | 0.44              |
| 20:R:84:ALA:O    | 20:R:88:PHE:HD1   | 2.00                     | 0.44              |
| 25:W:48:VAL:CG1  | 25:W:48:VAL:O     | 2.64                     | 0.44              |
| 30:2:36:ASN:HB3  | 30:2:39:ARG:NE    | 2.33                     | 0.44              |
| 1:0:566:A:H2'    | 1:0:567:U:O4'     | 2.18                     | 0.44              |
| 2:9:31:C:H1'     | 37:9:8392:HOH:O   | 2.17                     | 0.44              |
| 4:B:7:ARG:NH1    | 4:B:11:LEU:CD2    | 2.81                     | 0.44              |
| 4:B:195:ARG:HD2  | 4:B:324:ASP:OD1   | 2.18                     | 0.44              |
| 4:B:315:VAL:HG23 | 4:B:316:ARG:HG2   | 1.99                     | 0.44              |
| 10:H:26:SER:HA   | 10:H:59:HIS:CD2   | 2.53                     | 0.44              |
| 11:I:75:THR:HG22 | 11:I:79:ILE:CD1   | 2.48                     | 0.44              |
| 13:K:55:VAL:CG1  | 13:K:56:SER:N     | 2.81                     | 0.44              |
| 16:N:89:GLY:O    | 16:N:92:ALA:HB3   | 2.17                     | 0.44              |
| 18:P:10:ALA:CA   | 18:P:13:VAL:HG12  | 2.45                     | 0.44              |
| 29:1:8:GLN:HE22  | 29:1:11:LYS:HZ1   | 1.65                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:407:A:O5'    | 37:0:3965:HOH:O  | 2.21                     | 0.44              |
| 1:0:1120:U:H5'   | 1:0:1121:G:OP2   | 2.17                     | 0.44              |
| 1:0:1592:G:HO2'  | 1:0:1593:C:C4'   | 2.31                     | 0.44              |
| 1:0:1634:G:H2'   | 1:0:1635:U:C6    | 2.53                     | 0.44              |
| 1:0:1730:G:C5'   | 1:0:1731:C:H6    | 2.30                     | 0.44              |
| 1:0:2401:A:H5'   | 37:0:9000:HOH:O  | 2.16                     | 0.44              |
| 6:D:159:PRO:O    | 6:D:163:VAL:HG23 | 2.16                     | 0.44              |
| 14:L:6:ARG:NH2   | 37:L:8548:HOH:O  | 2.46                     | 0.44              |
| 14:L:34:GLY:C    | 14:L:36:ASP:H    | 2.26                     | 0.44              |
| 1:0:545:G:H2'    | 1:0:546:C:O4'    | 2.18                     | 0.44              |
| 1:0:834:G:H4'    | 1:0:835:U:OP2    | 2.18                     | 0.44              |
| 1:0:1029:U:O2'   | 1:0:1273:C:OP1   | 2.31                     | 0.44              |
| 1:0:1874:U:H2'   | 3:A:120:ARG:HG3  | 1.99                     | 0.44              |
| 1:0:2559:C:H4'   | 37:0:6747:HOH:O  | 2.17                     | 0.44              |
| 1:0:2730:G:O2'   | 1:0:2731:G:H5'   | 2.17                     | 0.44              |
| 4:B:27:ASN:HB3   | 37:B:8633:HOH:O  | 2.17                     | 0.44              |
| 4:B:60:SER:C     | 4:B:62:ARG:N     | 2.75                     | 0.44              |
| 6:D:173:GLU:O    | 6:D:174:VAL:C    | 2.61                     | 0.44              |
| 13:K:101:ASN:O   | 13:K:102:GLU:HB2 | 2.17                     | 0.44              |
| 16:N:32:PRO:HD2  | 16:N:99:GLU:O    | 2.18                     | 0.44              |
| 16:N:37:ARG:HA   | 16:N:37:ARG:HD3  | 1.72                     | 0.44              |
| 25:W:5:VAL:HG22  | 25:W:32:CYS:HB2  | 2.00                     | 0.44              |
| 25:W:88:THR:CG2  | 25:W:110:GLN:NE2 | 2.74                     | 0.44              |
| 1:0:1615:A:H4'   | 37:0:5386:HOH:O  | 2.17                     | 0.44              |
| 1:0:2251:G:H4'   | 37:0:6900:HOH:O  | 2.16                     | 0.44              |
| 37:0:9133:HOH:O  | 8:F:38:LYS:HE2   | 2.18                     | 0.44              |
| 2:9:28:U:H2'     | 2:9:29:C:C6      | 2.53                     | 0.44              |
| 4:B:248:ARG:O    | 4:B:251:VAL:CG1  | 2.66                     | 0.44              |
| 5:C:35:VAL:HG21  | 5:C:227:GLY:HA2  | 1.99                     | 0.44              |
| 5:C:162:VAL:HG12 | 5:C:162:VAL:O    | 2.18                     | 0.44              |
| 6:D:23:VAL:O     | 6:D:23:VAL:CG2   | 2.65                     | 0.44              |
| 9:G:64:ASN:O     | 9:G:68:GLU:HG3   | 2.17                     | 0.44              |
| 16:N:154:LEU:O   | 16:N:155:GLU:CB  | 2.66                     | 0.44              |
| 22:T:3:GLN:HA    | 22:T:4:PRO:HD3   | 1.80                     | 0.44              |
| 1:0:1211:G:O2'   | 1:0:1212:C:H5'   | 2.17                     | 0.43              |
| 1:0:1406:A:H4'   | 1:0:1407:A:H5''  | 1.99                     | 0.43              |
| 3:A:76:VAL:HG23  | 28:Z:63:LYS:HB3  | 1.99                     | 0.43              |
| 6:D:10:PHE:N     | 37:D:7345:HOH:O  | 2.51                     | 0.43              |
| 7:E:20:ILE:HD12  | 7:E:33:LEU:HD12  | 2.00                     | 0.43              |
| 11:I:122:THR:O   | 11:I:125:ALA:HB3 | 2.18                     | 0.43              |
| 13:K:49:LEU:HD21 | 13:K:74:VAL:O    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:1:17:THR:HA    | 30:2:49:GLU:HA    | 1.99                     | 0.43              |
| 1:0:894:A:C2      | 5:C:87:ARG:NH2    | 2.86                     | 0.43              |
| 1:0:1730:G:H5'    | 1:0:1731:C:H5     | 1.82                     | 0.43              |
| 1:0:1787:C:H4'    | 1:0:2883:A:O4'    | 2.18                     | 0.43              |
| 6:D:41:LEU:CA     | 6:D:44:ILE:HG22   | 2.47                     | 0.43              |
| 8:F:113:ASP:O     | 8:F:117:GLU:HG3   | 2.18                     | 0.43              |
| 15:M:115:LEU:HD13 | 15:M:116:ASN:HB2  | 2.00                     | 0.43              |
| 16:N:154:LEU:CG   | 16:N:155:GLU:H    | 2.28                     | 0.43              |
| 27:Y:154:ARG:HH12 | 27:Y:155:ARG:HG3  | 1.83                     | 0.43              |
| 28:Z:32:GLU:HA    | 28:Z:35:GLU:HG3   | 1.99                     | 0.43              |
| 30:2:40:ARG:HA    | 30:2:45:ASN:ND2   | 2.32                     | 0.43              |
| 1:0:1205:U:H2'    | 1:0:1206:U:H5'    | 1.99                     | 0.43              |
| 1:0:1329:A:C2     | 37:0:4183:HOH:O   | 2.56                     | 0.43              |
| 1:0:1926:G:H2'    | 1:0:1927:A:C8     | 2.54                     | 0.43              |
| 1:0:2314:G:C2'    | 1:0:2315:C:H5'    | 2.48                     | 0.43              |
| 3:A:100:PRO:O     | 3:A:103:VAL:HG23  | 2.17                     | 0.43              |
| 4:B:254:GLN:HG2   | 4:B:255:GLY:N     | 2.32                     | 0.43              |
| 9:G:12:ILE:HG13   | 37:G:6833:HOH:O   | 2.16                     | 0.43              |
| 22:T:37:GLN:OE1   | 22:T:118:SER:HA   | 2.17                     | 0.43              |
| 25:W:54:PHE:CZ    | 25:W:140:LYS:HB2  | 2.53                     | 0.43              |
| 29:1:2:GLY:O      | 29:1:6:PRO:HG2    | 2.18                     | 0.43              |
| 31:3:31:THR:HB    | 31:3:33:MET:HE3   | 1.99                     | 0.43              |
| 1:0:1171:A:H2'    | 1:0:1172:G:H5'    | 2.01                     | 0.43              |
| 1:0:2443:C:H3'    | 37:0:9982:HOH:O   | 2.18                     | 0.43              |
| 1:0:2672:C:H1'    | 37:B:8640:HOH:O   | 2.18                     | 0.43              |
| 4:B:154:VAL:HA    | 4:B:155:PRO:HD3   | 1.88                     | 0.43              |
| 4:B:205:VAL:HA    | 4:B:260:HIS:O     | 2.18                     | 0.43              |
| 10:H:169:GLY:C    | 10:H:170:ASN:HD22 | 2.26                     | 0.43              |
| 12:J:71:TYR:CD1   | 12:J:72:PRO:HD2   | 2.53                     | 0.43              |
| 17:O:43:VAL:HG12  | 17:O:44:ASN:O     | 2.18                     | 0.43              |
| 19:Q:32:GLU:O     | 19:Q:93:ARG:NH2   | 2.52                     | 0.43              |
| 31:3:65:THR:HB    | 31:3:83:TRP:H     | 1.83                     | 0.43              |
| 1:0:1172:G:H5''   | 37:0:6751:HOH:O   | 2.18                     | 0.43              |
| 1:0:1656:A:H2'    | 1:0:1657:A:O4'    | 2.19                     | 0.43              |
| 4:B:41:PHE:HB3    | 4:B:190:MET:CE    | 2.48                     | 0.43              |
| 5:C:107:ARG:CZ    | 37:C:8457:HOH:O   | 2.64                     | 0.43              |
| 6:D:18:ILE:HD13   | 6:D:84:LEU:HD12   | 2.00                     | 0.43              |
| 6:D:25:MET:HE1    | 6:D:37:ALA:HB1    | 2.01                     | 0.43              |
| 8:F:21:GLU:O      | 8:F:24:ARG:HG3    | 2.17                     | 0.43              |
| 12:J:39:VAL:CG1   | 12:J:107:ASN:HB2  | 2.48                     | 0.43              |
| 16:N:149:GLU:O    | 16:N:152:GLU:HB2  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:O:26:TRP:HA    | 17:O:26:TRP:CE3   | 2.52                     | 0.43              |
| 17:O:54:GLU:O     | 17:O:55:ASP:HB2   | 2.19                     | 0.43              |
| 18:P:120:ARG:NH2  | 18:P:123:TYR:CD2  | 2.86                     | 0.43              |
| 30:2:19:SER:O     | 30:2:36:ASN:ND2   | 2.52                     | 0.43              |
| 1:0:962:C:C1'     | 16:N:5:ARG:NH1    | 2.75                     | 0.43              |
| 1:0:1418:U:OP1    | 30:2:42:TRP:HB3   | 2.19                     | 0.43              |
| 1:0:1523:G:H2'    | 1:0:1524:U:C6     | 2.53                     | 0.43              |
| 1:0:1857:A:N6     | 1:0:2247:C:H1'    | 2.34                     | 0.43              |
| 1:0:1980:U:O2     | 1:0:2008:U:H4'    | 2.19                     | 0.43              |
| 1:0:2004:U:H1'    | 37:0:9700:HOH:O   | 2.19                     | 0.43              |
| 1:0:2825:C:H4'    | 1:0:2826:G:O5'    | 2.18                     | 0.43              |
| 3:A:26:ASP:OD1    | 3:A:28:GLU:HG3    | 2.18                     | 0.43              |
| 3:A:186:TRP:CG    | 3:A:187:PRO:HA    | 2.54                     | 0.43              |
| 6:D:35:ALA:C      | 6:D:37:ALA:N      | 2.76                     | 0.43              |
| 6:D:67:ASP:O      | 6:D:69:ILE:HG13   | 2.19                     | 0.43              |
| 14:L:121:ILE:HG12 | 14:L:141:GLU:HB2  | 2.00                     | 0.43              |
| 17:O:25:VAL:HG23  | 17:O:26:TRP:N     | 2.34                     | 0.43              |
| 23:U:6:CYS:HA     | 23:U:13:ILE:HD11  | 2.00                     | 0.43              |
| 25:W:88:THR:HG23  | 25:W:110:GLN:HB3  | 2.01                     | 0.43              |
| 26:X:43:VAL:HG22  | 26:X:76:ARG:NH1   | 2.34                     | 0.43              |
| 27:Y:106:THR:CG2  | 27:Y:107:PRO:HD2  | 2.48                     | 0.43              |
| 1:0:1163:G:N2     | 37:0:5548:HOH:O   | 2.52                     | 0.43              |
| 1:0:1669:A:H2'    | 1:0:1670:G:H8     | 1.82                     | 0.43              |
| 1:0:2653:A:H2'    | 1:0:2654:C:C6     | 2.54                     | 0.43              |
| 4:B:23:THR:CG2    | 4:B:162:MET:HE3   | 2.48                     | 0.43              |
| 7:E:133:VAL:HG12  | 7:E:141:VAL:HG13  | 2.00                     | 0.43              |
| 10:H:9:ILE:HG12   | 10:H:56:GLN:CG    | 2.49                     | 0.43              |
| 10:H:66:ARG:HB3   | 37:H:8382:HOH:O   | 2.18                     | 0.43              |
| 11:I:75:THR:CA    | 11:I:112:LYS:HE2  | 2.49                     | 0.43              |
| 11:I:131:THR:O    | 11:I:131:THR:HG22 | 2.17                     | 0.43              |
| 16:N:64:SER:C     | 16:N:66:LEU:N     | 2.74                     | 0.43              |
| 16:N:143:ARG:NH1  | 16:N:173:ASP:OD1  | 2.52                     | 0.43              |
| 19:Q:11:ARG:NH1   | 37:Q:5620:HOH:O   | 2.51                     | 0.43              |
| 25:W:41:TYR:CD2   | 25:W:44:MET:HE3   | 2.53                     | 0.43              |
| 1:0:284:C:C4'     | 1:0:285:A:O5'     | 2.64                     | 0.43              |
| 1:0:590:A:H2'     | 1:0:591:A:H5'     | 2.01                     | 0.43              |
| 1:0:661:G:C5      | 1:0:686:A:C2      | 3.06                     | 0.43              |
| 1:0:1180:U:H2'    | 1:0:1181:A:O4'    | 2.19                     | 0.43              |
| 1:0:1242:A:C5'    | 12:J:82:THR:HG23  | 2.28                     | 0.43              |
| 1:0:2256:G:C2'    | 1:0:2257:G:H5'    | 2.48                     | 0.43              |
| 1:0:2453:G:H4'    | 14:L:50:GLY:C     | 2.44                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 37:O:9183:HOH:O  | 5:C:214:THR:HB   | 2.18                     | 0.43              |
| 4:B:125:GLU:OE2  | 4:B:129:ARG:NH1  | 2.51                     | 0.43              |
| 5:C:7:ASP:OD1    | 5:C:11:ASN:O     | 2.37                     | 0.43              |
| 11:I:123:ASN:O   | 11:I:127:GLU:HG3 | 2.18                     | 0.43              |
| 13:K:75:ARG:HG2  | 13:K:90:PHE:CD2  | 2.54                     | 0.43              |
| 22:T:38:ARG:HG3  | 22:T:38:ARG:HH11 | 1.83                     | 0.43              |
| 28:Z:22:SER:O    | 28:Z:26:VAL:HG23 | 2.19                     | 0.43              |
| 1:O:151:A:H2'    | 1:O:152:A:O4'    | 2.19                     | 0.43              |
| 1:O:377:C:H5     | 37:O:9815:HOH:O  | 2.01                     | 0.43              |
| 1:O:834:G:H3'    | 1:O:835:U:H4'    | 2.00                     | 0.43              |
| 1:O:1545:C:H2'   | 1:O:1546:G:O4'   | 2.19                     | 0.43              |
