



## Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:01 PM UTC

PDB ID : 3T1Y / pdb\_00003t1y  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a human anti-codon stem loop (HASL) of transfer RNA Lysine 3 (TRNALYS3) bound to an mRNA with an AAG-codon in the A-site and paromomycin  
Authors : Murphy, F.V.; Vendeix, F.A.P.; Cantara, W.; Leszczynska, G.; Gustilo, E.M.; Sproat, B.; Malkiewicz, A.A.P.; Agris, P.F.  
Deposited on : 2011-07-22  
Resolution : 2.80 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](#) ①) were used in the production of this report:

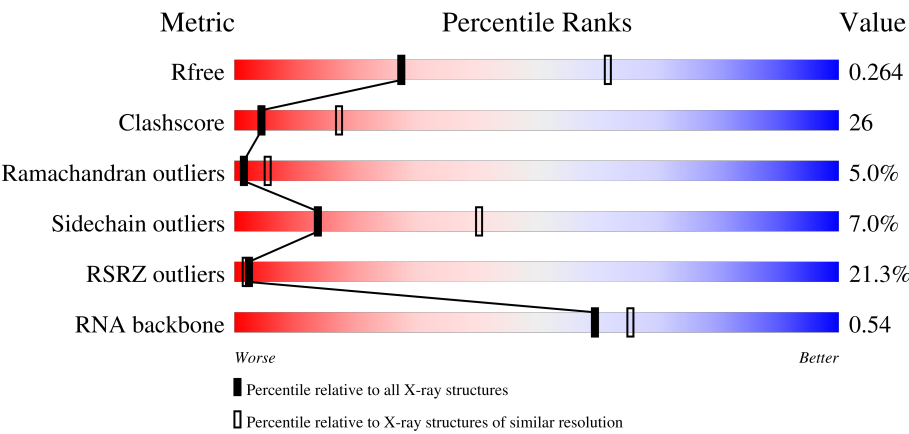
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |
| RNA backbone          | 3983                        | 1114 (3.00-2.60)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                 |
|-----|-------|--------|----------------------------------------------------------------------------------|
| 1   | A     | 1513   | <div><div>15%</div><div>42%</div><div>34%</div><div>15%</div><div>9%</div></div> |
| 2   | B     | 256    | <div><div>37%</div><div>32%</div><div>50%</div><div>9%</div><div>9%</div></div>  |
| 3   | C     | 239    | <div><div>36%</div><div>31%</div><div>45%</div><div>9%</div><div>14%</div></div> |
| 4   | D     | 209    | <div><div>12%</div><div>44%</div><div>48%</div><div>7%</div></div>               |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 162    |                  |
| 6   | F     | 101    |                  |
| 7   | G     | 156    |                  |
| 8   | H     | 138    |                  |
| 9   | I     | 128    |                  |
| 10  | J     | 105    |                  |
| 11  | K     | 129    |                  |
| 12  | L     | 132    |                  |
| 13  | M     | 126    |                  |
| 14  | N     | 61     |                  |
| 15  | O     | 89     |                  |
| 16  | P     | 88     |                  |
| 17  | Q     | 105    |                  |
| 18  | R     | 88     |                  |
| 19  | S     | 93     |                  |
| 20  | T     | 106    |                  |
| 21  | V     | 27     |                  |
| 22  | W     | 3      |                  |
| 23  | X     | 11     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24  | MG   | A     | 1603 | -         | -        | -       | X                |
| 24  | MG   | A     | 1604 | -         | -        | -       | X                |
| 24  | MG   | A     | 1605 | -         | -        | -       | X                |
| 24  | MG   | A     | 1607 | -         | -        | -       | X                |
| 24  | MG   | A     | 1608 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24  | MG   | A     | 1610 | -         | -        | -       | X                |
| 24  | MG   | A     | 1614 | -         | -        | -       | X                |
| 24  | MG   | A     | 1616 | -         | -        | -       | X                |
| 24  | MG   | A     | 1617 | -         | -        | -       | X                |
| 24  | MG   | A     | 1619 | -         | -        | -       | X                |
| 24  | MG   | A     | 1621 | -         | -        | -       | X                |
| 24  | MG   | A     | 1622 | -         | -        | -       | X                |
| 24  | MG   | A     | 1623 | -         | -        | -       | X                |
| 24  | MG   | A     | 1624 | -         | -        | -       | X                |
| 24  | MG   | A     | 1625 | -         | -        | -       | X                |
| 24  | MG   | A     | 1629 | -         | -        | -       | X                |
| 24  | MG   | A     | 1630 | -         | -        | -       | X                |
| 24  | MG   | A     | 1632 | -         | -        | -       | X                |
| 24  | MG   | A     | 1633 | -         | -        | -       | X                |
| 24  | MG   | A     | 1635 | -         | -        | -       | X                |
| 24  | MG   | A     | 1636 | -         | -        | -       | X                |
| 24  | MG   | A     | 1638 | -         | -        | -       | X                |
| 24  | MG   | A     | 1639 | -         | -        | -       | X                |
| 24  | MG   | A     | 1644 | -         | -        | -       | X                |
| 24  | MG   | A     | 1645 | -         | -        | -       | X                |
| 24  | MG   | A     | 1658 | -         | -        | -       | X                |
| 24  | MG   | A     | 1660 | -         | -        | -       | X                |
| 24  | MG   | A     | 1661 | -         | -        | -       | X                |
| 24  | MG   | A     | 1662 | -         | -        | -       | X                |
| 24  | MG   | A     | 1666 | -         | -        | -       | X                |
| 24  | MG   | A     | 1667 | -         | -        | -       | X                |
| 24  | MG   | A     | 1669 | -         | -        | -       | X                |
| 24  | MG   | A     | 1671 | -         | -        | -       | X                |
| 24  | MG   | A     | 1684 | -         | -        | -       | X                |
| 24  | MG   | A     | 1689 | -         | -        | -       | X                |
| 24  | MG   | A     | 1694 | -         | -        | -       | X                |
| 24  | MG   | A     | 1695 | -         | -        | -       | X                |
| 24  | MG   | A     | 1696 | -         | -        | -       | X                |
| 24  | MG   | A     | 1697 | -         | -        | -       | X                |
| 24  | MG   | A     | 1699 | -         | -        | -       | X                |
| 24  | MG   | A     | 1700 | -         | -        | -       | X                |
| 24  | MG   | A     | 1701 | -         | -        | -       | X                |
| 24  | MG   | A     | 1702 | -         | -        | -       | X                |
| 24  | MG   | A     | 1704 | -         | -        | -       | X                |
| 24  | MG   | A     | 1706 | -         | -        | -       | X                |
| 24  | MG   | A     | 1707 | -         | -        | -       | X                |
| 24  | MG   | A     | 1708 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24  | MG   | A     | 1712 | -         | -        | -       | X                |
| 24  | MG   | A     | 1715 | -         | -        | -       | X                |
| 24  | MG   | A     | 1716 | -         | -        | -       | X                |
| 24  | MG   | A     | 1717 | -         | -        | -       | X                |
| 24  | MG   | A     | 1719 | -         | -        | -       | X                |
| 24  | MG   | A     | 1722 | -         | -        | -       | X                |
| 24  | MG   | A     | 1724 | -         | -        | -       | X                |
| 24  | MG   | A     | 1725 | -         | -        | -       | X                |
| 24  | MG   | A     | 1727 | -         | -        | -       | X                |
| 24  | MG   | A     | 1730 | -         | -        | -       | X                |
| 24  | MG   | A     | 1731 | -         | -        | -       | X                |
| 24  | MG   | A     | 1733 | -         | -        | -       | X                |
| 24  | MG   | A     | 1734 | -         | -        | -       | X                |
| 24  | MG   | A     | 1736 | -         | -        | -       | X                |
| 24  | MG   | A     | 1739 | -         | -        | -       | X                |
| 24  | MG   | A     | 1741 | -         | -        | -       | X                |
| 24  | MG   | A     | 1745 | -         | -        | -       | X                |
| 24  | MG   | A     | 1750 | -         | -        | -       | X                |
| 24  | MG   | A     | 1751 | -         | -        | -       | X                |
| 24  | MG   | A     | 1752 | -         | -        | -       | X                |
| 24  | MG   | A     | 1753 | -         | -        | -       | X                |
| 24  | MG   | A     | 1754 | -         | -        | -       | X                |
| 24  | MG   | A     | 1757 | -         | -        | -       | X                |
| 24  | MG   | A     | 1758 | -         | -        | -       | X                |
| 24  | MG   | A     | 1759 | -         | -        | -       | X                |
| 24  | MG   | A     | 1760 | -         | -        | -       | X                |
| 24  | MG   | A     | 1767 | -         | -        | -       | X                |
| 24  | MG   | A     | 1768 | -         | -        | -       | X                |
| 24  | MG   | A     | 1773 | -         | -        | -       | X                |
| 24  | MG   | A     | 1776 | -         | -        | -       | X                |
| 24  | MG   | A     | 1777 | -         | -        | -       | X                |
| 24  | MG   | A     | 1780 | -         | -        | -       | X                |
| 24  | MG   | A     | 1785 | -         | -        | -       | X                |

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52289 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 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | A     | 1513     | Total | C     | N    | O     | P    | 22      | 0       | 0     |
|     |       |          | 32515 | 14472 | 6016 | 10514 | 1513 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| A     | 1517    | U        | -      | insertion | GB 55771382 |
| A     | 1518    | U        | -      | insertion | GB 55771382 |
| A     | 1519    | U        | -      | insertion | GB 55771382 |
| A     | 1520    | C        | -      | insertion | GB 55771382 |
| A     | 1521    | U        | -      | insertion | GB 55771382 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | I     | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 792   | 498 | 156 | 137 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | N     | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | O     | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | P     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | R     | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 647   | 414 | 119 | 112 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | T     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | V     | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |

- Molecule 22 is a RNA chain called mRNA A-site fragment.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 22  | W     | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 68    | 30 | 15 | 20 | 3 |         |         |       |

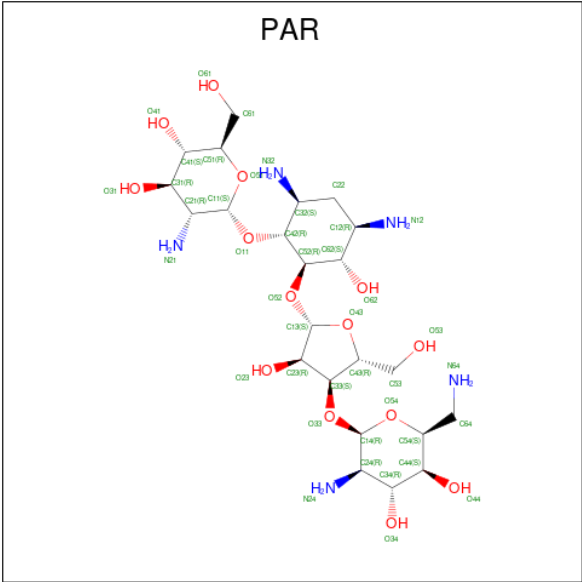
- Molecule 23 is a RNA chain called tRNA ASL human Lys3.

| Mol | Chain | Residues | Atoms |     |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---|---------|---------|-------|
| 23  | X     | 11       | Total | C   | N  | O  | P  | S | 0       | 0       | 0     |
|     |       |          | 247   | 112 | 37 | 85 | 11 | 2 |         |         |       |

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 24  | A     | 185      | Total | Mg  | 0       | 0       |
|     |       |          | 185   | 185 |         |         |
| 24  | B     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 25 is PAROMOMYCIN (CCD ID: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 25  | A     | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

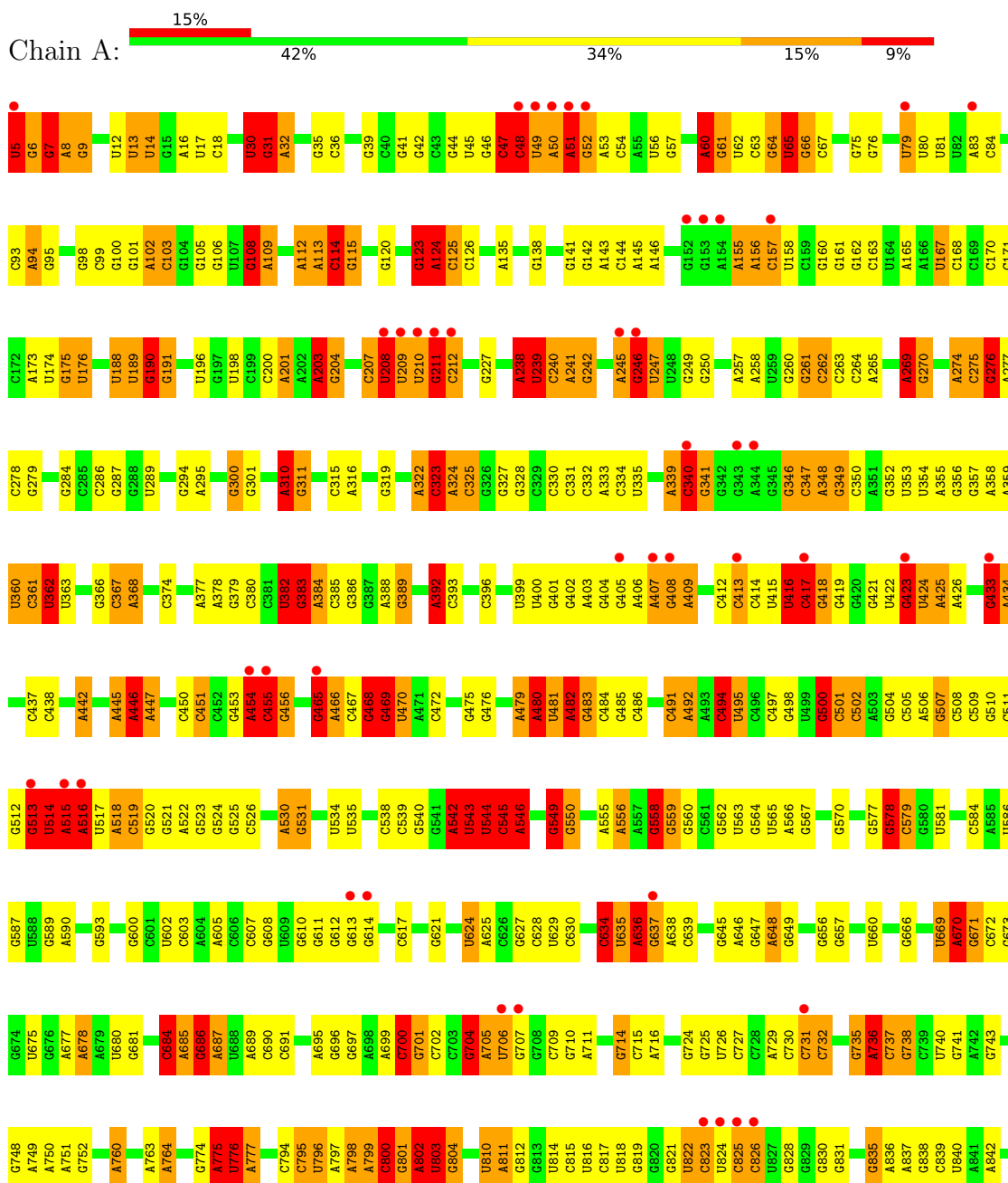
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