| 1:O:1625:U:H5''  | 37:O:5522:HOH:O  | 2.19                     | 0.43              |
| 1:O:2831:C:H2'   | 1:O:2832:C:H5'   | 2.01                     | 0.43              |
| 1:O:2904:U:H4'   | 26:X:8:ARG:NH1   | 2.34                     | 0.43              |
| 5:C:133:ARG:NE   | 5:C:138:VAL:HG22 | 2.34                     | 0.43              |
| 7:E:31:ARG:NH1   | 7:E:68:HIS:CD2   | 2.86                     | 0.43              |
| 8:F:48:VAL:HG23  | 8:F:74:PHE:CB    | 2.49                     | 0.43              |
| 11:I:75:THR:HA   | 11:I:112:LYS:CE  | 2.49                     | 0.43              |
| 11:I:99:ASP:OD1  | 11:I:138:THR:HB  | 2.19                     | 0.43              |
| 12:J:103:VAL:CG1 | 37:J:5907:HOH:O  | 2.65                     | 0.43              |
| 20:R:39:THR:CB   | 20:R:42:GLU:HG3  | 2.43                     | 0.43              |
| 22:T:1:SER:N     | 37:T:5837:HOH:O  | 2.52                     | 0.43              |
| 24:V:12:THR:OG1  | 24:V:13:PRO:HD2  | 2.19                     | 0.43              |
| 31:3:15:ASN:ND2  | 37:3:8546:HOH:O  | 2.52                     | 0.43              |
| 1:O:588:G:O6     | 25:W:154:ARG:NH1 | 2.52                     | 0.43              |
| 1:O:1058:A:H2'   | 1:O:1060:C:C5'   | 2.46                     | 0.43              |
| 1:O:1636:G:O2'   | 1:O:1637:A:H5'   | 2.18                     | 0.43              |
| 1:O:1878:G:H5''  | 37:O:9304:HOH:O  | 2.18                     | 0.43              |
| 1:O:1947:G:H2'   | 1:O:1948:G:C8    | 2.54                     | 0.43              |
| 1:O:2289:G:N2    | 1:O:2291:A:C2    | 2.78                     | 0.43              |
| 1:O:2420:G:H4'   | 37:O:3598:HOH:O  | 2.19                     | 0.43              |
| 2:9:107:C:H2'    | 2:9:108:C:C6     | 2.53                     | 0.43              |
| 5:C:133:ARG:HD2  | 37:C:8410:HOH:O  | 2.19                     | 0.43              |
| 6:D:167:GLU:C    | 6:D:169:THR:H    | 2.27                     | 0.43              |
| 10:H:46:GLN:CB   | 10:H:167:PRO:HD2 | 2.25                     | 0.43              |
| 15:M:125:ARG:NH1 | 37:M:8596:HOH:O  | 2.52                     | 0.43              |
| 16:N:63:SER:O    | 16:N:66:LEU:HB2  | 2.18                     | 0.43              |
| 24:V:60:GLN:O    | 24:V:65:ASP:N    | 2.51                     | 0.43              |
| 30:2:22:PRO:HG2  | 30:2:25:VAL:HG21 | 1.97                     | 0.43              |
| 1:O:559:U:H2'    | 1:O:560:C:O4'    | 2.19                     | 0.42              |
| 1:O:1158:G:O2'   | 1:O:1159:G:H5'   | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1236:A:C8     | 12:J:63:ILE:HD11  | 2.54                     | 0.42              |
| 1:0:1609:C:H2'    | 1:0:1610:G:H8     | 1.84                     | 0.42              |
| 1:0:2365:G:H4'    | 19:Q:45:PRO:O     | 2.18                     | 0.42              |
| 3:A:35:GLY:O      | 3:A:36:ASP:CB     | 2.61                     | 0.42              |
| 4:B:88:GLU:O      | 4:B:88:GLU:HG3    | 2.17                     | 0.42              |
| 10:H:46:GLN:HB3   | 10:H:167:PRO:CD   | 2.27                     | 0.42              |
| 10:H:151:ARG:HA   | 10:H:154:TYR:CE2  | 2.54                     | 0.42              |
| 13:K:27:ARG:HD2   | 37:K:4747:HOH:O   | 2.19                     | 0.42              |
| 14:L:73:VAL:HG11  | 14:L:118:LEU:HD21 | 2.00                     | 0.42              |
| 19:Q:66:LYS:HB2   | 19:Q:70:ALA:O     | 2.19                     | 0.42              |
| 1:0:653:C:H2'     | 1:0:654:A:C8      | 2.53                     | 0.42              |
| 1:0:660:A:H4'     | 1:0:661:G:O5'     | 2.19                     | 0.42              |
| 1:0:1109:U:O4     | 12:J:21:ARG:HA    | 2.19                     | 0.42              |
| 3:A:94:LEU:HG     | 3:A:99:ILE:CD1    | 2.47                     | 0.42              |
| 4:B:71:VAL:CG1    | 4:B:296:LEU:HB3   | 2.46                     | 0.42              |
| 4:B:175:LEU:C     | 4:B:175:LEU:CD2   | 2.92                     | 0.42              |
| 6:D:76:ARG:O      | 6:D:77:ASP:HB2    | 2.19                     | 0.42              |
| 11:I:78:LEU:HD12  | 11:I:112:LYS:NZ   | 2.34                     | 0.42              |
| 12:J:121:LEU:HD11 | 12:J:126:ASN:ND2  | 2.34                     | 0.42              |
| 14:L:128:GLY:O    | 14:L:132:LYS:HG3  | 2.19                     | 0.42              |
| 16:N:154:LEU:C    | 16:N:156:GLU:H    | 2.25                     | 0.42              |
| 25:W:38:THR:HB    | 37:W:5390:HOH:O   | 2.18                     | 0.42              |
| 25:W:90:TYR:CD1   | 25:W:90:TYR:N     | 2.86                     | 0.42              |
| 1:0:303:C:H2'     | 1:0:304:G:O4'     | 2.19                     | 0.42              |
| 1:0:1123:A:C2     | 1:0:1129:C:H4'    | 2.54                     | 0.42              |
| 1:0:1641:A:C2'    | 1:0:1642:A:H5'    | 2.49                     | 0.42              |
| 1:0:1947:G:H2'    | 1:0:1948:G:H8     | 1.83                     | 0.42              |
| 1:0:2266:A:H2'    | 1:0:2267:G:C8     | 2.55                     | 0.42              |
| 3:A:17:ARG:HD2    | 37:A:8542:HOH:O   | 2.20                     | 0.42              |
| 8:F:38:LYS:HZ3    | 15:M:3:SER:HA     | 1.85                     | 0.42              |
| 13:K:99:ASP:OD1   | 13:K:101:ASN:N    | 2.51                     | 0.42              |
| 15:M:78:LYS:HD3   | 37:M:8637:HOH:O   | 2.19                     | 0.42              |
| 15:M:95:LYS:HG2   | 15:M:99:ARG:HB3   | 2.01                     | 0.42              |
| 17:O:77:ALA:HA    | 17:O:96:VAL:O     | 2.19                     | 0.42              |
| 1:0:213:G:HO2'    | 1:0:214:U:P       | 2.42                     | 0.42              |
| 1:0:306:A:P       | 22:T:38:ARG:HH21  | 2.42                     | 0.42              |
| 1:0:513:A:H3'     | 37:O:3359:HOH:O   | 2.19                     | 0.42              |
| 1:0:793:A:H5''    | 18:P:83:LYS:HG2   | 2.02                     | 0.42              |
| 1:0:816:G:H5'     | 1:0:1598:A:H4'    | 2.00                     | 0.42              |
| 1:0:870:G:C3'     | 1:0:871:G:H5''    | 2.49                     | 0.42              |
| 1:0:1423:C:O2'    | 1:0:1424:A:H5'    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:2061:C:C2'    | 1:0:2062:A:H5'   | 2.49                     | 0.42              |
| 3:A:51:ARG:NH2    | 3:A:69:LEU:HD13  | 2.34                     | 0.42              |
| 5:C:33:LYS:HE2    | 37:C:8359:HOH:O  | 2.19                     | 0.42              |
| 6:D:77:ASP:HB3    | 6:D:78:GLU:H     | 1.57                     | 0.42              |
| 9:G:27:ILE:HD12   | 9:G:70:ALA:HB1   | 2.02                     | 0.42              |
| 11:I:102:VAL:HG12 | 11:I:106:LYS:HE3 | 2.02                     | 0.42              |
| 15:M:167:GLY:O    | 15:M:171:ARG:HG3 | 2.19                     | 0.42              |
| 21:S:29:ASP:OD1   | 21:S:31:ARG:NH1  | 2.52                     | 0.42              |
| 1:0:37:A:H2'      | 1:0:38:G:C8      | 2.55                     | 0.42              |
| 1:0:42:C:H1'      | 37:0:4176:HOH:O  | 2.19                     | 0.42              |
| 1:0:90:A:H2'      | 1:0:91:G:O4'     | 2.19                     | 0.42              |
| 1:0:736:A:H2'     | 1:0:737:A:O4'    | 2.19                     | 0.42              |
| 1:0:814:G:H4'     | 37:0:9639:HOH:O  | 2.19                     | 0.42              |
| 1:0:1168:C:H5'    | 37:I:5128:HOH:O  | 2.20                     | 0.42              |
| 1:0:1555:G:H4'    | 1:0:1630:A:H2    | 1.85                     | 0.42              |
| 1:0:1768:C:H2'    | 1:0:1769:C:O4'   | 2.19                     | 0.42              |
| 1:0:2561:C:OP1    | 7:E:153:ARG:NH2  | 2.53                     | 0.42              |
| 1:0:2649:A:H5'    | 1:0:2649:A:H8    | 1.84                     | 0.42              |
| 1:0:2691:A:OP1    | 1:0:2691:A:H8    | 2.01                     | 0.42              |
| 4:B:268:ARG:NE    | 37:B:8612:HOH:O  | 2.51                     | 0.42              |
| 4:B:279:THR:CG2   | 4:B:280:VAL:N    | 2.82                     | 0.42              |
| 7:E:84:MET:HB2    | 7:E:131:LEU:HB2  | 2.01                     | 0.42              |
| 10:H:43:TYR:HA    | 10:H:44:PRO:HD3  | 1.75                     | 0.42              |
| 12:J:130:VAL:CG1  | 12:J:131:THR:N   | 2.81                     | 0.42              |
| 13:K:14:LYS:CB    | 13:K:45:PRO:HG2  | 2.43                     | 0.42              |
| 1:0:40:C:H4'      | 37:0:6492:HOH:O  | 2.20                     | 0.42              |
| 1:0:162:C:H2'     | 1:0:163:U:H5'    | 2.00                     | 0.42              |
| 1:0:262:A:OP2     | 8:F:91:VAL:HG11  | 2.19                     | 0.42              |
| 1:0:289:G:O2'     | 1:0:290:C:H5'    | 2.20                     | 0.42              |
| 1:0:1162:G:O2'    | 11:I:117:LEU:HG  | 2.19                     | 0.42              |
| 1:0:2356:A:H2'    | 1:0:2357:G:O4'   | 2.19                     | 0.42              |
| 1:0:2359:G:H3'    | 37:0:5190:HOH:O  | 2.19                     | 0.42              |
| 1:0:2820:A:H2'    | 1:0:2821:C:C6    | 2.54                     | 0.42              |
| 6:D:64:ARG:NE     | 6:D:67:ASP:HB3   | 2.34                     | 0.42              |
| 12:J:22:VAL:O     | 12:J:26:VAL:HG23 | 2.18                     | 0.42              |
| 14:L:53:ARG:NH2   | 14:L:57:VAL:CG1  | 2.83                     | 0.42              |
| 16:N:47:LEU:HD12  | 16:N:92:ALA:CB   | 2.49                     | 0.42              |
| 16:N:138:ASP:O    | 16:N:139:TRP:C   | 2.62                     | 0.42              |
| 17:O:26:TRP:HA    | 17:O:26:TRP:HE3  | 1.83                     | 0.42              |
| 25:W:14:HIS:HB2   | 25:W:17:ILE:HD12 | 2.02                     | 0.42              |
| 1:0:249:G:O2'     | 1:0:250:C:H5'    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:2777:G:O2'    | 1:O:2778:A:H5'    | 2.20                     | 0.42              |
| 3:A:169:PHE:O     | 3:A:171:LYS:N     | 2.48                     | 0.42              |
| 4:B:254:GLN:NE2   | 37:B:8594:HOH:O   | 2.49                     | 0.42              |
| 11:I:81:ASP:O     | 11:I:84:GLY:N     | 2.53                     | 0.42              |
| 11:I:113:HIS:NE2  | 11:I:121:LEU:HD22 | 2.35                     | 0.42              |
| 11:I:128:VAL:C    | 11:I:130:GLY:H    | 2.27                     | 0.42              |
| 21:S:6:LYS:O      | 21:S:7:HIS:HB3    | 2.19                     | 0.42              |
| 25:W:64:THR:O     | 25:W:68:THR:HG22  | 2.19                     | 0.42              |
| 25:W:146:ILE:HG22 | 25:W:147:ASP:N    | 2.34                     | 0.42              |
| 1:O:1609:C:H2'    | 1:O:1610:G:C8     | 2.55                     | 0.42              |
| 1:O:2900:G:H2'    | 1:O:2901:C:O4'    | 2.20                     | 0.42              |
| 3:A:70:ALA:HA     | 3:A:71:PRO:HD3    | 1.78                     | 0.42              |
| 4:B:168:GLY:N     | 4:B:174:ARG:HD3   | 2.33                     | 0.42              |
| 4:B:305:ASP:O     | 4:B:306:LYS:CB    | 2.66                     | 0.42              |
| 5:C:139:VAL:CG1   | 37:C:8447:HOH:O   | 2.61                     | 0.42              |
| 5:C:165:ASP:O     | 5:C:168:ARG:HB3   | 2.20                     | 0.42              |
| 10:H:96:ARG:NH2   | 37:H:8336:HOH:O   | 2.51                     | 0.42              |
| 11:I:102:VAL:O    | 11:I:106:LYS:HG3  | 2.20                     | 0.42              |
| 12:J:63:ILE:HG22  | 12:J:64:GLY:N     | 2.33                     | 0.42              |
| 14:L:104:ASP:O    | 14:L:105:TYR:HB3  | 2.20                     | 0.42              |
| 16:N:73:ALA:N     | 37:N:8565:HOH:O   | 2.52                     | 0.42              |
| 22:T:40:VAL:HG22  | 22:T:41:ARG:N     | 2.35                     | 0.42              |
| 22:T:48:VAL:HG22  | 22:T:97:ARG:O     | 2.20                     | 0.42              |
| 31:3:91:GLN:O     | 31:3:92:GLU:HB2   | 2.19                     | 0.42              |
| 1:O:92:G:H4'      | 24:V:44:GLY:HA3   | 2.02                     | 0.42              |
| 1:O:1159:G:H1     | 1:O:1208:C:H42    | 1.67                     | 0.42              |
| 1:O:1268:C:O2'    | 1:O:1269:G:H5'    | 2.19                     | 0.42              |
| 1:O:1883:U:O2'    | 1:O:1884:G:H5'    | 2.19                     | 0.42              |
| 3:A:105:VAL:CG1   | 3:A:106:CYS:N     | 2.82                     | 0.42              |
| 4:B:55:ASN:HB3    | 4:B:64:GLY:H      | 1.85                     | 0.42              |
| 4:B:313:PRO:O     | 4:B:314:ALA:C     | 2.63                     | 0.42              |
| 6:D:166:ILE:O     | 6:D:169:THR:N     | 2.53                     | 0.42              |
| 16:N:100:ALA:O    | 16:N:129:ILE:HG23 | 2.20                     | 0.42              |
| 16:N:159:TYR:HD2  | 16:N:163:PHE:HD2  | 1.67                     | 0.42              |
| 22:T:71:VAL:CG1   | 22:T:72:ILE:N     | 2.82                     | 0.42              |
| 1:O:88:G:N7       | 30:2:28:LYS:HD2   | 2.34                     | 0.42              |
| 1:O:827:A:H2'     | 1:O:828:G:O4'     | 2.20                     | 0.42              |