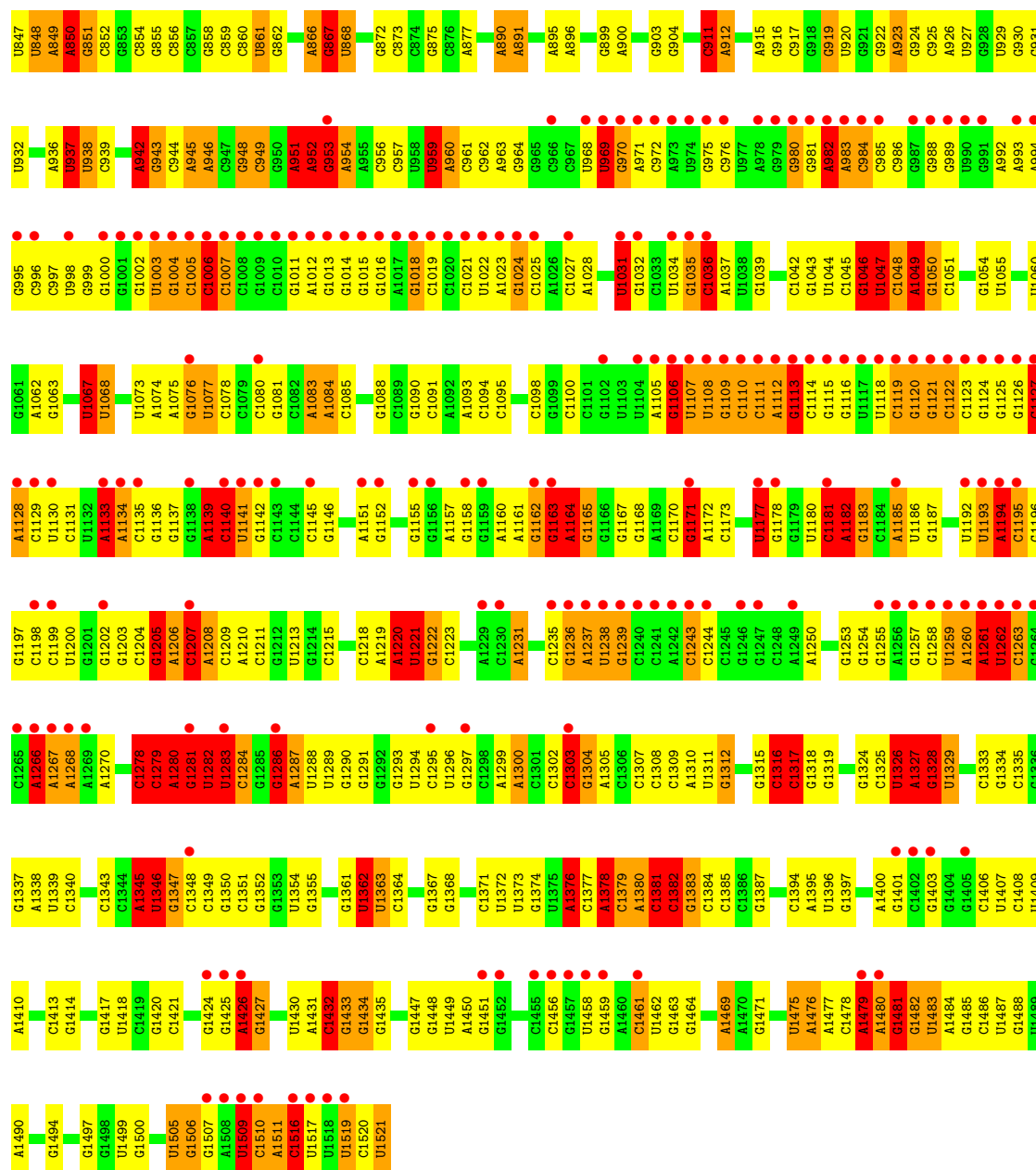
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 26  | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 26  | N     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

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

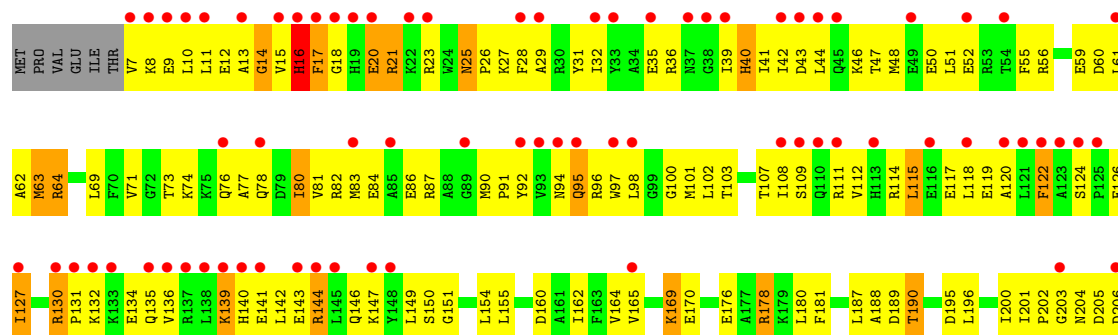
#### • Molecule 1: 16S rRNA

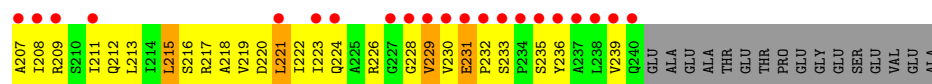




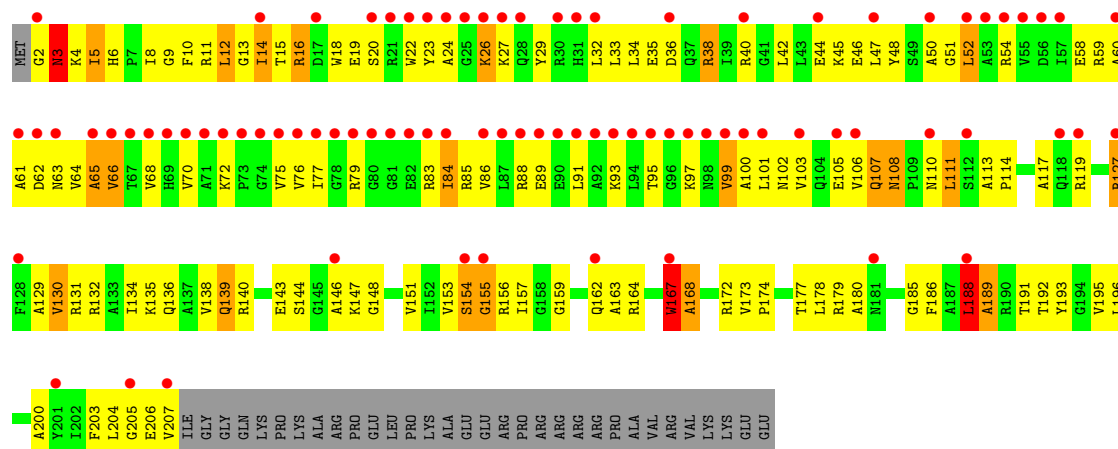
• Molecule 2: 30S ribosomal protein S2

Chain B:

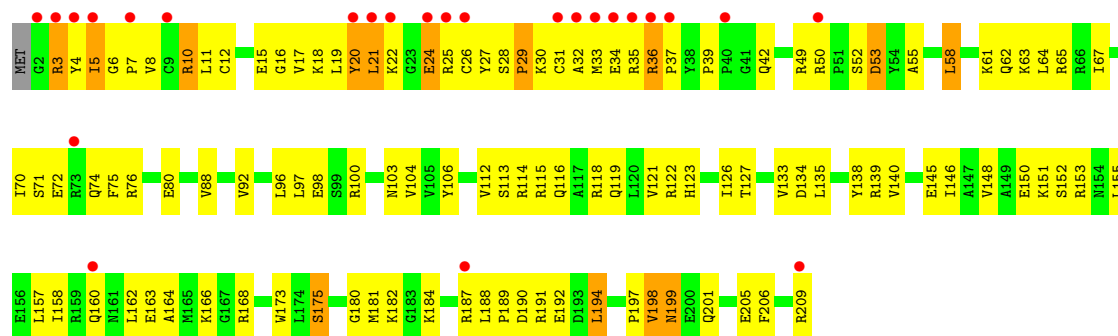
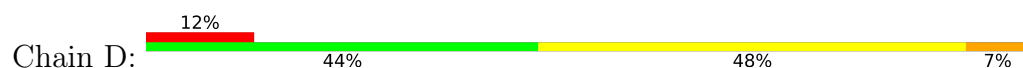