| 1:O:1139:U:H2'    | 1:O:1140:C:C6     | 2.55                     | 0.42              |
| 1:O:2361:A:H2'    | 1:O:2362:A:C8     | 2.55                     | 0.42              |
| 1:O:2741:A:H2'    | 1:O:2742:G:O4'    | 2.20                     | 0.42              |
| 7:E:112:ALA:HA    | 7:E:113:PRO:HD3   | 1.91                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:N:69:TYR:CE2  | 16:N:184:ILE:HD11 | 2.55                     | 0.42              |
| 20:R:132:ARG:NH2 | 37:R:8582:HOH:O   | 2.52                     | 0.42              |
| 26:X:51:ASP:O    | 26:X:53:SER:N     | 2.53                     | 0.42              |
| 1:O:1943:C:O4'   | 3:A:212:PRO:HA    | 2.20                     | 0.41              |
| 1:O:2115:U:H2'   | 1:O:2116:U:C6     | 2.55                     | 0.41              |
| 1:O:2237:G:H1'   | 37:O:4354:HOH:O   | 2.19                     | 0.41              |
| 1:O:2842:G:C2'   | 1:O:2843:A:H5'    | 2.49                     | 0.41              |
| 4:B:221:GLN:HE22 | 13:K:42:ASN:ND2   | 2.11                     | 0.41              |
| 5:C:153:VAL:O    | 5:C:157:LEU:HG    | 2.20                     | 0.41              |
| 7:E:47:VAL:HG11  | 7:E:69:ILE:HD13   | 2.01                     | 0.41              |
| 7:E:156:ASP:OD2  | 7:E:157:LYS:HG3   | 2.18                     | 0.41              |
| 9:G:12:ILE:HG22  | 9:G:17:GLN:NE2    | 2.35                     | 0.41              |
| 11:I:85:PHE:CD1  | 11:I:85:PHE:N     | 2.88                     | 0.41              |
| 14:L:148:GLU:HB2 | 37:L:8592:HOH:O   | 2.19                     | 0.41              |
| 17:O:41:ALA:HA   | 37:O:5104:HOH:O   | 2.18                     | 0.41              |
| 25:W:1:MET:HE3   | 25:W:101:LEU:HA   | 2.01                     | 0.41              |
| 1:O:777:U:O2'    | 29:1:11:LYS:HG2   | 2.20                     | 0.41              |
| 1:O:1014:A:H5''  | 2:9:101:G:O2'     | 2.20                     | 0.41              |
| 3:A:48:ASP:HB3   | 37:A:8609:HOH:O   | 2.21                     | 0.41              |
| 3:A:97:ALA:HB2   | 3:A:150:PRO:HB2   | 2.01                     | 0.41              |
| 5:C:129:HIS:HE1  | 5:C:231:ARG:HA    | 1.86                     | 0.41              |
| 5:C:234:VAL:O    | 5:C:234:VAL:HG22  | 2.20                     | 0.41              |
| 6:D:60:GLU:C     | 6:D:62:ASP:N      | 2.78                     | 0.41              |
| 12:J:26:VAL:HG13 | 12:J:36:VAL:HG11  | 2.01                     | 0.41              |
| 12:J:131:THR:HB  | 12:J:134:GLU:HG3  | 2.01                     | 0.41              |
| 15:M:42:ARG:HA   | 15:M:43:PRO:HD3   | 1.85                     | 0.41              |
| 1:O:321:A:H1'    | 37:O:6525:HOH:O   | 2.21                     | 0.41              |
| 1:O:1098:A:H2'   | 1:O:1099:G:O4'    | 2.20                     | 0.41              |
| 1:O:1235:G:C1'   | 12:J:63:ILE:HG23  | 2.50                     | 0.41              |
| 1:O:1973:A:H5'   | 1:O:1973:A:C8     | 2.46                     | 0.41              |
| 5:C:1:MET:HG2    | 5:C:2:GLN:NE2     | 2.36                     | 0.41              |
| 6:D:59:GLY:O     | 6:D:61:PHE:N      | 2.46                     | 0.41              |
| 10:H:162:ARG:NH1 | 37:H:8383:HOH:O   | 2.52                     | 0.41              |
| 13:K:55:VAL:HG12 | 13:K:56:SER:H     | 1.83                     | 0.41              |
| 23:U:9:CYS:O     | 23:U:52:THR:HG23  | 2.21                     | 0.41              |
| 31:3:74:CYS:N    | 37:3:8559:HOH:O   | 2.52                     | 0.41              |
| 1:O:245:C:H2'    | 1:O:246:G:H5'     | 2.01                     | 0.41              |
| 1:O:1477:C:C5'   | 1:O:1868:G:H5''   | 2.51                     | 0.41              |
| 3:A:36:ASP:CB    | 3:A:83:GLY:HA3    | 2.51                     | 0.41              |
| 7:E:152:THR:HG21 | 7:E:165:GLY:HA2   | 2.01                     | 0.41              |
| 14:L:144:ASP:HA  | 14:L:147:GLU:HG3  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:M:133:LEU:O    | 15:M:134:ILE:HD13 | 2.20                     | 0.41              |
| 16:N:175:LEU:HD12 | 16:N:175:LEU:HA   | 1.87                     | 0.41              |
| 18:P:94:TRP:CZ2   | 18:P:98:ILE:HG13  | 2.56                     | 0.41              |
| 22:T:48:VAL:HG22  | 22:T:97:ARG:C     | 2.45                     | 0.41              |
| 22:T:78:THR:HB    | 22:T:87:VAL:O     | 2.21                     | 0.41              |
| 26:X:15:ARG:HB3   | 26:X:15:ARG:NH1   | 2.32                     | 0.41              |
| 31:3:84:ARG:HD3   | 37:3:8549:HOH:O   | 2.21                     | 0.41              |
| 1:0:130:C:H5'     | 37:0:4710:HOH:O   | 2.20                     | 0.41              |
| 1:0:157:G:H4'     | 15:M:95:LYS:HE3   | 2.02                     | 0.41              |
| 1:0:1966:U:H2'    | 1:0:1967:U:C6     | 2.54                     | 0.41              |
| 1:0:2019:A:H5'    | 37:0:4042:HOH:O   | 2.20                     | 0.41              |
| 37:0:3915:HOH:O   | 3:A:11:ARG:CZ     | 2.69                     | 0.41              |
| 4:B:277:GLU:N     | 4:B:278:PRO:HD2   | 2.35                     | 0.41              |
| 6:D:104:PHE:CE2   | 6:D:132:VAL:HB    | 2.55                     | 0.41              |
| 7:E:20:ILE:O      | 7:E:30:THR:HA     | 2.20                     | 0.41              |
| 8:F:119:ARG:OXT   | 8:F:119:ARG:HD3   | 2.21                     | 0.41              |
| 13:K:22:ASP:C     | 13:K:22:ASP:OD1   | 2.64                     | 0.41              |
| 15:M:184:ARG:HG3  | 15:M:185:PRO:HA   | 2.02                     | 0.41              |
| 25:W:129:LYS:HG2  | 37:W:1990:HOH:O   | 2.21                     | 0.41              |
| 27:Y:99:ALA:HB2   | 27:Y:233:TYR:CZ   | 2.55                     | 0.41              |
| 27:Y:174:VAL:O    | 27:Y:174:VAL:HG12 | 2.20                     | 0.41              |
| 27:Y:189:ASN:HD22 | 27:Y:192:ASP:H    | 1.68                     | 0.41              |
| 1:0:1878:G:H5''   | 37:0:4663:HOH:O   | 2.19                     | 0.41              |
| 1:0:1923:G:H4'    | 31:3:31:THR:O     | 2.20                     | 0.41              |
| 1:0:2413:A:N7     | 16:N:109:PRO:HB3  | 2.35                     | 0.41              |
| 1:0:2415:A:N3     | 16:N:26:LEU:HD13  | 2.36                     | 0.41              |
| 1:0:2909:G:H2'    | 1:0:2910:A:H8     | 1.86                     | 0.41              |
| 6:D:20:LYS:HD3    | 6:D:76:ARG:NH2    | 2.35                     | 0.41              |
| 6:D:53:LYS:HA     | 6:D:67:ASP:O      | 2.20                     | 0.41              |
| 8:F:1:PRO:HB2     | 37:F:5897:HOH:O   | 2.21                     | 0.41              |
| 10:H:20:ILE:CG2   | 10:H:120:ILE:CD1  | 2.99                     | 0.41              |
| 11:I:130:GLY:C    | 37:I:3512:HOH:O   | 2.63                     | 0.41              |
| 16:N:43:VAL:HG13  | 16:N:118:ILE:HD11 | 2.03                     | 0.41              |
| 20:R:125:ARG:HG2  | 37:R:8542:HOH:O   | 2.21                     | 0.41              |
| 23:U:52:THR:HG21  | 23:U:54:THR:HB    | 2.02                     | 0.41              |
| 24:V:55:ARG:NE    | 37:V:4428:HOH:O   | 2.38                     | 0.41              |
| 26:X:12:ILE:HG23  | 26:X:36:HIS:CG    | 2.55                     | 0.41              |
| 28:Z:60:CYS:O     | 28:Z:61:ASP:CB    | 2.69                     | 0.41              |
| 1:0:396:U:H5'     | 31:3:42:ARG:NH1   | 2.35                     | 0.41              |
| 1:0:613:C:H2'     | 1:0:614:U:H6      | 1.85                     | 0.41              |
| 1:0:934:C:H2'     | 1:0:935:G:C8      | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:1385:G:O3'   | 26:X:49:ARG:NH1  | 2.53                     | 0.41              |
| 1:0:2011:A:H4'   | 1:0:2012:U:O5'   | 2.20                     | 0.41              |
| 37:0:3694:HOH:O  | 27:Y:186:ARG:HD2 | 2.21                     | 0.41              |
| 12:J:39:VAL:HG13 | 12:J:106:GLY:O   | 2.20                     | 0.41              |
| 14:L:92:ASP:OD1  | 14:L:94:ARG:HB2  | 2.20                     | 0.41              |
| 19:Q:25:PRO:HA   | 19:Q:26:PRO:HD3  | 1.84                     | 0.41              |
| 24:V:1:THR:HG23  | 24:V:2:VAL:N     | 2.25                     | 0.41              |
| 28:Z:27:ALA:O    | 28:Z:31:SER:HB2  | 2.21                     | 0.41              |
| 1:0:370:G:O2'    | 1:0:371:U:H5'    | 2.21                     | 0.41              |
| 1:0:412:C:H2'    | 1:0:413:G:O4'    | 2.21                     | 0.41              |
| 1:0:820:G:O2'    | 1:0:856:G:H4'    | 2.21                     | 0.41              |
| 1:0:949:U:H4'    | 19:Q:95:GLU:HA   | 2.02                     | 0.41              |
| 1:0:1116:U:H3    | 1:0:1246:A:N6    | 2.01                     | 0.41              |
| 1:0:2251:G:H2'   | 1:0:2252:A:H8    | 1.86                     | 0.41              |
| 1:0:2255:A:H2'   | 1:0:2256:G:O4'   | 2.21                     | 0.41              |
| 1:0:2712:G:H5'   | 37:K:4183:HOH:O  | 2.19                     | 0.41              |
| 4:B:82:VAL:O     | 4:B:82:VAL:CG1   | 2.67                     | 0.41              |
| 6:D:91:ALA:HB2   | 6:D:106:PHE:CD2  | 2.56                     | 0.41              |
| 16:N:103:ASP:OD1 | 16:N:103:ASP:C   | 2.64                     | 0.41              |
| 25:W:29:VAL:O    | 25:W:30:ASN:HB2  | 2.20                     | 0.41              |
| 1:0:40:C:H6      | 1:0:40:C:O5'     | 2.04                     | 0.41              |
| 1:0:56:G:H5''    | 24:V:50:ARG:NH1  | 2.36                     | 0.41              |
| 1:0:177:A:H2'    | 1:0:178:U:O4'    | 2.21                     | 0.41              |
| 1:0:324:G:O2'    | 1:0:325:U:H5'    | 2.21                     | 0.41              |
| 1:0:440:C:H2'    | 1:0:441:A:C8     | 2.56                     | 0.41              |
| 1:0:611:U:H2'    | 1:0:612:U:C6     | 2.56                     | 0.41              |
| 1:0:625:U:H5''   | 1:0:1044:C:N4    | 2.35                     | 0.41              |
| 1:0:764:C:H2'    | 1:0:765:G:O4'    | 2.21                     | 0.41              |
| 1:0:1515:A:H2'   | 1:0:1516:C:C6    | 2.55                     | 0.41              |
| 1:0:2421:G:H3'   | 1:0:2422:U:C5'   | 2.51                     | 0.41              |
| 1:0:2782:G:O6    | 1:0:2790:C:H5''  | 2.21                     | 0.41              |
| 1:0:2858:U:H2'   | 1:0:2859:C:C6    | 2.55                     | 0.41              |
| 2:9:8:G:O6       | 16:N:11:ARG:NH1  | 2.53                     | 0.41              |
| 2:9:14:G:O2'     | 16:N:1:ALA:HB2   | 2.21                     | 0.41              |
| 3:A:88:ILE:CD1   | 3:A:100:PRO:HD3  | 2.43                     | 0.41              |
| 3:A:103:VAL:HA   | 3:A:104:PRO:HD3  | 1.89                     | 0.41              |
| 4:B:127:GLN:HG3  | 37:B:8648:HOH:O  | 2.20                     | 0.41              |
| 4:B:129:ARG:NH2  | 4:B:176:ASP:OD1  | 2.51                     | 0.41              |
| 5:C:138:VAL:O    | 5:C:234:VAL:HA   | 2.21                     | 0.41              |
| 8:F:32:GLY:N     | 37:F:3111:HOH:O  | 2.52                     | 0.41              |
| 10:H:88:ARG:NH1  | 10:H:135:THR:OG1 | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:H:114:ARG:O    | 10:H:115:ALA:C    | 2.64                     | 0.41              |
| 10:H:116:ALA:O    | 10:H:117:PHE:C    | 2.61                     | 0.41              |
| 11:I:87:THR:HG22  | 11:I:88:GLY:H     | 1.85                     | 0.41              |
| 12:J:75:PRO:HD3   | 12:J:136:SER:OG   | 2.20                     | 0.41              |
| 14:L:10:SER:O     | 14:L:11:ARG:HB3   | 2.21                     | 0.41              |
| 14:L:72:ASN:O     | 14:L:76:LEU:HG    | 2.21                     | 0.41              |
| 14:L:143:THR:HG21 | 37:L:8537:HOH:O   | 2.20                     | 0.41              |
| 18:P:13:VAL:HG13  | 18:P:14:LEU:N     | 2.36                     | 0.41              |
| 21:S:32:ALA:HA    | 21:S:36:GLU:OE1   | 2.20                     | 0.41              |
| 22:T:48:VAL:HG13  | 22:T:49:GLU:N     | 2.35                     | 0.41              |
| 24:V:16:ARG:NH2   | 24:V:63:GLU:HG3   | 2.36                     | 0.41              |
| 24:V:45:ARG:C     | 24:V:47:LYS:N     | 2.77                     | 0.41              |
| 25:W:146:ILE:HD13 | 25:W:146:ILE:HA   | 1.89                     | 0.41              |
| 26:X:15:ARG:HH11  | 26:X:15:ARG:CB    | 2.32                     | 0.41              |
| 29:1:25:LYS:HD2   | 30:2:49:GLU:N     | 2.35                     | 0.41              |
| 1:0:794:U:H3      | 1:0:819:A:H61     | 1.68                     | 0.41              |
| 1:0:1175:G:H1'    | 1:0:1193:A:H2'    | 2.02                     | 0.41              |
| 1:0:1565:C:O4'    | 1:0:2738:G:H1'    | 2.21                     | 0.41              |
| 1:0:2679:G:H2'    | 1:0:2681:A:OP2    | 2.21                     | 0.41              |
| 2:9:1:U:H5''      | 2:9:3:A:OP1       | 2.21                     | 0.41              |
| 2:9:2:U:OP2       | 2:9:3:A:H5'       | 2.20                     | 0.41              |
| 4:B:53:LEU:HD12   | 4:B:327:VAL:HA    | 2.02                     | 0.41              |
| 4:B:146:THR:C     | 4:B:148:PRO:HD3   | 2.46                     | 0.41              |
| 5:C:115:LEU:HD12  | 5:C:115:LEU:HA    | 1.89                     | 0.41              |
| 7:E:35:TYR:HA     | 12:J:127:ILE:HD12 | 2.03                     | 0.41              |
| 10:H:9:ILE:HD12   | 10:H:54:THR:CG2   | 2.47                     | 0.41              |
| 10:H:112:GLY:N    | 37:H:8390:HOH:O   | 2.54                     | 0.41              |
| 13:K:30:LYS:C     | 13:K:55:VAL:HG13  | 2.46                     | 0.41              |
| 13:K:101:ASN:O    | 13:K:102:GLU:CB   | 2.69                     | 0.41              |
| 16:N:19:ASP:C     | 16:N:19:ASP:OD1   | 2.64                     | 0.41              |
| 22:T:14:ALA:HA    | 22:T:15:PRO:HD3   | 1.93                     | 0.41              |
| 1:0:517:U:H1'     | 37:0:7067:HOH:O   | 2.21                     | 0.40              |
| 1:0:1367:A:H2'    | 1:0:1368:U:O4'    | 2.21                     | 0.40              |
| 1:0:1592:G:O2'    | 1:0:1593:C:O5'    | 2.38                     | 0.40              |
| 1:0:2419:U:H5''   | 1:0:2420:G:C5'    | 2.50                     | 0.40              |
| 1:0:2478:U:O2'    | 1:0:2479:A:H5'    | 2.21                     | 0.40              |
| 1:0:2589:U:H2'    | 1:0:2590:U:C6     | 2.56                     | 0.40              |
| 1:0:2820:A:H2'    | 1:0:2821:C:O4'    | 2.21                     | 0.40              |
| 1:0:2821:C:H4'    | 4:B:116:PRO:CB    | 2.51                     | 0.40              |
| 37:0:3866:HOH:O   | 17:O:2:LYS:NZ     | 2.54                     | 0.40              |
| 3:A:36:ASP:HB2    | 3:A:84:VAL:N      | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:81:ALA:O      | 4:B:186:GLY:HA3   | 2.21                     | 0.40              |
| 5:C:57:PRO:O      | 5:C:58:ALA:C      | 2.63                     | 0.40              |
| 6:D:19:GLU:HG3    | 37:D:6165:HOH:O   | 2.20                     | 0.40              |
| 6:D:20:LYS:HA     | 6:D:75:LEU:O      | 2.22                     | 0.40              |
| 6:D:38:GLU:OE2    | 6:D:51:ARG:CZ     | 2.70                     | 0.40              |
| 6:D:59:GLY:C      | 6:D:61:PHE:N      | 2.80                     | 0.40              |
| 10:H:24:PRO:HD3   | 10:H:120:ILE:HG22 | 2.04                     | 0.40              |
| 13:K:72:VAL:HG11  | 13:K:121:PHE:CD1  | 2.56                     | 0.40              |
| 15:M:69:LYS:HG2   | 15:M:127:LYS:HG3  | 2.02                     | 0.40              |
| 15:M:134:ILE:O    | 15:M:136:PRO:HD3  | 2.21                     | 0.40              |
| 16:N:184:ILE:HG23 | 16:N:184:ILE:O    | 2.22                     | 0.40              |
| 22:T:38:ARG:NH1   | 22:T:38:ARG:HG3   | 2.35                     | 0.40              |
| 23:U:17:THR:CG2   | 23:U:18:GLY:N     | 2.84                     | 0.40              |
| 24:V:20:LEU:HD22  | 24:V:60:GLN:HE22  | 1.86                     | 0.40              |
| 25:W:151:GLU:O    | 25:W:154:ARG:HB3  | 2.21                     | 0.40              |
| 27:Y:189:ASN:C    | 27:Y:189:ASN:ND2  | 2.79                     | 0.40              |
| 1:O:290:C:O2'     | 1:O:291:C:H5'     | 2.21                     | 0.40              |
| 1:O:475:G:H5'     | 5:C:73:LEU:HD23   | 2.03                     | 0.40              |
| 1:O:553:G:OP2     | 27:Y:204:ARG:NH2  | 2.53                     | 0.40              |
| 1:O:926:A:O2'     | 14:L:41:HIS:CD2   | 2.74                     | 0.40              |
| 37:O:7200:HOH:O   | 5:C:94:THR:HG21   | 2.19                     | 0.40              |
| 4:B:41:PHE:CD2    | 4:B:190:MET:HE3   | 2.56                     | 0.40              |
| 6:D:24:HIS:HB2    | 6:D:72:LYS:CB     | 2.51                     | 0.40              |
| 6:D:67:ASP:HA     | 6:D:68:PRO:HD3    | 1.94                     | 0.40              |
| 7:E:69:ILE:HA     | 7:E:72:MET:HE3    | 2.01                     | 0.40              |
| 7:E:79:GLY:HA3    | 37:E:7046:HOH:O   | 2.20                     | 0.40              |
| 10:H:138:CYS:SG   | 10:H:146:VAL:HG11 | 2.61                     | 0.40              |
| 15:M:59:GLY:HA3   | 15:M:141:ILE:HD12 | 2.03                     | 0.40              |
| 16:N:66:LEU:HD12  | 16:N:66:LEU:HA    | 1.95                     | 0.40              |
| 19:Q:16:ASN:HD22  | 19:Q:16:ASN:HA    | 1.76                     | 0.40              |
| 21:S:76:GLU:HB3   | 37:S:8343:HOH:O   | 2.20                     | 0.40              |
| 25:W:1:MET:HB2    | 25:W:103:GLU:HG2  | 2.02                     | 0.40              |
| 1:O:317:A:OP1     | 22:T:52:ARG:O     | 2.40                     | 0.40              |
| 1:O:1165:G:H1'    | 1:O:1174:A:H1'    | 2.03                     | 0.40              |
| 1:O:2780:C:H1'    | 7:E:143:GLN:NE2   | 2.35                     | 0.40              |
| 2:9:24:U:H3'      | 2:9:25:G:C5'      | 2.52                     | 0.40              |
| 3:A:114:ASP:OD1   | 3:A:114:ASP:C     | 2.64                     | 0.40              |
| 5:C:16:VAL:CG1    | 5:C:17:ASP:N      | 2.83                     | 0.40              |
| 6:D:18:ILE:HD13   | 6:D:84:LEU:CD1    | 2.52                     | 0.40              |
| 6:D:23:VAL:HG23   | 6:D:41:LEU:HD22   | 2.03                     | 0.40              |
| 12:J:39:VAL:HG11  | 12:J:107:ASN:HB2  | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:J:39:VAL:HG12 | 12:J:40:ASN:ND2  | 2.36                     | 0.40              |
| 20:R:7:GLU:HG3   | 37:R:8580:HOH:O  | 2.21                     | 0.40              |
| 1:0:1413:A:H2'   | 1:0:1414:A:O4'   | 2.22                     | 0.40              |
| 1:0:1753:C:O2    | 4:B:229:ARG:NH2  | 2.49                     | 0.40              |
| 1:0:2050:G:H5''  | 20:R:80:TYR:O    | 2.21                     | 0.40              |
| 1:0:2281:C:C2'   | 1:0:2282:U:H5'   | 2.51                     | 0.40              |
| 1:0:2851:G:C2'   | 1:0:2852:A:H5'   | 2.52                     | 0.40              |
| 5:C:91:PRO:O     | 5:C:93:LYS:HG3   | 2.21                     | 0.40              |
| 10:H:29:ALA:C    | 10:H:30:GLN:HG3  | 2.46                     | 0.40              |
| 10:H:40:ALA:HB1  | 10:H:137:TYR:CE2 | 2.57                     | 0.40              |
| 11:I:134:SER:CB  | 37:I:7330:HOH:O  | 2.70                     | 0.40              |
| 14:L:24:ALA:HB2  | 14:L:30:ARG:HD2  | 2.04                     | 0.40              |
| 22:T:26:THR:HA   | 22:T:39:ASN:HB3  | 2.03                     | 0.40              |
| 25:W:5:VAL:O     | 25:W:52:VAL:CG2  | 2.70                     | 0.40              |
| 29:1:28:HIS:HD2  | 29:1:31:LYS:H    | 1.69                     | 0.40              |
| 1:0:475:G:OP1    | 5:C:73:LEU:CD2   | 2.70                     | 0.40              |
| 1:0:932:U:H2'    | 1:0:933:C:C6     | 2.57                     | 0.40              |
| 1:0:1298:U:H2'   | 1:0:1299:G:C8    | 2.56                     | 0.40              |
| 1:0:1477:C:O2'   | 1:0:1478:U:H5'   | 2.21                     | 0.40              |
| 1:0:1972:U:C2'   | 1:0:1973:A:H5''  | 2.51                     | 0.40              |
| 1:0:2089:A:O2'   | 1:0:2090:G:H5'   | 2.22                     | 0.40              |
| 1:0:2462:G:N7    | 31:3:60:LYS:NZ   | 2.67                     | 0.40              |
| 2:9:59:C:H6      | 2:9:59:C:O5'     | 2.05                     | 0.40              |
| 3:A:72:GLU:HG3   | 28:Z:66:GLY:HA2  | 2.04                     | 0.40              |
| 6:D:25:MET:HE1   | 6:D:37:ALA:O     | 2.22                     | 0.40              |
| 7:E:11:VAL:HG11  | 7:E:22:VAL:HG13  | 2.02                     | 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   | A     | 235/240 (98%)   | 217 (92%)  | 15 (6%)  | 3 (1%)   | 9           | 14  |
| 4   | B     | 335/338 (99%)   | 314 (94%)  | 14 (4%)  | 7 (2%)   | 5           | 7   |
| 5   | C     | 244/246 (99%)   | 224 (92%)  | 20 (8%)  | 0        | 100         | 100 |
| 6   | D     | 134/177 (76%)   | 104 (78%)  | 23 (17%) | 7 (5%)   | 1           | 1   |
| 7   | E     | 170/178 (96%)   | 159 (94%)  | 10 (6%)  | 1 (1%)   | 21          | 32  |
| 8   | F     | 117/120 (98%)   | 105 (90%)  | 10 (8%)  | 2 (2%)   | 7           | 10  |
| 9   | G     | 25/348 (7%)     | 24 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 10  | H     | 156/171 (91%)   | 145 (93%)  | 9 (6%)   | 2 (1%)   | 9           | 14  |
| 11  | I     | 68/162 (42%)    | 53 (78%)   | 12 (18%) | 3 (4%)   | 2           | 1   |
| 12  | J     | 140/145 (97%)   | 132 (94%)  | 5 (4%)   | 3 (2%)   | 5           | 7   |
| 13  | K     | 130/132 (98%)   | 120 (92%)  | 8 (6%)   | 2 (2%)   | 8           | 12  |
| 14  | L     | 141/165 (86%)   | 120 (85%)  | 20 (14%) | 1 (1%)   | 18          | 28  |
| 15  | M     | 192/194 (99%)   | 186 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 16  | N     | 184/187 (98%)   | 171 (93%)  | 8 (4%)   | 5 (3%)   | 4           | 4   |
| 17  | O     | 113/116 (97%)   | 108 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 18  | P     | 141/149 (95%)   | 138 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 19  | Q     | 93/96 (97%)     | 89 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 20  | R     | 148/155 (96%)   | 143 (97%)  | 4 (3%)   | 1 (1%)   | 18          | 28  |
| 21  | S     | 79/85 (93%)     | 75 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 22  | T     | 117/120 (98%)   | 111 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 23  | U     | 51/66 (77%)     | 47 (92%)   | 4 (8%)   | 0        | 100         | 100 |
| 24  | V     | 63/71 (89%)     | 58 (92%)   | 3 (5%)   | 2 (3%)   | 3           | 3   |
| 25  | W     | 152/154 (99%)   | 147 (97%)  | 4 (3%)   | 1 (1%)   | 18          | 28  |
| 26  | X     | 80/92 (87%)     | 71 (89%)   | 7 (9%)   | 2 (2%)   | 4           | 5   |
| 27  | Y     | 140/241 (58%)   | 140 (100%) | 0        | 0        | 100         | 100 |
| 28  | Z     | 71/73 (97%)     | 61 (86%)   | 9 (13%)  | 1 (1%)   | 9           | 13  |
| 29  | 1     | 54/57 (95%)     | 52 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 30  | 2     | 42/50 (84%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 31  | 3     | 90/92 (98%)     | 86 (96%)   | 2 (2%)   | 2 (2%)   | 5           | 6   |
| All | All   | 3705/4420 (84%) | 3442 (93%) | 218 (6%) | 45 (1%)  | 10          | 16  |

All (45) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 139 | ASP  |
| 6   | D     | 137 | PRO  |
| 6   | D     | 173 | GLU  |
| 10  | H     | 166 | SER  |
| 10  | H     | 168 | ALA  |
| 14  | L     | 80  | ASP  |
| 16  | N     | 154 | LEU  |
| 28  | Z     | 81  | ARG  |
| 3   | A     | 34  | ASP  |
| 3   | A     | 37  | VAL  |
| 3   | A     | 132 | ASP  |
| 4   | B     | 34  | GLY  |
| 4   | B     | 169 | GLY  |
| 4   | B     | 184 | ASP  |
| 6   | D     | 171 | ASP  |
| 12  | J     | 5   | GLU  |
| 16  | N     | 167 | ASP  |
| 24  | V     | 43  | PRO  |
| 31  | 3     | 56  | PRO  |
| 31  | 3     | 57  | GLY  |
| 6   | D     | 61  | PHE  |
| 8   | F     | 101 | ALA  |
| 11  | I     | 80  | LYS  |
| 12  | J     | 7   | ASP  |
| 12  | J     | 143 | LYS  |
| 13  | K     | 126 | SER  |
| 16  | N     | 139 | TRP  |
| 16  | N     | 164 | ASP  |
| 25  | W     | 77  | ALA  |
| 26  | X     | 77  | PHE  |
| 4   | B     | 107 | SER  |
| 8   | F     | 64  | PRO  |
| 13  | K     | 119 | GLN  |
| 16  | N     | 65  | ASP  |
| 4   | B     | 185 | GLY  |
| 6   | D     | 27  | ILE  |
| 6   | D     | 170 | TYR  |
| 24  | V     | 40  | PRO  |
| 4   | B     | 2   | GLN  |
| 7   | E     | 44  | GLY  |
| 6   | D     | 16  | PRO  |
| 11  | I     | 74  | PRO  |
| 11  | I     | 92  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | R     | 81  | PRO  |
| 26  | X     | 52  | 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   | A     | 179/182 (98%)  | 167 (93%) | 12 (7%)  | 15          | 26  |
| 4   | B     | 282/283 (100%) | 262 (93%) | 20 (7%)  | 13          | 23  |
| 5   | C     | 193/193 (100%) | 179 (93%) | 14 (7%)  | 13          | 22  |
| 6   | D     | 117/148 (79%)  | 110 (94%) | 7 (6%)   | 17          | 31  |
| 7   | E     | 152/156 (97%)  | 148 (97%) | 4 (3%)   | 40          | 63  |
| 8   | F     | 93/94 (99%)    | 91 (98%)  | 2 (2%)   | 45          | 67  |
| 9   | G     | 27/283 (10%)   | 27 (100%) | 0        | 100         | 100 |
| 10  | H     | 132/138 (96%)  | 124 (94%) | 8 (6%)   | 17          | 30  |
| 11  | I     | 58/130 (45%)   | 53 (91%)  | 5 (9%)   | 10          | 16  |
| 12  | J     | 118/121 (98%)  | 111 (94%) | 7 (6%)   | 18          | 31  |
| 13  | K     | 106/106 (100%) | 103 (97%) | 3 (3%)   | 38          | 60  |
| 14  | L     | 113/127 (89%)  | 110 (97%) | 3 (3%)   | 39          | 62  |
| 15  | M     | 158/158 (100%) | 152 (96%) | 6 (4%)   | 29          | 49  |
| 16  | N     | 149/150 (99%)  | 141 (95%) | 8 (5%)   | 20          | 35  |
| 17  | O     | 93/94 (99%)    | 88 (95%)  | 5 (5%)   | 20          | 35  |
| 18  | P     | 113/117 (97%)  | 110 (97%) | 3 (3%)   | 39          | 62  |
| 19  | Q     | 79/80 (99%)    | 74 (94%)  | 5 (6%)   | 16          | 29  |
| 20  | R     | 117/122 (96%)  | 114 (97%) | 3 (3%)   | 40          | 63  |
| 21  | S     | 71/74 (96%)    | 70 (99%)  | 1 (1%)   | 59          | 79  |