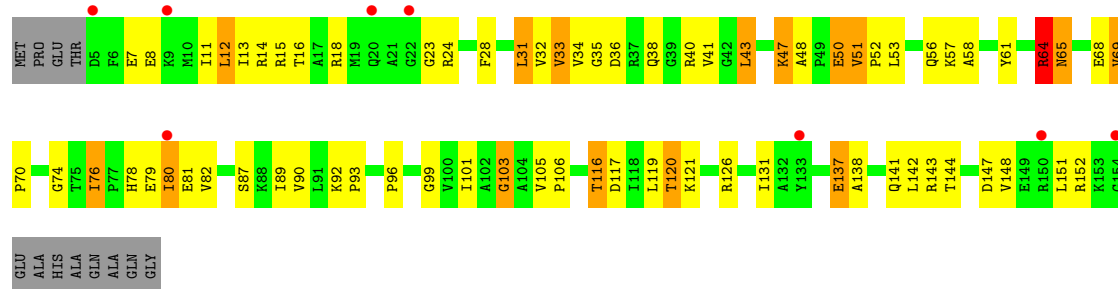
• Molecule 3: 30S ribosomal protein S3



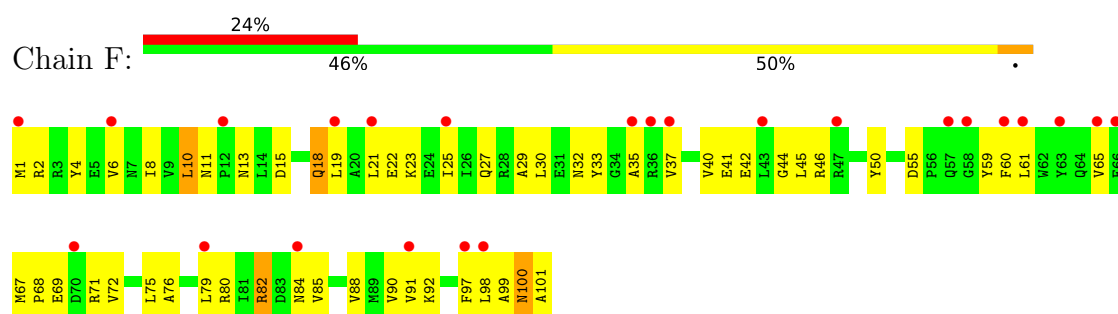
• Molecule 4: 30S ribosomal protein S4



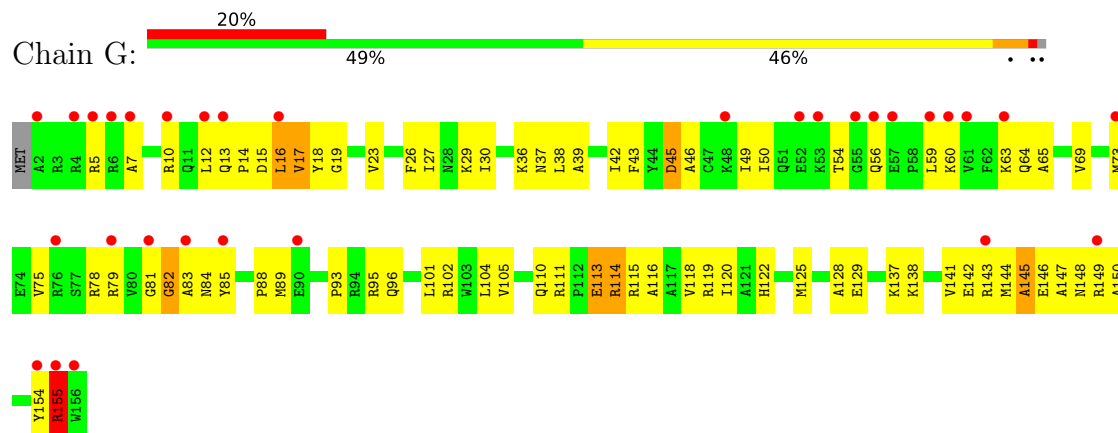
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



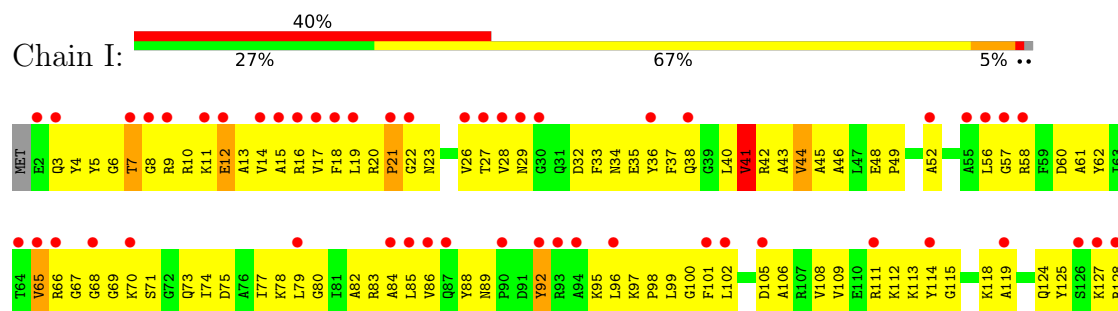
- Molecule 7: 30S ribosomal protein S7



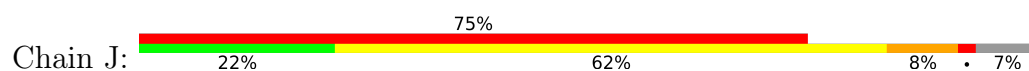
- Molecule 8: 30S ribosomal protein S8

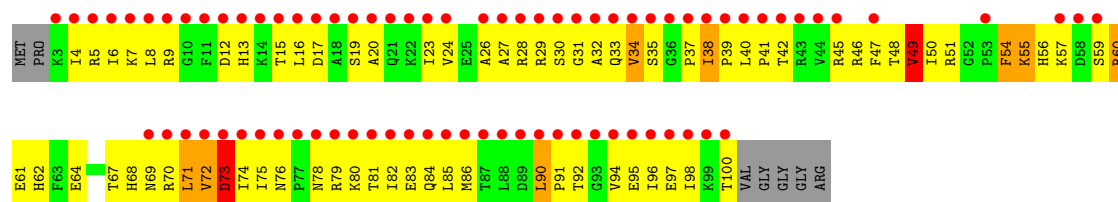


- Molecule 9: 30S ribosomal protein S9

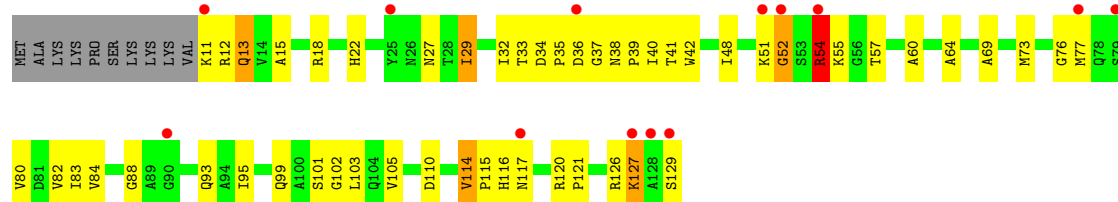


- Molecule 10: 30S ribosomal protein S10

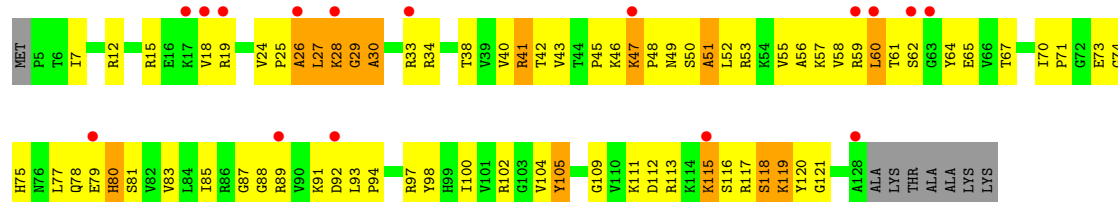




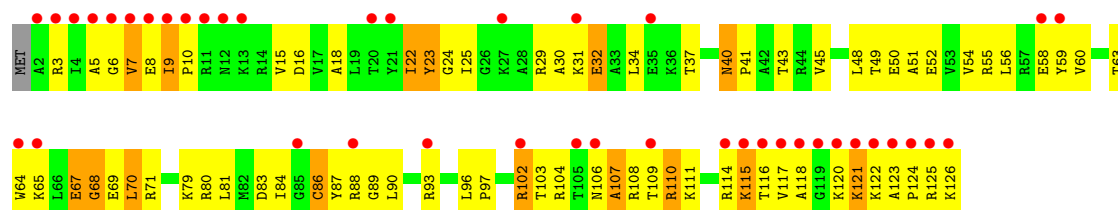
• Molecule 11: 30S ribosomal protein S11



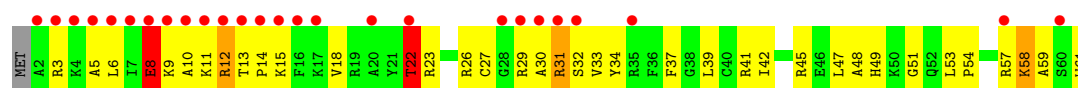
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



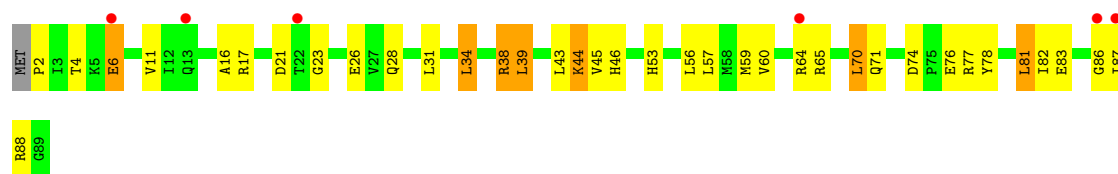
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 15: 30S ribosomal protein S15







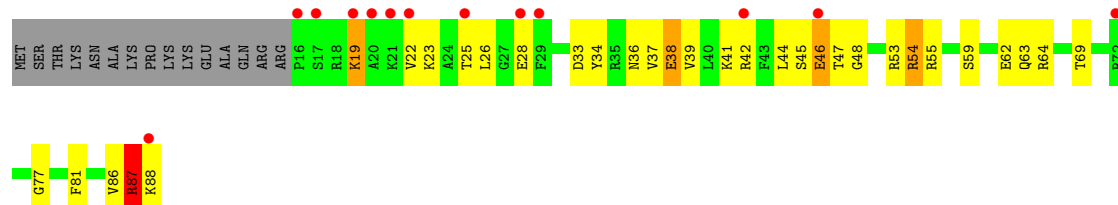
- Molecule 16: 30S ribosomal protein S16



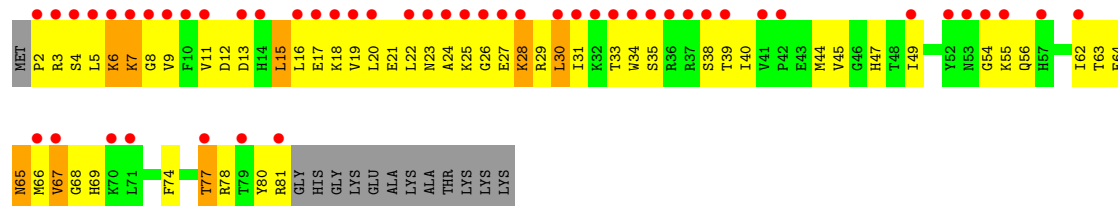
- Molecule 17: 30S ribosomal protein S17



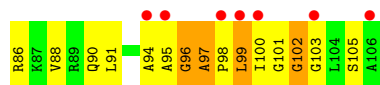
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



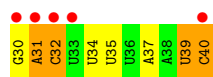
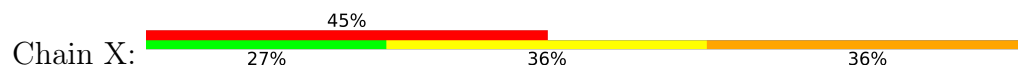
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA A-site fragment



- Molecule 23: tRNA ASL human Lys3



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 400.97Å 400.97Å 174.65Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.89 – 2.80<br>29.89 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (29.89-2.80)<br>99.1 (29.89-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.84 (at 2.77Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.3                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.245 , 0.268<br>0.242 , 0.264                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 17248 reflections (4.92%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 59.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.205                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 86.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 52289                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 65.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% 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: PSU, 70U, ZN, PAR, MG, 12A

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.45         | 1/36395 (0.0%) | 0.91        | 188/56801 (0.3%) |
| 2   | B     | 0.43         | 0/1935         | 0.94        | 1/2609 (0.0%)    |
| 3   | C     | 0.47         | 0/1636         | 0.93        | 5/2205 (0.2%)    |
| 4   | D     | 0.46         | 0/1733         | 0.91        | 8/2318 (0.3%)    |
| 5   | E     | 0.55         | 0/1162         | 1.09        | 7/1564 (0.4%)    |
| 6   | F     | 0.42         | 0/856          | 0.83        | 1/1154 (0.1%)    |
| 7   | G     | 0.46         | 0/1276         | 0.90        | 3/1709 (0.2%)    |
| 8   | H     | 0.55         | 0/1136         | 1.14        | 10/1527 (0.7%)   |
| 9   | I     | 0.43         | 0/1029         | 0.93        | 2/1378 (0.1%)    |
| 10  | J     | 0.48         | 0/805          | 0.93        | 3/1082 (0.3%)    |
| 11  | K     | 0.56         | 0/900          | 1.00        | 3/1213 (0.2%)    |
| 12  | L     | 0.58         | 0/986          | 1.11        | 4/1320 (0.3%)    |
| 13  | M     | 0.49         | 0/1008         | 0.98        | 5/1347 (0.4%)    |
| 14  | N     | 0.47         | 0/501          | 0.89        | 0/664            |
| 15  | O     | 0.46         | 0/745          | 0.88        | 1/992 (0.1%)     |
| 16  | P     | 0.54         | 0/716          | 1.04        | 6/963 (0.6%)     |
| 17  | Q     | 0.53         | 0/870          | 1.10        | 5/1159 (0.4%)    |
| 18  | R     | 0.43         | 0/603          | 0.96        | 2/799 (0.3%)     |
| 19  | S     | 0.44         | 0/661          | 0.95        | 1/890 (0.1%)     |
| 20  | T     | 0.56         | 0/764          | 1.11        | 4/1006 (0.4%)    |
| 21  | V     | 0.50         | 0/212          | 0.78        | 0/277            |
| 22  | W     | 0.74         | 0/76           | 0.90        | 0/115            |
| 23  | X     | 0.60         | 0/184          | 0.97        | 0/277            |
| All | All   | 0.46         | 1/56189 (0.0%) | 0.93        | 259/83369 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 42                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 634 | C    | O3'-P | 5.98 | 1.70        | 1.61     |