| 22  | T     | 105/106 (99%)  | 100 (95%) | 5 (5%)   | 23          | 40  |
| 23  | U     | 44/52 (85%)    | 44 (100%) | 0        | 100         | 100 |
| 24  | V     | 51/57 (90%)    | 50 (98%)  | 1 (2%)   | 48          | 70  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 25  | W     | 130/130 (100%)  | 122 (94%)  | 8 (6%)   | 16          | 29  |
| 26  | X     | 66/74 (89%)     | 63 (96%)   | 3 (4%)   | 24          | 42  |
| 27  | Y     | 120/196 (61%)   | 110 (92%)  | 10 (8%)  | 10          | 17  |
| 28  | Z     | 60/60 (100%)    | 60 (100%)  | 0        | 100         | 100 |
| 29  | 1     | 46/47 (98%)     | 46 (100%)  | 0        | 100         | 100 |
| 30  | 2     | 42/46 (91%)     | 41 (98%)   | 1 (2%)   | 43          | 65  |
| 31  | 3     | 79/79 (100%)    | 75 (95%)   | 4 (5%)   | 21          | 37  |
| All | All   | 3093/3603 (86%) | 2945 (95%) | 148 (5%) | 23          | 40  |

All (148) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 3   | ARG  |
| 3   | A     | 33  | GLU  |
| 3   | A     | 36  | ASP  |
| 3   | A     | 55  | VAL  |
| 3   | A     | 68  | ILE  |
| 3   | A     | 69  | LEU  |
| 3   | A     | 94  | LEU  |
| 3   | A     | 131 | HIS  |
| 3   | A     | 153 | ARG  |
| 3   | A     | 175 | LYS  |
| 3   | A     | 179 | MET  |
| 3   | A     | 217 | ARG  |
| 4   | B     | 7   | ARG  |
| 4   | B     | 11  | LEU  |
| 4   | B     | 27  | ASN  |
| 4   | B     | 33  | ASP  |
| 4   | B     | 53  | LEU  |
| 4   | B     | 63  | GLU  |
| 4   | B     | 84  | LEU  |
| 4   | B     | 97  | LEU  |
| 4   | B     | 98  | THR  |
| 4   | B     | 103 | ASP  |
| 4   | B     | 190 | MET  |
| 4   | B     | 195 | ARG  |
| 4   | B     | 251 | VAL  |
| 4   | B     | 254 | GLN  |
| 4   | B     | 256 | GLN  |
| 4   | B     | 257 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 264 | GLU  |
| 4   | B     | 277 | GLU  |
| 4   | B     | 307 | ARG  |
| 4   | B     | 312 | ARG  |
| 5   | C     | 2   | GLN  |
| 5   | C     | 67  | GLN  |
| 5   | C     | 78  | ARG  |
| 5   | C     | 94  | THR  |
| 5   | C     | 115 | LEU  |
| 5   | C     | 136 | VAL  |
| 5   | C     | 187 | ARG  |
| 5   | C     | 214 | THR  |
| 5   | C     | 222 | ASP  |
| 5   | C     | 223 | LEU  |
| 5   | C     | 234 | VAL  |
| 5   | C     | 236 | THR  |
| 5   | C     | 240 | LEU  |
| 5   | C     | 243 | VAL  |
| 6   | D     | 24  | HIS  |
| 6   | D     | 50  | VAL  |
| 6   | D     | 99  | ASP  |
| 6   | D     | 131 | THR  |
| 6   | D     | 136 | ARG  |
| 6   | D     | 137 | PRO  |
| 6   | D     | 149 | ARG  |
| 7   | E     | 7   | ILE  |
| 7   | E     | 36  | PRO  |
| 7   | E     | 86  | VAL  |
| 7   | E     | 102 | VAL  |
| 8   | F     | 46  | GLU  |
| 8   | F     | 78  | GLU  |
| 10  | H     | 18  | GLU  |
| 10  | H     | 30  | GLN  |
| 10  | H     | 62  | LEU  |
| 10  | H     | 84  | LYS  |
| 10  | H     | 88  | ARG  |
| 10  | H     | 132 | GLN  |
| 10  | H     | 146 | VAL  |
| 10  | H     | 170 | ASN  |
| 11  | I     | 86  | GLU  |
| 11  | I     | 93  | GLN  |
| 11  | I     | 108 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | I     | 138 | THR  |
| 11  | I     | 140 | GLU  |
| 12  | J     | 46  | ILE  |
| 12  | J     | 74  | ARG  |
| 12  | J     | 93  | ARG  |
| 12  | J     | 120 | SER  |
| 12  | J     | 125 | SER  |
| 12  | J     | 127 | ILE  |
| 12  | J     | 131 | THR  |
| 13  | K     | 7   | ASP  |
| 13  | K     | 10  | GLN  |
| 13  | K     | 98  | VAL  |
| 14  | L     | 35  | ARG  |
| 14  | L     | 117 | GLU  |
| 14  | L     | 140 | VAL  |
| 15  | M     | 46  | LEU  |
| 15  | M     | 81  | ARG  |
| 15  | M     | 93  | ARG  |
| 15  | M     | 99  | ARG  |
| 15  | M     | 158 | ARG  |
| 15  | M     | 164 | THR  |
| 16  | N     | 26  | LEU  |
| 16  | N     | 43  | VAL  |
| 16  | N     | 47  | LEU  |
| 16  | N     | 127 | LEU  |
| 16  | N     | 128 | ASP  |
| 16  | N     | 135 | VAL  |
| 16  | N     | 152 | GLU  |
| 16  | N     | 180 | LEU  |
| 17  | O     | 3   | THR  |
| 17  | O     | 25  | VAL  |
| 17  | O     | 28  | ASP  |
| 17  | O     | 98  | LEU  |
| 17  | O     | 111 | VAL  |
| 18  | P     | 52  | LYS  |
| 18  | P     | 91  | LYS  |
| 18  | P     | 98  | ILE  |
| 19  | Q     | 11  | ARG  |
| 19  | Q     | 16  | ASN  |
| 19  | Q     | 57  | ASP  |
| 19  | Q     | 81  | GLU  |
| 19  | Q     | 95  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | R     | 13  | THR  |
| 20  | R     | 39  | THR  |
| 20  | R     | 82  | GLU  |
| 21  | S     | 10  | VAL  |
| 22  | T     | 26  | THR  |
| 22  | T     | 39  | ASN  |
| 22  | T     | 47  | THR  |
| 22  | T     | 48  | VAL  |
| 22  | T     | 96  | VAL  |
| 24  | V     | 43  | PRO  |
| 25  | W     | 4   | LEU  |
| 25  | W     | 35  | VAL  |
| 25  | W     | 52  | VAL  |
| 25  | W     | 73  | LEU  |
| 25  | W     | 122 | ARG  |
| 25  | W     | 142 | ASP  |
| 25  | W     | 146 | ILE  |
| 25  | W     | 154 | ARG  |
| 26  | X     | 15  | ARG  |
| 26  | X     | 72  | VAL  |
| 26  | X     | 84  | ILE  |
| 27  | Y     | 103 | THR  |
| 27  | Y     | 141 | THR  |
| 27  | Y     | 154 | ARG  |
| 27  | Y     | 163 | THR  |
| 27  | Y     | 172 | THR  |
| 27  | Y     | 189 | ASN  |
| 27  | Y     | 200 | THR  |
| 27  | Y     | 203 | VAL  |
| 27  | Y     | 231 | PRO  |
| 27  | Y     | 235 | GLU  |
| 30  | 2     | 18  | ASN  |
| 31  | 3     | 14  | CYS  |
| 31  | 3     | 42  | ARG  |
| 31  | 3     | 56  | PRO  |
| 31  | 3     | 65  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 92  | ASN  |
| 3   | A     | 127 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 199 | HIS  |
| 3   | A     | 218 | ASN  |
| 4   | B     | 27  | ASN  |
| 4   | B     | 55  | ASN  |
| 4   | B     | 94  | GLN  |
| 4   | B     | 145 | HIS  |
| 4   | B     | 221 | GLN  |
| 4   | B     | 238 | ASN  |
| 4   | B     | 243 | ASN  |
| 4   | B     | 256 | GLN  |
| 4   | B     | 260 | HIS  |
| 4   | B     | 318 | ASN  |
| 4   | B     | 320 | GLN  |
| 5   | C     | 2   | GLN  |
| 5   | C     | 39  | GLN  |
| 5   | C     | 67  | GLN  |
| 5   | C     | 129 | HIS  |
| 5   | C     | 163 | HIS  |
| 5   | C     | 178 | GLN  |
| 6   | D     | 11  | HIS  |
| 6   | D     | 103 | ASN  |
| 6   | D     | 133 | ASN  |
| 7   | E     | 15  | GLN  |
| 7   | E     | 66  | GLN  |
| 7   | E     | 106 | ASN  |
| 7   | E     | 119 | HIS  |
| 7   | E     | 143 | GLN  |
| 9   | G     | 17  | GLN  |
| 9   | G     | 64  | ASN  |
| 10  | H     | 30  | GLN  |
| 10  | H     | 46  | GLN  |
| 10  | H     | 56  | GLN  |
| 10  | H     | 59  | HIS  |
| 10  | H     | 72  | HIS  |
| 10  | H     | 132 | GLN  |
| 10  | H     | 155 | ASN  |
| 10  | H     | 170 | ASN  |
| 11  | I     | 111 | GLN  |
| 12  | J     | 52  | GLN  |
| 12  | J     | 107 | ASN  |
| 12  | J     | 126 | ASN  |
| 12  | J     | 142 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | K     | 10  | GLN  |
| 14  | L     | 18  | HIS  |
| 14  | L     | 41  | HIS  |
| 14  | L     | 42  | ASN  |
| 14  | L     | 58  | GLN  |
| 14  | L     | 116 | HIS  |
| 15  | M     | 24  | GLN  |
| 15  | M     | 26  | GLN  |
| 15  | M     | 52  | GLN  |
| 15  | M     | 58  | GLN  |
| 15  | M     | 143 | ASN  |
| 15  | M     | 170 | ASN  |
| 16  | N     | 21  | HIS  |
| 16  | N     | 22  | GLN  |
| 16  | N     | 107 | ASN  |
| 16  | N     | 140 | GLN  |
| 16  | N     | 153 | GLN  |
| 17  | O     | 53  | GLN  |
| 18  | P     | 50  | GLN  |
| 18  | P     | 66  | GLN  |
| 18  | P     | 73  | HIS  |
| 18  | P     | 118 | GLN  |
| 19  | Q     | 40  | HIS  |
| 20  | R     | 61  | GLN  |
| 20  | R     | 94  | ASN  |
| 20  | R     | 98  | ASN  |
| 20  | R     | 113 | HIS  |
| 20  | R     | 117 | HIS  |
| 21  | S     | 51  | GLN  |
| 21  | S     | 53  | ASN  |
| 21  | S     | 55  | GLN  |
| 21  | S     | 56  | ASN  |
| 22  | T     | 39  | ASN  |
| 22  | T     | 43  | ASN  |
| 22  | T     | 73  | HIS  |
| 23  | U     | 39  | ASN  |
| 24  | V     | 4   | HIS  |
| 24  | V     | 6   | GLN  |
| 24  | V     | 60  | GLN  |
| 25  | W     | 6   | GLN  |
| 25  | W     | 27  | HIS  |
| 25  | W     | 110 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | W     | 119 | HIS  |
| 25  | W     | 125 | HIS  |
| 25  | W     | 141 | HIS  |
| 26  | X     | 23  | HIS  |
| 26  | X     | 36  | HIS  |
| 27  | Y     | 119 | GLN  |
| 27  | Y     | 133 | HIS  |
| 27  | Y     | 134 | HIS  |
| 27  | Y     | 149 | GLN  |
| 27  | Y     | 189 | ASN  |
| 29  | 1     | 8   | GLN  |
| 29  | 1     | 16  | HIS  |
| 29  | 1     | 28  | HIS  |
| 30  | 2     | 16  | ASN  |
| 30  | 2     | 17  | GLN  |
| 30  | 2     | 18  | ASN  |
| 30  | 2     | 37  | HIS  |
| 30  | 2     | 41  | HIS  |
| 30  | 2     | 45  | ASN  |
| 31  | 3     | 2   | GLN  |
| 31  | 3     | 30  | GLN  |
| 31  | 3     | 48  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 0     | 2746/2922 (93%) | 251 (9%)          | 34 (1%)         |
| 2   | 9     | 121/122 (99%)   | 18 (14%)          | 2 (1%)          |
| All | All   | 2867/3044 (94%) | 269 (9%)          | 36 (1%)         |

All (269) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 11  | A    |
| 1   | 0     | 31  | C    |
| 1   | 0     | 60  | A    |
| 1   | 0     | 67  | A    |
| 1   | 0     | 69  | A    |
| 1   | 0     | 70  | A    |
| 1   | 0     | 71  | G    |
| 1   | 0     | 87  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 88  | G    |
| 1   | 0     | 114 | A    |
| 1   | 0     | 115 | U    |
| 1   | 0     | 120 | A    |
| 1   | 0     | 130 | C    |
| 1   | 0     | 139 | C    |
| 1   | 0     | 141 | C    |
| 1   | 0     | 151 | A    |
| 1   | 0     | 166 | A    |
| 1   | 0     | 169 | A    |
| 1   | 0     | 170 | U    |
| 1   | 0     | 186 | A    |
| 1   | 0     | 191 | A    |
| 1   | 0     | 192 | A    |
| 1   | 0     | 200 | U    |
| 1   | 0     | 219 | G    |
| 1   | 0     | 237 | G    |
| 1   | 0     | 271 | C    |
| 1   | 0     | 272 | A    |
| 1   | 0     | 273 | G    |
| 1   | 0     | 283 | U    |
| 1   | 0     | 284 | C    |
| 1   | 0     | 285 | A    |
| 1   | 0     | 308 | U    |
| 1   | 0     | 309 | C    |
| 1   | 0     | 318 | C    |
| 1   | 0     | 336 | G    |
| 1   | 0     | 337 | A    |
| 1   | 0     | 338 | C    |
| 1   | 0     | 339 | A    |
| 1   | 0     | 345 | G    |
| 1   | 0     | 358 | G    |
| 1   | 0     | 381 | G    |
| 1   | 0     | 397 | A    |
| 1   | 0     | 417 | G    |
| 1   | 0     | 461 | C    |
| 1   | 0     | 473 | A    |
| 1   | 0     | 487 | G    |
| 1   | 0     | 498 | A    |
| 1   | 0     | 510 | U    |
| 1   | 0     | 511 | A    |
| 1   | 0     | 514 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 537  | G    |
| 1   | 0     | 538  | C    |
| 1   | 0     | 539  | G    |
| 1   | 0     | 542  | A    |
| 1   | 0     | 545  | G    |
| 1   | 0     | 553  | G    |
| 1   | 0     | 559  | U    |
| 1   | 0     | 588  | G    |
| 1   | 0     | 604  | G    |
| 1   | 0     | 620  | A    |
| 1   | 0     | 632  | A    |
| 1   | 0     | 644  | G    |
| 1   | 0     | 660  | A    |
| 1   | 0     | 688  | A    |
| 1   | 0     | 701  | U    |
| 1   | 0     | 759  | C    |
| 1   | 0     | 777  | U    |
| 1   | 0     | 809  | G    |
| 1   | 0     | 821  | U    |
| 1   | 0     | 835  | U    |
| 1   | 0     | 840  | U    |
| 1   | 0     | 857  | A    |
| 1   | 0     | 858  | U    |
| 1   | 0     | 868  | G    |
| 1   | 0     | 869  | G    |
| 1   | 0     | 871  | G    |
| 1   | 0     | 872  | U    |
| 1   | 0     | 875  | A    |
| 1   | 0     | 877  | G    |
| 1   | 0     | 878  | G    |
| 1   | 0     | 884  | C    |
| 1   | 0     | 898  | G    |
| 1   | 0     | 905  | C    |
| 1   | 0     | 921  | G    |
| 1   | 0     | 923  | A    |
| 1   | 0     | 953  | G    |
| 1   | 0     | 960  | G    |
| 1   | 0     | 961  | A    |
| 1   | 0     | 1006 | A    |
| 1   | 0     | 1008 | C    |
| 1   | 0     | 1029 | U    |
| 1   | 0     | 1045 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 1059 | G    |
| 1   | 0     | 1060 | C    |
| 1   | 0     | 1072 | G    |
| 1   | 0     | 1081 | A    |
| 1   | 0     | 1088 | A    |
| 1   | 0     | 1109 | U    |
| 1   | 0     | 1110 | G    |
| 1   | 0     | 1119 | G    |
| 1   | 0     | 1130 | U    |
| 1   | 0     | 1161 | A    |
| 1   | 0     | 1162 | G    |
| 1   | 0     | 1164 | U    |
| 1   | 0     | 1165 | G    |
| 1   | 0     | 1166 | A    |
| 1   | 0     | 1174 | A    |
| 1   | 0     | 1175 | G    |
| 1   | 0     | 1185 | U    |
| 1   | 0     | 1192 | A    |
| 1   | 0     | 1193 | A    |
| 1   | 0     | 1206 | U    |
| 1   | 0     | 1208 | C    |
| 1   | 0     | 1216 | G    |
| 1   | 0     | 1232 | A    |
| 1   | 0     | 1233 | A    |
| 1   | 0     | 1237 | U    |
| 1   | 0     | 1238 | C    |
| 1   | 0     | 1239 | G    |
| 1   | 0     | 1246 | A    |
| 1   | 0     | 1247 | A    |
| 1   | 0     | 1279 | U    |
| 1   | 0     | 1289 | C    |
| 1   | 0     | 1342 | C    |
| 1   | 0     | 1353 | C    |
| 1   | 0     | 1360 | C    |
| 1   | 0     | 1377 | C    |
| 1   | 0     | 1378 | G    |
| 1   | 0     | 1407 | A    |
| 1   | 0     | 1409 | G    |
| 1   | 0     | 1451 | C    |
| 1   | 0     | 1474 | C    |
| 1   | 0     | 1485 | A    |
| 1   | 0     | 1488 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 1505 | U    |
| 1   | 0     | 1506 | U    |
| 1   | 0     | 1524 | U    |
| 1   | 0     | 1525 | G    |