All (259) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | A     | 801  | G    | C2'-C3'-O3' | 12.51  | 128.26      | 109.50   |
| 1   | A     | 634  | C    | P-O3'-C3'   | -12.37 | 101.65      | 120.20   |
| 1   | A     | 686  | G    | C2'-C3'-O3' | 12.01  | 127.52      | 109.50   |
| 1   | A     | 500  | G    | C2'-C3'-O3' | 11.21  | 126.32      | 109.50   |
| 20  | T     | 12   | ALA  | N-CA-C      | -11.20 | 99.60       | 113.38   |
| 1   | A     | 276  | G    | C2'-C3'-O3' | 11.16  | 126.25      | 109.50   |
| 17  | Q     | 67   | LYS  | N-CA-C      | -11.12 | 96.74       | 110.41   |
| 1   | A     | 578  | G    | C2'-C3'-O3' | 11.09  | 126.13      | 109.50   |
| 5   | E     | 64   | ARG  | N-CA-C      | -11.01 | 93.99       | 110.28   |
| 1   | A     | 65   | U    | C2'-C3'-O3' | 10.77  | 125.65      | 109.50   |
| 1   | A     | 1047 | U    | C2'-C3'-O3' | 10.56  | 125.33      | 109.50   |
| 1   | A     | 542  | A    | C2'-C3'-O3' | 10.32  | 124.98      | 109.50   |
| 1   | A     | 1483 | U    | C2'-C3'-O3' | 10.24  | 124.86      | 109.50   |
| 8   | H     | 79   | VAL  | N-CA-C      | -9.96  | 101.02      | 111.58   |
| 1   | A     | 1278 | C    | C2'-C3'-O3' | 9.89   | 124.34      | 109.50   |
| 1   | A     | 953  | G    | C4'-C3'-O3' | -9.89  | 94.56       | 109.40   |
| 1   | A     | 861  | U    | C2'-C3'-O3' | 9.73   | 124.10      | 109.50   |
| 18  | R     | 46   | GLU  | N-CA-C      | -9.47  | 100.81      | 111.71   |
| 1   | A     | 239  | U    | C2'-C3'-O3' | 9.29   | 123.44      | 109.50   |
| 1   | A     | 1141 | U    | C2'-C3'-O3' | 9.19   | 123.29      | 109.50   |
| 1   | A     | 47   | C    | C2'-C3'-O3' | 9.12   | 123.17      | 109.50   |
| 1   | A     | 1345 | A    | C2'-C3'-O3' | 9.08   | 123.12      | 109.50   |
| 12  | L     | 26   | ALA  | N-CA-C      | -9.08  | 100.85      | 113.20   |
| 1   | A     | 775  | A    | C2'-C3'-O3' | 9.01   | 123.01      | 109.50   |
| 1   | A     | 238  | A    | C2'-C3'-O3' | 8.97   | 122.96      | 109.50   |
| 15  | O     | 44   | LYS  | N-CA-C      | -8.85  | 101.72      | 111.36   |
| 1   | A     | 1282 | U    | C2'-C3'-O3' | 8.84   | 122.77      | 109.50   |
| 1   | A     | 445  | A    | C2'-C3'-O3' | 8.83   | 122.75      | 109.50   |
| 1   | A     | 480  | A    | C2'-C3'-O3' | 8.81   | 122.72      | 109.50   |
| 1   | A     | 704  | G    | C2'-C3'-O3' | 8.79   | 122.68      | 109.50   |
| 1   | A     | 1286 | G    | C2'-C3'-O3' | 8.76   | 122.64      | 109.50   |
| 1   | A     | 1362 | U    | C2'-C3'-O3' | 8.69   | 122.53      | 109.50   |
| 1   | A     | 1505 | U    | C2'-C3'-O3' | 8.61   | 122.42      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 513  | G    | C2'-C3'-O3' | 8.53  | 122.29      | 109.50   |
| 1   | A     | 454  | A    | C2'-C3'-O3' | 8.45  | 122.18      | 109.50   |
| 12  | L     | 119  | LYS  | N-CA-C      | -8.38 | 99.23       | 110.55   |
| 1   | A     | 1317 | C    | C2'-C3'-O3' | 8.19  | 121.79      | 109.50   |
| 1   | A     | 1283 | U    | C2'-C3'-O3' | 8.18  | 121.77      | 109.50   |
| 1   | A     | 951  | A    | C2'-C3'-O3' | 8.12  | 121.69      | 109.50   |
| 1   | A     | 1521 | U    | C4'-C3'-O3' | -8.08 | 97.29       | 109.40   |
| 1   | A     | 1046 | G    | C2'-C3'-O3' | 7.92  | 121.39      | 109.50   |
| 1   | A     | 1432 | C    | C2'-C3'-O3' | 7.79  | 121.19      | 109.50   |
| 1   | A     | 1220 | A    | C2'-C3'-O3' | 7.75  | 121.12      | 109.50   |
| 13  | M     | 107  | ALA  | N-CA-C      | -7.74 | 100.85      | 112.54   |
| 1   | A     | 323  | C    | C2'-C3'-O3' | 7.72  | 121.08      | 109.50   |
| 1   | A     | 558  | G    | C2'-C3'-O3' | 7.69  | 121.03      | 109.50   |
| 1   | A     | 1261 | A    | C2'-C3'-O3' | 7.66  | 120.99      | 109.50   |
| 1   | A     | 1279 | C    | C2'-C3'-O3' | 7.65  | 120.97      | 109.50   |
| 17  | Q     | 83   | ASP  | N-CA-C      | -7.65 | 103.02      | 111.36   |
| 1   | A     | 982  | A    | C4'-C3'-O3' | 7.64  | 124.47      | 113.00   |
| 1   | A     | 1381 | C    | C2'-C3'-O3' | 7.62  | 120.93      | 109.50   |
| 11  | K     | 116  | HIS  | N-CA-C      | -7.54 | 102.00      | 112.25   |
| 1   | A     | 959  | U    | C2'-C3'-O3' | 7.52  | 120.78      | 109.50   |
| 1   | A     | 776  | U    | C4'-C3'-O3' | 7.50  | 120.65      | 109.40   |
| 1   | A     | 1376 | A    | C2'-C3'-O3' | 7.48  | 120.72      | 109.50   |
| 1   | A     | 300  | G    | C2'-C3'-O3' | 7.40  | 120.60      | 109.50   |
| 1   | A     | 937  | U    | N1-C1'-C2'  | 7.34  | 125.02      | 114.00   |
| 1   | A     | 417  | C    | C2'-C3'-O3' | 7.31  | 120.46      | 109.50   |
| 1   | A     | 1516 | C    | O4'-C4'-C3' | -7.30 | 96.70       | 104.00   |
| 1   | A     | 867  | G    | C2'-C3'-O3' | 7.28  | 120.42      | 109.50   |
| 1   | A     | 558  | G    | N9-C1'-C2'  | 7.28  | 124.91      | 114.00   |
| 1   | A     | 7    | G    | C2'-C3'-O3' | 7.25  | 120.37      | 109.50   |
| 1   | A     | 513  | G    | N9-C1'-C2'  | 7.21  | 124.82      | 114.00   |
| 11  | K     | 37   | GLY  | N-CA-C      | 7.21  | 123.62      | 114.25   |
| 1   | A     | 1177 | U    | C2'-C3'-O3' | 7.17  | 120.25      | 109.50   |
| 1   | A     | 446  | A    | C2'-C3'-O3' | 7.16  | 120.23      | 109.50   |
| 8   | H     | 134  | ILE  | N-CA-C      | 7.15  | 117.23      | 110.30   |
| 1   | A     | 736  | A    | C2'-C3'-O3' | 7.14  | 120.21      | 109.50   |
| 5   | E     | 69   | VAL  | CA-C-N      | 7.08  | 128.69      | 119.84   |
| 5   | E     | 69   | VAL  | C-N-CA      | 7.08  | 128.69      | 119.84   |
| 1   | A     | 64   | G    | C2'-C3'-O3' | 6.99  | 119.99      | 109.50   |
| 1   | A     | 1326 | U    | C2'-C3'-O3' | 6.93  | 119.89      | 109.50   |
| 1   | A     | 1221 | U    | C2'-C3'-O3' | 6.90  | 119.85      | 109.50   |
| 1   | A     | 1163 | G    | C4'-C3'-O3' | -6.89 | 102.67      | 113.00   |
| 1   | A     | 124  | A    | C2'-C3'-O3' | 6.87  | 119.80      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 937  | U    | C2'-C3'-O3' | 6.86  | 119.79      | 109.50   |
| 2   | B     | 90   | MET  | N-CA-C      | 6.84  | 118.27      | 109.65   |
| 1   | A     | 1481 | G    | C2'-C3'-O3' | 6.81  | 119.72      | 109.50   |
| 4   | D     | 163  | GLU  | N-CA-C      | -6.81 | 103.78      | 111.14   |
| 1   | A     | 1316 | C    | C2'-C3'-O3' | 6.81  | 119.72      | 109.50   |
| 1   | A     | 383  | G    | C2'-C3'-O3' | 6.81  | 119.71      | 109.50   |
| 1   | A     | 953  | G    | O4'-C1'-C2' | 6.79  | 112.59      | 105.80   |
| 1   | A     | 1327 | A    | C2'-C3'-O3' | 6.79  | 119.69      | 109.50   |
| 1   | A     | 1346 | U    | C2'-C3'-O3' | 6.78  | 119.67      | 109.50   |
| 1   | A     | 392  | A    | C5'-C4'-C3' | -6.76 | 105.86      | 116.00   |
| 1   | A     | 1049 | A    | C2'-C3'-O3' | 6.76  | 119.64      | 109.50   |
| 1   | A     | 1521 | U    | C2'-C3'-O3' | 6.73  | 119.60      | 109.50   |
| 4   | D     | 12   | CYS  | N-CA-C      | -6.73 | 103.87      | 111.07   |
| 1   | A     | 1480 | A    | C2'-C3'-O3' | 6.72  | 119.58      | 109.50   |
| 1   | A     | 1280 | A    | N9-C1'-C2'  | 6.71  | 122.07      | 112.00   |
| 1   | A     | 5    | U    | C2'-C3'-O3' | 6.69  | 119.53      | 109.50   |
| 1   | A     | 1300 | A    | N9-C1'-C2'  | 6.67  | 122.01      | 112.00   |
| 1   | A     | 1182 | A    | C2'-C3'-O3' | 6.66  | 119.49      | 109.50   |
| 1   | A     | 802  | A    | C2'-C3'-O3' | 6.65  | 119.48      | 109.50   |
| 1   | A     | 700  | C    | C2'-C3'-O3' | 6.61  | 119.42      | 109.50   |
| 1   | A     | 175  | G    | C2'-C3'-O3' | 6.61  | 119.42      | 109.50   |
| 1   | A     | 340  | C    | C2'-C3'-O3' | 6.60  | 119.40      | 109.50   |
| 9   | I     | 60   | ASP  | N-CA-C      | -6.58 | 99.04       | 109.23   |
| 8   | H     | 44   | PHE  | N-CA-C      | -6.53 | 105.44      | 113.41   |
| 1   | A     | 735  | G    | N9-C1'-C2'  | 6.51  | 123.76      | 114.00   |
| 1   | A     | 684  | C    | C2'-C3'-O3' | 6.50  | 119.25      | 109.50   |
| 1   | A     | 624  | U    | C2'-C3'-O3' | -6.48 | 99.78       | 109.50   |
| 1   | A     | 1517 | U    | C4'-C3'-O3' | 6.43  | 122.65      | 113.00   |
| 1   | A     | 238  | A    | N9-C1'-C2'  | 6.42  | 123.63      | 114.00   |
| 1   | A     | 482  | A    | C2'-C3'-O3' | 6.42  | 119.13      | 109.50   |
| 1   | A     | 624  | U    | C4'-C3'-O3' | 6.33  | 118.90      | 109.40   |
| 1   | A     | 1205 | G    | C2'-C3'-O3' | 6.33  | 119.00      | 109.50   |
| 1   | A     | 455  | C    | C2'-C3'-O3' | 6.31  | 118.97      | 109.50   |
| 1   | A     | 636  | A    | P-O3'-C3'   | 6.27  | 129.61      | 120.20   |
| 1   | A     | 1031 | U    | C2'-C3'-O3' | 6.24  | 118.86      | 109.50   |
| 1   | A     | 123  | G    | C2'-C3'-O3' | 6.23  | 118.84      | 109.50   |
| 3   | C     | 127  | ARG  | N-CA-C      | 6.20  | 119.97      | 111.54   |
| 1   | A     | 543  | U    | N1-C1'-C2'  | 6.20  | 121.29      | 112.00   |
| 1   | A     | 1127 | C    | C2'-C3'-O3' | -6.20 | 104.41      | 113.70   |
| 1   | A     | 1328 | G    | C2'-C3'-O3' | 6.18  | 118.77      | 109.50   |
| 1   | A     | 114  | C    | C2'-C3'-O3' | -6.16 | 100.26      | 109.50   |
| 1   | A     | 1511 | A    | C1'-C2'-O2' | -6.15 | 99.17       | 108.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1483 | U    | N1-C1'-C2'  | 6.14  | 123.21      | 114.00   |
| 1   | A     | 545  | C    | C2'-C3'-O3' | 6.13  | 118.70      | 109.50   |
| 1   | A     | 469  | G    | N9-C1'-C2'  | 6.13  | 123.19      | 114.00   |
| 5   | E     | 23   | GLY  | N-CA-C      | 6.12  | 119.72      | 110.18   |
| 1   | A     | 423  | G    | C2'-C3'-O3' | 6.12  | 118.67      | 109.50   |
| 1   | A     | 48   | C    | C2'-C3'-O3' | 6.11  | 118.66      | 109.50   |
| 1   | A     | 1047 | U    | N1-C1'-C2'  | 6.09  | 123.14      | 114.00   |
| 1   | A     | 803  | U    | C4'-C3'-O3' | 6.09  | 118.53      | 109.40   |
| 1   | A     | 14   | U    | C5'-C4'-C3' | -6.08 | 106.89      | 116.00   |
| 1   | A     | 1382 | C    | C2'-C3'-O3' | -6.07 | 100.40      | 109.50   |
| 13  | M     | 50   | GLU  | N-CA-C      | -6.07 | 104.67      | 111.28   |
| 1   | A     | 468  | G    | C2'-C3'-O3' | 6.06  | 118.59      | 109.50   |
| 1   | A     | 942  | A    | C2'-C3'-O3' | 6.02  | 118.53      | 109.50   |
| 1   | A     | 1139 | A    | C2'-C3'-O3' | 6.01  | 118.51      | 109.50   |
| 1   | A     | 1312 | G    | N9-C1'-C2'  | 5.99  | 120.98      | 112.00   |
| 1   | A     | 1036 | C    | N1-C1'-C2'  | -5.98 | 103.03      | 112.00   |
| 13  | M     | 40   | ASN  | CA-C-N      | 5.98  | 126.14      | 119.32   |
| 13  | M     | 40   | ASN  | C-N-CA      | 5.98  | 126.14      | 119.32   |
| 1   | A     | 1133 | A    | C4'-C3'-O3' | 5.94  | 118.32      | 109.40   |
| 1   | A     | 494  | C    | C4'-C3'-O3' | 5.94  | 118.31      | 109.40   |
| 16  | P     | 4    | ILE  | N-CA-C      | -5.93 | 97.28       | 107.24   |
| 1   | A     | 1106 | G    | C4'-C3'-O3' | 5.92  | 118.28      | 109.40   |
| 1   | A     | 1511 | A    | C3'-C2'-O2' | 5.91  | 119.56      | 110.70   |
| 1   | A     | 1140 | C    | N1-C1'-C2'  | 5.91  | 120.86      | 112.00   |
| 7   | G     | 110  | GLN  | N-CA-C      | -5.86 | 106.67      | 113.88   |
| 1   | A     | 60   | A    | C2'-C3'-O3' | 5.85  | 118.27      | 109.50   |
| 1   | A     | 1426 | A    | C2'-C3'-O3' | 5.83  | 118.25      | 109.50   |
| 1   | A     | 1378 | A    | C2'-C3'-O3' | 5.80  | 118.20      | 109.50   |
| 19  | S     | 54   | GLY  | N-CA-C      | -5.79 | 107.80      | 114.69   |
| 1   | A     | 1171 | G    | C4'-C3'-O3' | -5.78 | 104.34      | 113.00   |
| 1   | A     | 1076 | G    | C4'-C3'-O3' | -5.77 | 104.34      | 113.00   |
| 1   | A     | 112  | A    | C2'-C3'-O3' | 5.77  | 118.16      | 109.50   |
| 1   | A     | 1266 | A    | C2'-C3'-O3' | 5.77  | 118.15      | 109.50   |
| 11  | K     | 54   | ARG  | N-CA-C      | -5.77 | 105.34      | 112.38   |
| 5   | E     | 48   | ALA  | N-CA-C      | 5.76  | 113.41      | 108.22   |
| 9   | I     | 115  | GLY  | N-CA-C      | -5.72 | 107.34      | 115.30   |
| 1   | A     | 797  | A    | C5'-C4'-C3' | -5.72 | 107.42      | 116.00   |
| 3   | C     | 99   | VAL  | N-CA-C      | 5.71  | 115.89      | 107.15   |
| 1   | A     | 1479 | A    | N9-C1'-C2'  | 5.71  | 122.56      | 114.00   |
| 1   | A     | 310  | A    | C2'-C3'-O3' | 5.69  | 118.04      | 109.50   |
| 1   | A     | 13   | U    | C2'-C3'-O3' | 5.69  | 118.04      | 109.50   |
| 1   | A     | 1036 | C    | C4'-C3'-O3' | 5.68  | 121.52      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 362  | U    | C2'-C3'-O3' | 5.67  | 118.01      | 109.50   |
| 1   | A     | 1281 | G    | N9-C1'-C2'  | 5.67  | 120.51      | 112.00   |
| 1   | A     | 1303 | C    | C4'-C3'-O3' | 5.67  | 117.91      | 109.40   |
| 1   | A     | 30   | U    | C2'-C3'-O3' | 5.66  | 117.99      | 109.50   |
| 1   | A     | 945  | A    | C2'-C3'-O3' | 5.64  | 117.96      | 109.50   |