| 1   | 0     | 1526 | A    |
| 1   | 0     | 1564 | C    |
| 1   | 0     | 1580 | A    |
| 1   | 0     | 1592 | G    |
| 1   | 0     | 1603 | A    |
| 1   | 0     | 1625 | U    |
| 1   | 0     | 1626 | A    |
| 1   | 0     | 1633 | C    |
| 1   | 0     | 1634 | G    |
| 1   | 0     | 1656 | A    |
| 1   | 0     | 1667 | A    |
| 1   | 0     | 1682 | A    |
| 1   | 0     | 1684 | A    |
| 1   | 0     | 1685 | A    |
| 1   | 0     | 1692 | C    |
| 1   | 0     | 1693 | A    |
| 1   | 0     | 1701 | A    |
| 1   | 0     | 1710 | A    |
| 1   | 0     | 1722 | U    |
| 1   | 0     | 1723 | G    |
| 1   | 0     | 1725 | C    |
| 1   | 0     | 1731 | C    |
| 1   | 0     | 1752 | G    |
| 1   | 0     | 1778 | A    |
| 1   | 0     | 1798 | C    |
| 1   | 0     | 1820 | G    |
| 1   | 0     | 1829 | A    |
| 1   | 0     | 1856 | C    |
| 1   | 0     | 1857 | A    |
| 1   | 0     | 1879 | U    |
| 1   | 0     | 1904 | A    |
| 1   | 0     | 1919 | A    |
| 1   | 0     | 1942 | A    |
| 1   | 0     | 1943 | C    |
| 1   | 0     | 1971 | G    |
| 1   | 0     | 1973 | A    |
| 1   | 0     | 1974 | G    |
| 1   | 0     | 1978 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 1979 | G    |
| 1   | 0     | 1980 | U    |
| 1   | 0     | 1996 | U    |
| 1   | 0     | 2004 | U    |
| 1   | 0     | 2008 | U    |
| 1   | 0     | 2011 | A    |
| 1   | 0     | 2012 | U    |
| 1   | 0     | 2013 | G    |
| 1   | 0     | 2033 | G    |
| 1   | 0     | 2034 | U    |
| 1   | 0     | 2064 | U    |
| 1   | 0     | 2072 | G    |
| 1   | 0     | 2073 | G    |
| 1   | 0     | 2074 | A    |
| 1   | 0     | 2096 | A    |
| 1   | 0     | 2101 | A    |
| 1   | 0     | 2102 | G    |
| 1   | 0     | 2110 | G    |
| 1   | 0     | 2238 | A    |
| 1   | 0     | 2258 | A    |
| 1   | 0     | 2271 | G    |
| 1   | 0     | 2272 | G    |
| 1   | 0     | 2291 | A    |
| 1   | 0     | 2317 | C    |
| 1   | 0     | 2321 | A    |
| 1   | 0     | 2346 | C    |
| 1   | 0     | 2354 | A    |
| 1   | 0     | 2361 | A    |
| 1   | 0     | 2369 | A    |
| 1   | 0     | 2422 | U    |
| 1   | 0     | 2462 | G    |
| 1   | 0     | 2469 | A    |
| 1   | 0     | 2476 | C    |
| 1   | 0     | 2480 | G    |
| 1   | 0     | 2483 | A    |
| 1   | 0     | 2507 | G    |
| 1   | 0     | 2511 | A    |
| 1   | 0     | 2526 | C    |
| 1   | 0     | 2527 | U    |
| 1   | 0     | 2533 | C    |
| 1   | 0     | 2537 | G    |
| 1   | 0     | 2541 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 2553 | A    |
| 1   | 0     | 2564 | G    |
| 1   | 0     | 2589 | U    |
| 1   | 0     | 2601 | A    |
| 1   | 0     | 2602 | G    |
| 1   | 0     | 2608 | C    |
| 1   | 0     | 2613 | G    |
| 1   | 0     | 2638 | G    |
| 1   | 0     | 2649 | A    |
| 1   | 0     | 2664 | A    |
| 1   | 0     | 2681 | A    |
| 1   | 0     | 2682 | C    |
| 1   | 0     | 2718 | C    |
| 1   | 0     | 2719 | A    |
| 1   | 0     | 2726 | U    |
| 1   | 0     | 2727 | A    |
| 1   | 0     | 2747 | C    |
| 1   | 0     | 2748 | G    |
| 1   | 0     | 2749 | U    |
| 1   | 0     | 2750 | G    |
| 1   | 0     | 2762 | C    |
| 1   | 0     | 2768 | A    |
| 1   | 0     | 2786 | G    |
| 1   | 0     | 2792 | A    |
| 1   | 0     | 2800 | A    |
| 1   | 0     | 2811 | A    |
| 1   | 0     | 2825 | C    |
| 1   | 0     | 2840 | A    |
| 1   | 0     | 2850 | C    |
| 1   | 0     | 2876 | G    |
| 1   | 0     | 2890 | A    |
| 1   | 0     | 2896 | A    |
| 1   | 0     | 2914 | A    |
| 2   | 9     | 2    | U    |
| 2   | 9     | 11   | A    |
| 2   | 9     | 14   | G    |
| 2   | 9     | 22   | G    |
| 2   | 9     | 23   | U    |
| 2   | 9     | 24   | U    |
| 2   | 9     | 25   | G    |
| 2   | 9     | 41   | C    |
| 2   | 9     | 43   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 9     | 44  | A    |
| 2   | 9     | 52  | A    |
| 2   | 9     | 57  | A    |
| 2   | 9     | 66  | G    |
| 2   | 9     | 77  | A    |
| 2   | 9     | 103 | A    |
| 2   | 9     | 104 | A    |
| 2   | 9     | 114 | G    |
| 2   | 9     | 122 | C    |

All (36) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 10   | U    |
| 1   | 0     | 69   | A    |
| 1   | 0     | 129  | A    |
| 1   | 0     | 169  | A    |
| 1   | 0     | 284  | C    |
| 1   | 0     | 338  | C    |
| 1   | 0     | 603  | A    |
| 1   | 0     | 699  | C    |
| 1   | 0     | 834  | G    |
| 1   | 0     | 857  | A    |
| 1   | 0     | 871  | G    |
| 1   | 0     | 877  | G    |
| 1   | 0     | 1080 | C    |
| 1   | 0     | 1232 | A    |
| 1   | 0     | 1237 | U    |
| 1   | 0     | 1246 | A    |
| 1   | 0     | 1352 | A    |
| 1   | 0     | 1377 | C    |
| 1   | 0     | 1450 | C    |
| 1   | 0     | 1563 | G    |
| 1   | 0     | 1692 | C    |
| 1   | 0     | 1856 | C    |
| 1   | 0     | 1942 | A    |
| 1   | 0     | 1979 | G    |
| 1   | 0     | 2011 | A    |
| 1   | 0     | 2313 | C    |
| 1   | 0     | 2467 | A    |
| 1   | 0     | 2526 | C    |
| 1   | 0     | 2536 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 0     | 2649 | A    |
| 1   | 0     | 2718 | C    |
| 1   | 0     | 2726 | U    |
| 1   | 0     | 2761 | A    |
| 1   | 0     | 2791 | U    |
| 2   | 9     | 65   | A    |
| 2   | 9     | 103  | A    |

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 1   | 1MA  | 0     | 628  | 1    | 21,25,26     | 0.72 | 1 (4%)      | 30,37,40    | 0.75 | 1 (3%)      |
| 1   | OMG  | 0     | 2588 | 1    | 23,26,27     | 0.30 | 0           | 32,38,41    | 0.37 | 0           |
| 1   | OMU  | 0     | 2587 | 1    | 19,22,23     | 0.21 | 0           | 25,31,34    | 0.41 | 0           |
| 1   | PSU  | 0     | 2621 | 1    | 18,21,22     | 1.48 | 2 (11%)     | 21,30,33    | 1.30 | 3 (14%)     |
| 1   | UR3  | 0     | 2619 | 1    | 19,22,23     | 0.49 | 0           | 26,32,35    | 0.73 | 1 (3%)      |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 1MA  | 0     | 628  | 1    | -       | 2/7/25/26 | 0/3/3/3 |
| 1   | OMG  | 0     | 2588 | 1    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMU  | 0     | 2587 | 1    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | PSU  | 0     | 2621 | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | UR3  | 0     | 2619 | 1    | -       | 0/7/25/26 | 0/2/2/2 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | 0     | 2621 | PSU  | C2-N1 | 5.02 | 1.43        | 1.36     |
| 1   | 0     | 2621 | PSU  | C6-C5 | 2.96 | 1.38        | 1.35     |
| 1   | 0     | 628  | 1MA  | C6-N6 | 2.48 | 1.34        | 1.28     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 0     | 2621 | PSU  | C6-N1-C2 | -3.22 | 119.70      | 122.69   |
| 1   | 0     | 2621 | PSU  | C6-C5-C4 | 3.07  | 120.25      | 118.17   |
| 1   | 0     | 2621 | PSU  | O2-C2-N1 | 2.73  | 125.60      | 122.79   |
| 1   | 0     | 628  | 1MA  | N1-C2-N3 | 2.73  | 129.24      | 126.00   |
| 1   | 0     | 2619 | UR3  | C4-N3-C2 | 2.69  | 126.75      | 124.58   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 1   | 0     | 628 | 1MA  | C2'-C1'-N9-C8 |
| 1   | 0     | 628 | 1MA  | C2'-C1'-N9-C4 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 0     | 2587 | OMU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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   | 0     | 2749/2922 (94%) | -0.77  | 49 (1%) 67 63 | 18, 37, 80, 136       | 0     |
| 2   | 9     | 122/122 (100%)  | -0.20  | 4 (3%) 49 45  | 32, 54, 75, 144       | 0     |
| 3   | A     | 237/240 (98%)   | -0.28  | 4 (1%) 69 65  | 20, 39, 73, 93        | 0     |
| 4   | B     | 337/338 (99%)   | -0.13  | 5 (1%) 72 68  | 21, 46, 72, 83        | 0     |
| 5   | C     | 246/246 (100%)  | -0.32  | 1 (0%) 88 86  | 15, 36, 58, 70        | 0     |
| 6   | D     | 140/177 (79%)   | 1.32   | 30 (21%) 2 2  | 44, 89, 112, 117      | 0     |
| 7   | E     | 172/178 (96%)   | 0.27   | 3 (1%) 69 65  | 38, 59, 78, 83        | 0     |
| 8   | F     | 119/120 (99%)   | 0.52   | 7 (5%) 28 24  | 38, 58, 83, 90        | 0     |
| 9   | G     | 29/348 (8%)     | 1.14   | 3 (10%) 12 9  | 65, 81, 89, 93        | 0     |
| 10  | H     | 160/171 (93%)   | -0.05  | 3 (1%) 66 62  | 32, 47, 77, 88        | 0     |
| 11  | I     | 70/162 (43%)    | 2.67   | 46 (65%) 0 0  | 88, 102, 119, 122     | 0     |
| 12  | J     | 142/145 (97%)   | -0.18  | 0 100 100     | 30, 43, 63, 85        | 0     |
| 13  | K     | 132/132 (100%)  | -0.17  | 2 (1%) 72 68  | 28, 43, 62, 71        | 0     |
| 14  | L     | 145/165 (87%)   | 0.20   | 14 (9%) 13 10 | 20, 55, 93, 106       | 0     |
| 15  | M     | 194/194 (100%)  | -0.62  | 1 (0%) 87 85  | 19, 32, 46, 54        | 0     |
| 16  | N     | 186/187 (99%)   | 0.37   | 21 (11%) 10 7 | 32, 51, 94, 109       | 0     |
| 17  | O     | 115/116 (99%)   | -0.00  | 3 (2%) 57 53  | 28, 44, 61, 69        | 0     |
| 18  | P     | 143/149 (95%)   | -0.14  | 0 100 100     | 31, 45, 57, 64        | 0     |
| 19  | Q     | 95/96 (98%)     | -0.40  | 1 (1%) 78 74  | 27, 35, 52, 59        | 0     |
| 20  | R     | 150/155 (96%)   | -0.57  | 0 100 100     | 23, 36, 54, 63        | 0     |
| 21  | S     | 81/85 (95%)     | -0.10  | 0 100 100     | 32, 47, 68, 72        | 0     |
| 22  | T     | 119/120 (99%)   | 0.00   | 2 (1%) 69 65  | 29, 46, 67, 82        | 0     |
| 23  | U     | 53/66 (80%)     | 0.06   | 0 100 100     | 34, 47, 64, 73        | 0     |
| 24  | V     | 65/71 (91%)     | 0.54   | 5 (7%) 19 16  | 40, 59, 99, 103       | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25  | W     | 154/154 (100%)  | -0.25  | 0 100 100      | 28, 42, 58, 67        | 0     |
| 26  | X     | 82/92 (89%)     | 0.26   | 6 (7%) 21 17   | 36, 49, 74, 91        | 0     |
| 27  | Y     | 142/241 (58%)   | -0.35  | 1 (0%) 84 81   | 22, 36, 60, 75        | 0     |
| 28  | Z     | 73/73 (100%)    | 0.19   | 3 (4%) 41 37   | 37, 49, 68, 85        | 0     |
| 29  | 1     | 56/57 (98%)     | -0.85  | 0 100 100      | 18, 25, 33, 37        | 0     |
| 30  | 2     | 46/50 (92%)     | 0.19   | 2 (4%) 40 36   | 29, 50, 75, 86        | 0     |
| 31  | 3     | 92/92 (100%)    | -0.08  | 2 (2%) 62 58   | 24, 45, 59, 73        | 0     |
| All | All   | 6646/7464 (89%) | -0.32  | 218 (3%) 49 45 | 15, 42, 85, 144       | 0     |

All (218) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | I     | 133  | THR  | 9.9  |
| 24  | V     | 1    | THR  | 7.5  |
| 11  | I     | 96   | PHE  | 6.5  |
| 26  | X     | 88   | GLU  | 6.4  |
| 3   | A     | 37   | VAL  | 6.3  |
| 8   | F     | 105  | ASP  | 5.5  |
| 11  | I     | 90   | GLY  | 5.3  |
| 16  | N     | 166  | ALA  | 5.1  |
| 6   | D     | 10   | PHE  | 5.0  |
| 4   | B     | 1    | PRO  | 5.0  |
| 6   | D     | 63   | ILE  | 4.7  |
| 1   | 0     | 1173 | A    | 4.7  |
| 11  | I     | 82   | GLU  | 4.5  |
| 24  | V     | 40   | PRO  | 4.4  |
| 1   | 0     | 10   | U    | 4.4  |
| 1   | 0     | 1169 | U    | 4.4  |
| 14  | L     | 78   | ALA  | 4.4  |
| 30  | 2     | 49   | GLU  | 4.3  |
| 11  | I     | 137  | VAL  | 4.3  |
| 11  | I     | 121  | LEU  | 4.3  |
| 16  | N     | 163  | PHE  | 4.3  |
| 8   | F     | 103  | GLU  | 4.2  |
| 11  | I     | 93   | GLN  | 4.2  |
| 16  | N     | 186  | LEU  | 4.2  |
| 11  | I     | 88   | GLY  | 4.2  |
| 1   | 0     | 1525 | G    | 4.2  |
| 30  | 2     | 31   | ARG  | 4.1  |
| 11  | I     | 138  | THR  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | G     | 26   | MET  | 4.1  |
| 11  | I     | 95   | ASP  | 4.0  |
| 24  | V     | 39   | ALA  | 4.0  |
| 11  | I     | 92   | PRO  | 4.0  |
| 11  | I     | 85   | PHE  | 3.9  |
| 11  | I     | 100  | LEU  | 3.9  |
| 11  | I     | 97   | VAL  | 3.8  |
| 2   | 9     | 2    | U    | 3.8  |
| 16  | N     | 161  | GLY  | 3.8  |
| 7   | E     | 10   | ASP  | 3.8  |
| 6   | D     | 172  | VAL  | 3.7  |
| 24  | V     | 2    | VAL  | 3.7  |
| 1   | 0     | 1168 | C    | 3.7  |
| 6   | D     | 171  | ASP  | 3.6  |
| 1   | 0     | 1175 | G    | 3.6  |
| 8   | F     | 107  | ASP  | 3.6  |
| 11  | I     | 72   | VAL  | 3.5  |
| 27  | Y     | 235  | GLU  | 3.5  |
| 16  | N     | 154  | LEU  | 3.5  |
| 16  | N     | 168  | LEU  | 3.5  |
| 26  | X     | 83   | ALA  | 3.5  |
| 15  | M     | 194  | ALA  | 3.5  |
| 8   | F     | 102  | GLY  | 3.5  |
| 14  | L     | 77   | ALA  | 3.4  |
| 9   | G     | 12   | ILE  | 3.4  |
| 3   | A     | 36   | ASP  | 3.4  |
| 11  | I     | 139  | ILE  | 3.4  |
| 17  | O     | 23   | GLY  | 3.4  |
| 22  | T     | 1    | SER  | 3.3  |
| 2   | 9     | 1    | U    | 3.3  |
| 6   | D     | 62   | ASP  | 3.2  |
| 1   | 0     | 1176 | C    | 3.2  |
| 1   | 0     | 960  | G    | 3.2  |
| 6   | D     | 170  | TYR  | 3.2  |
| 6   | D     | 54   | ALA  | 3.2  |
| 11  | I     | 83   | ALA  | 3.2  |
| 14  | L     | 99   | GLU  | 3.2  |
| 1   | 0     | 283  | U    | 3.2  |
| 16  | N     | 152  | GLU  | 3.1  |
| 11  | I     | 94   | GLU  | 3.1  |
| 6   | D     | 59   | GLY  | 3.1  |
| 16  | N     | 164  | ASP  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | D     | 69   | ILE  | 3.1  |
| 11  | I     | 117  | LEU  | 3.1  |
| 7   | E     | 87   | PHE  | 3.0  |
| 14  | L     | 82   | ALA  | 3.0  |
| 1   | 0     | 128  | A    | 3.0  |
| 16  | N     | 167  | ASP  | 3.0  |
| 8   | F     | 101  | ALA  | 3.0  |
| 24  | V     | 43   | PRO  | 3.0  |
| 1   | 0     | 2506 | A    | 3.0  |
| 11  | I     | 87   | THR  | 3.0  |
| 1   | 0     | 970  | U    | 3.0  |
| 6   | D     | 61   | PHE  | 3.0  |
| 6   | D     | 58   | VAL  | 2.9  |
| 1   | 0     | 1172 | G    | 2.9  |
| 1   | 0     | 1192 | A    | 2.9  |
| 16  | N     | 165  | ALA  | 2.9  |
| 11  | I     | 78   | LEU  | 2.9  |
| 1   | 0     | 1170 | U    | 2.9  |
| 26  | X     | 82   | GLU  | 2.9  |
| 7   | E     | 45   | ASP  | 2.9  |
| 11  | I     | 102  | VAL  | 2.8  |
| 1   | 0     | 1184 | C    | 2.8  |
| 11  | I     | 124  | ALA  | 2.8  |
| 11  | I     | 135  | LEU  | 2.8  |
| 8   | F     | 110  | ASP  | 2.8  |
| 26  | X     | 80   | GLU  | 2.8  |
| 1   | 0     | 284  | C    | 2.8  |
| 10  | H     | 168  | ALA  | 2.8  |
| 14  | L     | 147  | GLU  | 2.8  |
| 14  | L     | 148  | GLU  | 2.8  |
| 11  | I     | 116  | LEU  | 2.8  |
| 16  | N     | 1    | ALA  | 2.8  |
| 1   | 0     | 1524 | U    | 2.7  |
| 11  | I     | 136  | GLY  | 2.7  |
| 6   | D     | 96   | SER  | 2.7  |
| 6   | D     | 174  | VAL  | 2.7  |
| 11  | I     | 89   | SER  | 2.7  |
| 6   | D     | 85   | GLN  | 2.7  |
| 11  | I     | 113  | HIS  | 2.7  |
| 16  | N     | 162  | ASP  | 2.7  |
| 11  | I     | 71   | GLY  | 2.7  |
| 1   | 0     | 1174 | A    | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | I     | 120  | ASP  | 2.7  |
| 1   | 0     | 1181 | A    | 2.7  |
| 11  | I     | 128  | VAL  | 2.7  |
| 6   | D     | 11   | HIS  | 2.7  |
| 14  | L     | 81   | VAL  | 2.6  |
| 11  | I     | 119  | TYR  | 2.6  |
| 1   | 0     | 1964 | U    | 2.6  |
| 9   | G     | 71   | LEU  | 2.6  |
| 6   | D     | 107  | GLY  | 2.6  |
| 6   | D     | 64   | ARG  | 2.6  |
| 1   | 0     | 138  | U    | 2.6  |
| 1   | 0     | 1164 | U    | 2.5  |
| 2   | 9     | 23   | U    | 2.5  |
| 2   | 9     | 24   | U    | 2.5  |
| 11  | I     | 98   | ALA  | 2.5  |
| 1   | 0     | 2345 | A    | 2.5  |
| 11  | I     | 129  | VAL  | 2.5  |
| 26  | X     | 87   | ALA  | 2.5  |
| 6   | D     | 27   | ILE  | 2.4  |
| 1   | 0     | 1171 | A    | 2.4  |
| 11  | I     | 134  | SER  | 2.4  |
| 3   | A     | 35   | GLY  | 2.4  |
| 4   | B     | 56   | ASP  | 2.4  |
| 11  | I     | 79   | ILE  | 2.4  |
| 1   | 0     | 1202 | A    | 2.4  |
| 1   | 0     | 2251 | G    | 2.4  |
| 11  | I     | 105  | VAL  | 2.4  |
| 1   | 0     | 1166 | A    | 2.4  |
| 31  | 3     | 18   | GLN  | 2.4  |
| 6   | D     | 20   | LYS  | 2.4  |
| 4   | B     | 57   | GLU  | 2.4  |
| 11  | I     | 118  | SER  | 2.3  |
| 11  | I     | 106  | LYS  | 2.3  |
| 1   | 0     | 1929 | G    | 2.3  |
| 16  | N     | 185  | GLU  | 2.3  |
| 6   | D     | 68   | PRO  | 2.3  |
| 1   | 0     | 2914 | A    | 2.3  |
| 6   | D     | 105  | SER  | 2.3  |
| 13  | K     | 119  | GLN  | 2.3  |
| 14  | L     | 145  | LEU  | 2.3  |
| 1   | 0     | 1179 | C    | 2.3  |
| 11  | I     | 114  | PRO  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | N     | 169  | PRO  | 2.3  |
| 14  | L     | 146  | GLY  | 2.3  |
| 1   | 0     | 1185 | U    | 2.3  |
| 16  | N     | 181  | ASP  | 2.3  |
| 6   | D     | 50   | VAL  | 2.3  |
| 4   | B     | 119  | HIS  | 2.3  |
| 1   | 0     | 1165 | G    | 2.3  |
| 16  | N     | 179  | LEU  | 2.3  |
| 1   | 0     | 1161 | A    | 2.3  |
| 5   | C     | 132  | ASP  | 2.3  |
| 11  | I     | 140  | GLU  | 2.3  |
| 14  | L     | 150  | GLN  | 2.2  |
| 6   | D     | 67   | ASP  | 2.2  |
| 1   | 0     | 1163 | G    | 2.2  |
| 1   | 0     | 1197 | G    | 2.2  |
| 1   | 0     | 2508 | C    | 2.2  |
| 16  | N     | 158  | LEU  | 2.2  |
| 10  | H     | 166  | SER  | 2.2  |
| 19  | Q     | 95   | GLU  | 2.2  |
| 1   | 0     | 1167 | G    | 2.2  |
| 14  | L     | 130  | ARG  | 2.2  |
| 1   | 0     | 1183 | C    | 2.2  |
| 11  | I     | 109  | ALA  | 2.2  |
| 11  | I     | 112  | LYS  | 2.2  |
| 11  | I     | 75   | THR  | 2.2  |
| 6   | D     | 66   | GLY  | 2.2  |
| 14  | L     | 75   | LEU  | 2.2  |
| 16  | N     | 160  | SER  | 2.2  |
| 3   | A     | 64   | ASP  | 2.2  |
| 14  | L     | 102  | ASP  | 2.2  |
| 1   | 0     | 1195 | G    | 2.2  |
| 6   | D     | 74   | THR  | 2.2  |
| 31  | 3     | 57   | GLY  | 2.2  |
| 14  | L     | 149  | ARG  | 2.2  |
| 1   | 0     | 1189 | A    | 2.1  |
| 1   | 0     | 1190 | G    | 2.1  |
| 28  | Z     | 81   | ARG  | 2.1  |
| 13  | K     | 132  | VAL  | 2.1  |
| 1   | 0     | 1180 | U    | 2.1  |
| 10  | H     | 171  | ALA  | 2.1  |
| 6   | D     | 47   | GLN  | 2.1  |
| 1   | 0     | 1198 | U    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 0     | 1561 | U    | 2.1  |
| 17  | O     | 24   | ALA  | 2.1  |
| 6   | D     | 52   | THR  | 2.1  |
| 1   | 0     | 282  | C    | 2.1  |
| 16  | N     | 180  | LEU  | 2.1  |
| 17  | O     | 22   | GLY  | 2.1  |
| 28  | Z     | 24   | ARG  | 2.1  |
| 6   | D     | 12   | GLU  | 2.1  |
| 11  | I     | 127  | GLU  | 2.1  |
| 22  | T     | 115  | GLU  | 2.1  |
| 11  | I     | 115  | ASP  | 2.1  |
| 16  | N     | 183  | ASP  | 2.1  |
| 1   | 0     | 1201 | C    | 2.1  |
| 26  | X     | 85   | VAL  | 2.0  |
| 8   | F     | 117  | GLU  | 2.0  |
| 6   | D     | 44   | ILE  | 2.0  |
| 1   | 0     | 1162 | G    | 2.0  |
| 4   | B     | 183  | GLU  | 2.0  |
| 6   | D     | 154  | LYS  | 2.0  |
| 16  | N     | 184  | ILE  | 2.0  |
| 1   | 0     | 2511 | A    | 2.0  |
| 28  | Z     | 82   | SER  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1   | OMU  | 0     | 2587 | 21/22 | 0.98 | 0.05 | 24,26,28,30                | 0     |
| 1   | OMG  | 0     | 2588 | 24/25 | 0.98 | 0.05 | 22,25,27,30                | 0     |
| 1   | UR3  | 0     | 2619 | 21/22 | 0.98 | 0.05 | 23,27,31,37                | 0     |
| 1   | 1MA  | 0     | 628  | 23/24 | 0.99 | 0.04 | 21,24,25,27                | 0     |
| 1   | PSU  | 0     | 2621 | 20/21 | 0.99 | 0.04 | 20,25,28,28                | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 32  | MG   | 0     | 8087 | 1/1   | 0.62 | 0.24 | 71,71,71,71                | 0     |
| 32  | MG   | 0     | 8102 | 1/1   | 0.70 | 0.10 | 54,54,54,54                | 0     |
| 32  | MG   | 9     | 8095 | 1/1   | 0.73 | 0.24 | 67,67,67,67                | 0     |
| 34  | NA   | R     | 8386 | 1/1   | 0.75 | 0.25 | 75,75,75,75                | 0     |
| 32  | MG   | 0     | 8050 | 1/1   | 0.76 | 0.08 | 62,62,62,62                | 0     |
| 34  | NA   | 0     | 8370 | 1/1   | 0.81 | 0.24 | 60,60,60,60                | 0     |
| 32  | MG   | 0     | 8070 | 1/1   | 0.81 | 0.06 | 41,41,41,41                | 0     |
| 34  | NA   | 9     | 8351 | 1/1   | 0.83 | 0.18 | 43,43,43,43                | 0     |
| 34  | NA   | 9     | 8383 | 1/1   | 0.84 | 0.18 | 44,44,44,44                | 0     |
| 34  | NA   | 0     | 8340 | 1/1   | 0.85 | 0.13 | 46,46,46,46                | 0     |
| 32  | MG   | 0     | 8090 | 1/1   | 0.85 | 0.10 | 55,55,55,55                | 0     |
| 34  | NA   | 0     | 8376 | 1/1   | 0.85 | 0.10 | 40,40,40,40                | 0     |
| 32  | MG   | 0     | 8103 | 1/1   | 0.86 | 0.09 | 57,57,57,57                | 0     |
| 34  | NA   | 0     | 8307 | 1/1   | 0.86 | 0.07 | 42,42,42,42                | 0     |
| 34  | NA   | 0     | 8329 | 1/1   | 0.86 | 0.08 | 50,50,50,50                | 0     |
| 32  | MG   | 0     | 8105 | 1/1   | 0.87 | 0.06 | 43,43,43,43                | 0     |
| 32  | MG   | 0     | 8101 | 1/1   | 0.87 | 0.11 | 48,48,48,48                | 0     |
| 34  | NA   | 0     | 8324 | 1/1   | 0.88 | 0.18 | 51,51,51,51                | 0     |
| 34  | NA   | 0     | 8366 | 1/1   | 0.88 | 0.10 | 57,57,57,57                | 0     |
| 34  | NA   | 0     | 8384 | 1/1   | 0.88 | 0.10 | 54,54,54,54                | 0     |
| 32  | MG   | 0     | 8082 | 1/1   | 0.89 | 0.15 | 59,59,59,59                | 0     |
| 34  | NA   | 0     | 8311 | 1/1   | 0.90 | 0.09 | 48,48,48,48                | 0     |
| 34  | NA   | 0     | 8350 | 1/1   | 0.90 | 0.08 | 36,36,36,36                | 0     |
| 34  | NA   | 0     | 8364 | 1/1   | 0.90 | 0.11 | 38,38,38,38                | 0     |
| 32  | MG   | 0     | 8076 | 1/1   | 0.90 | 0.04 | 43,43,43,43                | 0     |
| 32  | MG   | 0     | 8094 | 1/1   | 0.90 | 0.13 | 62,62,62,62                | 0     |
| 32  | MG   | 0     | 8047 | 1/1   | 0.91 | 0.11 | 55,55,55,55                | 0     |
| 34  | NA   | 0     | 8369 | 1/1   | 0.91 | 0.11 | 41,41,41,41                | 0     |
| 32  | MG   | 0     | 8043 | 1/1   | 0.91 | 0.06 | 34,34,34,34                | 0     |
| 34  | NA   | H     | 8322 | 1/1   | 0.91 | 0.14 | 53,53,53,53                | 0     |
| 34  | NA   | R     | 8337 | 1/1   | 0.91 | 0.05 | 34,34,34,34                | 0     |
| 32  | MG   | 0     | 8066 | 1/1   | 0.91 | 0.15 | 76,76,76,76                | 0     |
| 34  | NA   | 0     | 8371 | 1/1   | 0.92 | 0.14 | 52,52,52,52                | 0     |
| 34  | NA   | 0     | 8357 | 1/1   | 0.92 | 0.06 | 40,40,40,40                | 0     |
| 34  | NA   | 0     | 8358 | 1/1   | 0.92 | 0.39 | 67,67,67,67                | 0     |
| 34  | NA   | 0     | 8341 | 1/1   | 0.92 | 0.08 | 38,38,38,38                | 0     |
| 34  | NA   | 0     | 8373 | 1/1   | 0.93 | 0.06 | 44,44,44,44                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | NA   | 0     | 8363 | 1/1   | 0.93 | 0.12 | 52,52,52,52                 | 0     |
| 34  | NA   | 0     | 8314 | 1/1   | 0.93 | 0.08 | 39,39,39,39                 | 0     |
| 32  | MG   | 0     | 8113 | 1/1   | 0.93 | 0.04 | 36,36,36,36                 | 0     |
| 34  | NA   | 0     | 8327 | 1/1   | 0.93 | 0.11 | 38,38,38,38                 | 0     |
| 32  | MG   | 0     | 8049 | 1/1   | 0.93 | 0.08 | 55,55,55,55                 | 0     |
| 34  | NA   | 0     | 8330 | 1/1   | 0.93 | 0.08 | 38,38,38,38                 | 0     |
| 34  | NA   | 0     | 8372 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 32  | MG   | 0     | 8093 | 1/1   | 0.94 | 0.05 | 37,37,37,37                 | 0     |
| 32  | MG   | 0     | 8104 | 1/1   | 0.94 | 0.04 | 47,47,47,47                 | 0     |
| 32  | MG   | 0     | 8046 | 1/1   | 0.94 | 0.05 | 38,38,38,38                 | 0     |
| 34  | NA   | 0     | 8379 | 1/1   | 0.94 | 0.15 | 49,49,49,49                 | 0     |
| 32  | MG   | 0     | 8112 | 1/1   | 0.94 | 0.06 | 38,38,38,38                 | 0     |
| 32  | MG   | 0     | 8099 | 1/1   | 0.94 | 0.05 | 43,43,43,43                 | 0     |
| 32  | MG   | 0     | 8072 | 1/1   | 0.94 | 0.06 | 51,51,51,51                 | 0     |
| 34  | NA   | 0     | 8336 | 1/1   | 0.94 | 0.04 | 37,37,37,37                 | 0     |
| 32  | MG   | 0     | 8092 | 1/1   | 0.94 | 0.10 | 68,68,68,68                 | 0     |
| 34  | NA   | 0     | 8310 | 1/1   | 0.94 | 0.08 | 28,28,28,28                 | 0     |
| 32  | MG   | 0     | 8114 | 1/1   | 0.95 | 0.04 | 37,37,37,37                 | 0     |
| 34  | NA   | 0     | 8334 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 34  | NA   | 0     | 8374 | 1/1   | 0.95 | 0.09 | 44,44,44,44                 | 0     |
| 34  | NA   | 0     | 8360 | 1/1   | 0.95 | 0.07 | 43,43,43,43                 | 0     |
| 34  | NA   | 0     | 8362 | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 34  | NA   | 0     | 8381 | 1/1   | 0.95 | 0.06 | 42,42,42,42                 | 0     |
| 34  | NA   | 0     | 8382 | 1/1   | 0.95 | 0.07 | 66,66,66,66                 | 0     |
| 32  | MG   | 0     | 8116 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |
| 34  | NA   | 0     | 8385 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 32  | MG   | 0     | 8091 | 1/1   | 0.95 | 0.04 | 42,42,42,42                 | 0     |
| 32  | MG   | 0     | 8062 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 34  | NA   | 0     | 8349 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 34  | NA   | Q     | 8348 | 1/1   | 0.95 | 0.04 | 32,32,32,32                 | 0     |
| 32  | MG   | 0     | 8053 | 1/1   | 0.95 | 0.14 | 29,29,29,29                 | 0     |
| 34  | NA   | 0     | 8352 | 1/1   | 0.95 | 0.05 | 40,40,40,40                 | 0     |
| 34  | NA   | S     | 8312 | 1/1   | 0.95 | 0.05 | 28,28,28,28                 | 0     |
| 34  | NA   | 0     | 8365 | 1/1   | 0.96 | 0.21 | 30,30,30,30                 | 0     |
| 32  | MG   | 0     | 8100 | 1/1   | 0.96 | 0.07 | 62,62,62,62                 | 0     |
| 34  | NA   | 0     | 8367 | 1/1   | 0.96 | 0.05 | 45,45,45,45                 | 0     |
| 34  | NA   | 0     | 8368 | 1/1   | 0.96 | 0.11 | 50,50,50,50                 | 0     |
| 32  | MG   | 0     | 8067 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 32  | MG   | 0     | 8012 | 1/1   | 0.96 | 0.07 | 34,34,34,34                 | 0     |
| 33  | K    | 0     | 8201 | 1/1   | 0.96 | 0.12 | 64,64,64,64                 | 0     |
| 34  | NA   | 0     | 8335 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 34  | NA   | 0     | 8302 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | 0     | 8071 | 1/1   | 0.96 | 0.05 | 61,61,61,61                 | 0     |
| 32  | MG   | 0     | 8048 | 1/1   | 0.96 | 0.04 | 40,40,40,40                 | 0     |
| 34  | NA   | 0     | 8377 | 1/1   | 0.96 | 0.08 | 51,51,51,51                 | 0     |
| 34  | NA   | 0     | 8378 | 1/1   | 0.96 | 0.12 | 42,42,42,42                 | 0     |
| 34  | NA   | 0     | 8342 | 1/1   | 0.96 | 0.05 | 33,33,33,33                 | 0     |
| 32  | MG   | 0     | 8064 | 1/1   | 0.96 | 0.04 | 26,26,26,26                 | 0     |
| 34  | NA   | 0     | 8313 | 1/1   | 0.96 | 0.05 | 48,48,48,48                 | 0     |
| 32  | MG   | 0     | 8051 | 1/1   | 0.96 | 0.07 | 56,56,56,56                 | 0     |
| 34  | NA   | 0     | 8356 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 34  | NA   | 0     | 8316 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 34  | NA   | 0     | 8318 | 1/1   | 0.96 | 0.11 | 51,51,51,51                 | 0     |
| 34  | NA   | C     | 8304 | 1/1   | 0.96 | 0.04 | 32,32,32,32                 | 0     |
| 34  | NA   | 0     | 8319 | 1/1   | 0.96 | 0.03 | 29,29,29,29                 | 0     |
| 34  | NA   | J     | 8346 | 1/1   | 0.96 | 0.04 | 36,36,36,36                 | 0     |
| 34  | NA   | 0     | 8361 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 32  | MG   | 0     | 8085 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 34  | NA   | 0     | 8325 | 1/1   | 0.96 | 0.08 | 49,49,49,49                 | 0     |
| 34  | NA   | 0     | 8326 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 35  | CL   | J     | 8502 | 1/1   | 0.96 | 0.04 | 53,53,53,53                 | 0     |
| 35  | CL   | J     | 8521 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 32  | MG   | 0     | 8096 | 1/1   | 0.97 | 0.04 | 38,38,38,38                 | 0     |
| 34  | NA   | 0     | 8375 | 1/1   | 0.97 | 0.18 | 43,43,43,43                 | 0     |
| 32  | MG   | 0     | 8024 | 1/1   | 0.97 | 0.03 | 23,23,23,23                 | 0     |
| 32  | MG   | 0     | 8052 | 1/1   | 0.97 | 0.04 | 47,47,47,47                 | 0     |
| 34  | NA   | 0     | 8321 | 1/1   | 0.97 | 0.12 | 40,40,40,40                 | 0     |
| 32  | MG   | 0     | 8089 | 1/1   | 0.97 | 0.05 | 52,52,52,52                 | 0     |
| 34  | NA   | 0     | 8359 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 32  | MG   | K     | 8069 | 1/1   | 0.97 | 0.04 | 47,47,47,47                 | 0     |
| 32  | MG   | Y     | 8108 | 1/1   | 0.97 | 0.05 | 27,27,27,27                 | 0     |
| 32  | MG   | 3     | 8078 | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 32  | MG   | 0     | 8037 | 1/1   | 0.97 | 0.03 | 34,34,34,34                 | 0     |
| 34  | NA   | 0     | 8301 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 34  | NA   | 0     | 8333 | 1/1   | 0.97 | 0.04 | 25,25,25,25                 | 0     |
| 34  | NA   | H     | 8309 | 1/1   | 0.97 | 0.03 | 28,28,28,28                 | 0     |
| 32  | MG   | 0     | 8040 | 1/1   | 0.97 | 0.04 | 38,38,38,38                 | 0     |
| 32  | MG   | 0     | 8075 | 1/1   | 0.97 | 0.05 | 30,30,30,30                 | 0     |
| 34  | NA   | L     | 8380 | 1/1   | 0.97 | 0.28 | 42,42,42,42                 | 0     |
| 34  | NA   | M     | 8347 | 1/1   | 0.97 | 0.04 | 20,20,20,20                 | 0     |
| 34  | NA   | 0     | 8308 | 1/1   | 0.97 | 0.05 | 43,43,43,43                 | 0     |
| 32  | MG   | 0     | 8014 | 1/1   | 0.97 | 0.09 | 25,25,25,25                 | 0     |
| 32  | MG   | 0     | 8107 | 1/1   | 0.97 | 0.09 | 65,65,65,65                 | 0     |
| 32  | MG   | 0     | 8111 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | NA   | T     | 8343 | 1/1   | 0.97 | 0.04 | 31,31,31,31                 | 0     |
| 35  | CL   | 0     | 8515 | 1/1   | 0.97 | 0.10 | 50,50,50,50                 | 0     |
| 35  | CL   | 0     | 8517 | 1/1   | 0.97 | 0.05 | 50,50,50,50                 | 0     |
| 35  | CL   | A     | 8509 | 1/1   | 0.97 | 0.04 | 49,49,49,49                 | 0     |
| 34  | NA   | 0     | 8344 | 1/1   | 0.97 | 0.07 | 25,25,25,25                 | 0     |
| 32  | MG   | 0     | 8045 | 1/1   | 0.97 | 0.05 | 51,51,51,51                 | 0     |
| 35  | CL   | L     | 8510 | 1/1   | 0.97 | 0.08 | 38,38,38,38                 | 0     |
| 34  | NA   | 0     | 8315 | 1/1   | 0.98 | 0.06 | 32,32,32,32                 | 0     |
| 32  | MG   | 0     | 8115 | 1/1   | 0.98 | 0.03 | 44,44,44,44                 | 0     |
| 32  | MG   | 0     | 8097 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 34  | NA   | 0     | 8354 | 1/1   | 0.98 | 0.05 | 26,26,26,26                 | 0     |
| 34  | NA   | 0     | 8355 | 1/1   | 0.98 | 0.12 | 48,48,48,48                 | 0     |
| 32  | MG   | 0     | 8098 | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 34  | NA   | 0     | 8320 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 32  | MG   | B     | 8055 | 1/1   | 0.98 | 0.03 | 43,43,43,43                 | 0     |
| 32  | MG   | 0     | 8041 | 1/1   | 0.98 | 0.10 | 34,34,34,34                 | 0     |
| 32  | MG   | T     | 8073 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 32  | MG   | 0     | 8025 | 1/1   | 0.98 | 0.03 | 37,37,37,37                 | 0     |
| 32  | MG   | 0     | 8086 | 1/1   | 0.98 | 0.04 | 33,33,33,33                 | 0     |
| 32  | MG   | 0     | 8044 | 1/1   | 0.98 | 0.03 | 33,33,33,33                 | 0     |
| 32  | MG   | 0     | 8088 | 1/1   | 0.98 | 0.07 | 21,21,21,21                 | 0     |
| 34  | NA   | 0     | 8331 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 34  | NA   | 0     | 8332 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 32  | MG   | 0     | 8034 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 34  | NA   | 0     | 8306 | 1/1   | 0.98 | 0.13 | 31,31,31,31                 | 0     |
| 32  | MG   | 0     | 8007 | 1/1   | 0.98 | 0.03 | 22,22,22,22                 | 0     |
| 32  | MG   | 0     | 8074 | 1/1   | 0.98 | 0.03 | 35,35,35,35                 | 0     |
| 35  | CL   | 0     | 8503 | 1/1   | 0.98 | 0.03 | 42,42,42,42                 | 0     |
| 35  | CL   | 0     | 8505 | 1/1   | 0.98 | 0.04 | 42,42,42,42                 | 0     |
| 35  | CL   | 0     | 8511 | 1/1   | 0.98 | 0.03 | 38,38,38,38                 | 0     |
| 35  | CL   | 0     | 8513 | 1/1   | 0.98 | 0.04 | 45,45,45,45                 | 0     |
| 35  | CL   | 0     | 8514 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 34  | NA   | 0     | 8338 | 1/1   | 0.98 | 0.03 | 38,38,38,38                 | 0     |
| 35  | CL   | 0     | 8516 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 34  | NA   | 0     | 8339 | 1/1   | 0.98 | 0.03 | 21,21,21,21                 | 0     |
| 35  | CL   | 0     | 8522 | 1/1   | 0.98 | 0.20 | 46,46,46,46                 | 0     |
| 32  | MG   | 0     | 8039 | 1/1   | 0.98 | 0.03 | 34,34,34,34                 | 0     |
| 35  | CL   | B     | 8519 | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 35  | CL   | J     | 8501 | 1/1   | 0.98 | 0.04 | 46,46,46,46                 | 0     |
| 32  | MG   | 0     | 8003 | 1/1   | 0.98 | 0.02 | 22,22,22,22                 | 0     |
| 32  | MG   | 0     | 8080 | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 32  | MG   | 0     | 8081 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35  | CL   | M     | 8518 | 1/1   | 0.98 | 0.03 | 35,35,35,35                 | 0     |
| 35  | CL   | R     | 8506 | 1/1   | 0.98 | 0.04 | 40,40,40,40                 | 0     |
| 35  | CL   | Y     | 8520 | 1/1   | 0.98 | 0.06 | 39,39,39,39                 | 0     |
| 36  | CD   | O     | 8405 | 1/1   | 0.98 | 0.04 | 73,73,73,73                 | 0     |
| 32  | MG   | 0     | 8068 | 1/1   | 0.99 | 0.03 | 45,45,45,45                 | 0     |
| 32  | MG   | 0     | 8106 | 1/1   | 0.99 | 0.02 | 31,31,31,31                 | 0     |
| 32  | MG   | 0     | 8035 | 1/1   | 0.99 | 0.02 | 37,37,37,37                 | 0     |
| 34  | NA   | 0     | 8328 | 1/1   | 0.99 | 0.09 | 30,30,30,30                 | 0     |
| 32  | MG   | 0     | 8109 | 1/1   | 0.99 | 0.02 | 26,26,26,26                 | 0     |
| 32  | MG   | 0     | 8110 | 1/1   | 0.99 | 0.05 | 32,32,32,32                 | 0     |
| 32  | MG   | 0     | 8036 | 1/1   | 0.99 | 0.03 | 36,36,36,36                 | 0     |
| 32  | MG   | 0     | 8011 | 1/1   | 0.99 | 0.02 | 24,24,24,24                 | 0     |
| 32  | MG   | 0     | 8038 | 1/1   | 0.99 | 0.02 | 23,23,23,23                 | 0     |
| 32  | MG   | 0     | 8006 | 1/1   | 0.99 | 0.05 | 27,27,27,27                 | 0     |
| 32  | MG   | 0     | 8013 | 1/1   | 0.99 | 0.03 | 22,22,22,22                 | 0     |
| 32  | MG   | 0     | 8077 | 1/1   | 0.99 | 0.02 | 24,24,24,24                 | 0     |
| 34  | NA   | A     | 8345 | 1/1   | 0.99 | 0.03 | 47,47,47,47                 | 0     |
| 32  | MG   | 0     | 8079 | 1/1   | 0.99 | 0.02 | 20,20,20,20                 | 0     |
| 32  | MG   | A     | 8065 | 1/1   | 0.99 | 0.05 | 24,24,24,24                 | 0     |
| 32  | MG   | 0     | 8002 | 1/1   | 0.99 | 0.04 | 28,28,28,28                 | 0     |
| 32  | MG   | 0     | 8042 | 1/1   | 0.99 | 0.06 | 29,29,29,29                 | 0     |
| 32  | MG   | 0     | 8015 | 1/1   | 0.99 | 0.02 | 27,27,27,27                 | 0     |
| 32  | MG   | 0     | 8016 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 32  | MG   | 0     | 8017 | 1/1   | 0.99 | 0.03 | 13,13,13,13                 | 0     |
| 32  | MG   | 0     | 8018 | 1/1   | 0.99 | 0.03 | 29,29,29,29                 | 0     |
| 33  | K    | 0     | 8202 | 1/1   | 0.99 | 0.14 | 38,38,38,38                 | 0     |
| 34  | NA   | 0     | 8353 | 1/1   | 0.99 | 0.05 | 20,20,20,20                 | 0     |
| 32  | MG   | 0     | 8022 | 1/1   | 0.99 | 0.03 | 31,31,31,31                 | 0     |
| 32  | MG   | 0     | 8023 | 1/1   | 0.99 | 0.02 | 31,31,31,31                 | 0     |
| 34  | NA   | 0     | 8303 | 1/1   | 0.99 | 0.08 | 34,34,34,34                 | 0     |
| 34  | NA   | 0     | 8305 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 35  | CL   | 0     | 8512 | 1/1   | 0.99 | 0.03 | 35,35,35,35                 | 0     |
| 32  | MG   | 0     | 8008 | 1/1   | 0.99 | 0.03 | 24,24,24,24                 | 0     |
| 32  | MG   | 0     | 8009 | 1/1   | 0.99 | 0.03 | 25,25,25,25                 | 0     |
| 32  | MG   | 0     | 8027 | 1/1   | 0.99 | 0.02 | 36,36,36,36                 | 0     |
| 32  | MG   | 0     | 8028 | 1/1   | 0.99 | 0.02 | 26,26,26,26                 | 0     |
| 32  | MG   | 0     | 8029 | 1/1   | 0.99 | 0.03 | 36,36,36,36                 | 0     |
| 32  | MG   | 0     | 8056 | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 32  | MG   | 0     | 8057 | 1/1   | 0.99 | 0.04 | 36,36,36,36                 | 0     |
| 32  | MG   | 0     | 8059 | 1/1   | 0.99 | 0.05 | 26,26,26,26                 | 0     |
| 32  | MG   | 0     | 8060 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 34  | NA   | 0     | 8317 | 1/1   | 0.99 | 0.02 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MG   | 0     | 8031 | 1/1   | 0.99 | 0.02 | 24,24,24,24                 | 0     |
| 32  | MG   | 0     | 8063 | 1/1   | 0.99 | 0.05 | 62,62,62,62                 | 0     |
| 32  | MG   | 0     | 8032 | 1/1   | 0.99 | 0.04 | 24,24,24,24                 | 0     |
| 35  | CL   | N     | 8507 | 1/1   | 0.99 | 0.05 | 46,46,46,46                 | 0     |
| 35  | CL   | O     | 8508 | 1/1   | 0.99 | 0.03 | 53,53,53,53                 | 0     |
| 32  | MG   | 0     | 8033 | 1/1   | 0.99 | 0.01 | 20,20,20,20                 | 0     |
| 34  | NA   | 0     | 8323 | 1/1   | 0.99 | 0.10 | 32,32,32,32                 | 0     |
| 35  | CL   | 3     | 8504 | 1/1   | 0.99 | 0.03 | 45,45,45,45                 | 0     |
| 32  | MG   | 0     | 8010 | 1/1   | 0.99 | 0.02 | 25,25,25,25                 | 0     |
| 36  | CD   | U     | 8401 | 1/1   | 0.99 | 0.02 | 52,52,52,52                 | 0     |
| 36  | CD   | Z     | 8403 | 1/1   | 0.99 | 0.04 | 48,48,48,48                 | 0     |
| 36  | CD   | 3     | 8404 | 1/1   | 0.99 | 0.01 | 49,49,49,49                 | 0     |
| 32  | MG   | 0     | 8004 | 1/1   | 1.00 | 0.02 | 22,22,22,22                 | 0     |
| 32  | MG   | 0     | 8054 | 1/1   | 1.00 | 0.02 | 18,18,18,18                 | 0     |
| 32  | MG   | 0     | 8030 | 1/1   | 1.00 | 0.03 | 22,22,22,22                 | 0     |
| 32  | MG   | 0     | 8083 | 1/1   | 1.00 | 0.02 | 30,30,30,30                 | 0     |
| 32  | MG   | 0     | 8084 | 1/1   | 1.00 | 0.04 | 39,39,39,39                 | 0     |
| 32  | MG   | 0     | 8005 | 1/1   | 1.00 | 0.02 | 24,24,24,24                 | 0     |
| 32  | MG   | 0     | 8058 | 1/1   | 1.00 | 0.03 | 28,28,28,28                 | 0     |
| 32  | MG   | 0     | 8001 | 1/1   | 1.00 | 0.02 | 25,25,25,25                 | 0     |
| 32  | MG   | 0     | 8019 | 1/1   | 1.00 | 0.01 | 25,25,25,25                 | 0     |
| 32  | MG   | 0     | 8061 | 1/1   | 1.00 | 0.01 | 34,34,34,34                 | 0     |
| 32  | MG   | 0     | 8026 | 1/1   | 1.00 | 0.01 | 27,27,27,27                 | 0     |
| 32  | MG   | 0     | 8020 | 1/1   | 1.00 | 0.02 | 25,25,25,25                 | 0     |
| 36  | CD   | 1     | 8402 | 1/1   | 1.00 | 0.06 | 44,44,44,44                 | 0     |
| 32  | MG   | 0     | 8021 | 1/1   | 1.00 | 0.02 | 24,24,24,24                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.