| 8   | H     | 20   | TYR  | N-CA-C      | 5.63  | 119.20      | 111.54   |
| 1   | A     | 578  | G    | N9-C1'-C2'  | 5.61  | 122.42      | 114.00   |
| 1   | A     | 549  | G    | C4'-C3'-O3' | 5.61  | 117.81      | 109.40   |
| 1   | A     | 433  | G    | C4'-C3'-O3' | 5.60  | 117.80      | 109.40   |
| 20  | T     | 68   | LYS  | N-CA-C      | -5.59 | 105.27      | 111.36   |
| 1   | A     | 700  | C    | C4'-C3'-O3' | -5.57 | 101.05      | 109.40   |
| 6   | F     | 60   | PHE  | N-CA-C      | 5.57  | 119.14      | 110.17   |
| 1   | A     | 360  | U    | N1-C1'-C2'  | 5.57  | 120.35      | 112.00   |
| 1   | A     | 491  | C    | O4'-C1'-C2' | 5.54  | 111.34      | 105.80   |
| 1   | A     | 1155 | G    | C3'-C2'-O2' | 5.53  | 119.00      | 110.70   |
| 18  | R     | 81   | PHE  | N-CA-C      | -5.52 | 106.68      | 113.41   |
| 1   | A     | 382  | U    | C5'-C4'-C3' | -5.51 | 107.73      | 116.00   |
| 20  | T     | 13   | LEU  | N-CA-C      | -5.50 | 105.28      | 111.28   |
| 12  | L     | 58   | VAL  | N-CA-C      | 5.49  | 115.76      | 107.80   |
| 4   | D     | 50   | ARG  | CA-C-N      | 5.47  | 125.42      | 119.78   |
| 4   | D     | 50   | ARG  | C-N-CA      | 5.47  | 125.42      | 119.78   |
| 17  | Q     | 13   | ASP  | N-CA-C      | -5.47 | 107.86      | 114.75   |
| 16  | P     | 51   | VAL  | N-CA-C      | 5.46  | 120.69      | 109.34   |
| 1   | A     | 969  | U    | C2'-C3'-O3' | 5.45  | 117.67      | 109.50   |
| 1   | A     | 1509 | U    | C4'-C3'-O3' | 5.44  | 121.16      | 113.00   |
| 1   | A     | 63   | C    | C5'-C4'-C3' | -5.41 | 107.89      | 116.00   |
| 3   | C     | 111  | LEU  | N-CA-C      | -5.41 | 104.38      | 112.54   |
| 16  | P     | 27   | LYS  | N-CA-C      | -5.40 | 103.00      | 110.35   |
| 1   | A     | 911  | C    | C2'-C3'-O3' | -5.39 | 101.41      | 109.50   |
| 1   | A     | 51   | A    | C2'-C3'-O3' | 5.38  | 117.58      | 109.50   |
| 1   | A     | 246  | G    | N9-C1'-C2'  | 5.37  | 122.06      | 114.00   |
| 1   | A     | 1046 | G    | O4'-C1'-C2' | 5.37  | 111.17      | 105.80   |
| 1   | A     | 716  | A    | C4'-C3'-O3' | -5.35 | 104.97      | 113.00   |
| 1   | A     | 516  | A    | C2'-C3'-O3' | 5.35  | 117.52      | 109.50   |
| 8   | H     | 75   | ARG  | CA-C-N      | 5.34  | 125.28      | 119.78   |
| 8   | H     | 75   | ARG  | C-N-CA      | 5.34  | 125.28      | 119.78   |
| 16  | P     | 25   | ARG  | N-CA-C      | 5.34  | 119.64      | 113.18   |
| 8   | H     | 68   | ARG  | N-CA-C      | -5.34 | 103.44      | 110.43   |
| 1   | A     | 190  | G    | C2'-C3'-O3' | 5.33  | 117.49      | 109.50   |
| 1   | A     | 1382 | C    | C4'-C3'-O3' | 5.32  | 117.39      | 109.40   |
| 1   | A     | 1312 | G    | C4'-C3'-O3' | -5.31 | 105.03      | 113.00   |
| 17  | Q     | 65   | ILE  | N-CA-C      | -5.31 | 107.21      | 113.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | E     | 51   | VAL  | CB-CA-C     | -5.30 | 107.06      | 114.00   |
| 1   | A     | 323  | C    | N1-C1'-C2'  | 5.29  | 121.94      | 114.00   |
| 20  | T     | 21   | LYS  | N-CA-C      | -5.29 | 105.59      | 111.36   |
| 1   | A     | 636  | A    | C4'-C3'-O3' | 5.29  | 117.33      | 109.40   |
| 16  | P     | 11   | SER  | N-CA-C      | -5.29 | 100.88      | 108.60   |
| 1   | A     | 911  | C    | C4'-C3'-O3' | 5.27  | 117.30      | 109.40   |
| 1   | A     | 413  | C    | C3'-C2'-O2' | 5.26  | 118.59      | 110.70   |
| 1   | A     | 1194 | A    | C2'-C3'-O3' | 5.25  | 117.38      | 109.50   |
| 10  | J     | 38   | ILE  | CA-C-N      | 5.25  | 124.43      | 118.97   |
| 10  | J     | 38   | ILE  | C-N-CA      | 5.25  | 124.43      | 118.97   |
| 10  | J     | 49   | VAL  | N-CA-C      | 5.25  | 116.29      | 108.46   |
| 1   | A     | 700  | C    | N1-C1'-C2'  | 5.25  | 121.87      | 114.00   |
| 8   | H     | 56   | LYS  | CA-C-N      | 5.25  | 126.40      | 119.84   |
| 8   | H     | 56   | LYS  | C-N-CA      | 5.25  | 126.40      | 119.84   |
| 1   | A     | 269  | A    | C2'-C3'-O3' | 5.23  | 117.34      | 109.50   |
| 3   | C     | 100  | ALA  | N-CA-C      | -5.23 | 103.59      | 110.33   |
| 1   | A     | 392  | A    | C4'-C3'-O3' | -5.23 | 105.16      | 113.00   |
| 1   | A     | 1164 | A    | C2'-C3'-O3' | 5.22  | 117.34      | 109.50   |
| 8   | H     | 28   | ALA  | N-CA-C      | 5.22  | 118.07      | 109.76   |
| 1   | A     | 1506 | G    | C2'-C3'-O3' | 5.22  | 117.33      | 109.50   |
| 1   | A     | 803  | U    | C2'-C3'-O3' | -5.21 | 101.68      | 109.50   |
| 1   | A     | 546  | A    | C4'-C3'-O3' | -5.21 | 105.19      | 113.00   |
| 1   | A     | 1181 | C    | C2'-C3'-O3' | -5.20 | 105.91      | 113.70   |
| 13  | M     | 22   | ILE  | N-CA-C      | -5.19 | 102.39      | 109.55   |
| 1   | A     | 114  | C    | C4'-C3'-O3' | 5.18  | 117.18      | 109.40   |
| 4   | D     | 139  | ARG  | N-CA-C      | 5.18  | 116.75      | 108.41   |
| 1   | A     | 670  | A    | C2'-C3'-O3' | 5.18  | 117.27      | 109.50   |
| 1   | A     | 802  | A    | N9-C1'-C2'  | 5.18  | 121.77      | 114.00   |
| 4   | D     | 39   | PRO  | CA-C-N      | 5.15  | 125.13      | 120.03   |
| 4   | D     | 39   | PRO  | C-N-CA      | 5.15  | 125.13      | 120.03   |
| 1   | A     | 31   | G    | C4'-C3'-O3' | 5.14  | 117.12      | 109.40   |
| 4   | D     | 198  | VAL  | N-CA-C      | 5.14  | 115.68      | 108.17   |
| 1   | A     | 451  | C    | C3'-C2'-O2' | 5.14  | 118.41      | 110.70   |
| 17  | Q     | 62   | SER  | N-CA-C      | 5.14  | 117.22      | 109.41   |
| 1   | A     | 775  | A    | N9-C1'-C2'  | 5.14  | 121.70      | 114.00   |
| 1   | A     | 416  | U    | C2'-C3'-O3' | 5.13  | 117.20      | 109.50   |
| 1   | A     | 558  | G    | C4'-C3'-C2' | 5.13  | 107.73      | 102.60   |
| 7   | G     | 145  | ALA  | N-CA-C      | -5.12 | 101.80      | 109.79   |
| 1   | A     | 465  | G    | C2'-C3'-O3' | -5.11 | 101.83      | 109.50   |
| 1   | A     | 800  | C    | O3'-P-O5'   | 5.11  | 111.66      | 104.00   |
| 1   | A     | 1006 | C    | N1-C1'-C2'  | -5.10 | 104.35      | 112.00   |
| 7   | G     | 114  | ARG  | N-CA-C      | 5.10  | 116.64      | 111.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 848  | U    | C4'-C3'-O3' | 5.09  | 117.04      | 109.40   |
| 1   | A     | 800  | C    | O4'-C1'-C2' | 5.09  | 110.89      | 105.80   |
| 1   | A     | 1259 | U    | N1-C1'-C2'  | 5.08  | 119.62      | 112.00   |
| 1   | A     | 246  | G    | C2'-C3'-O3' | 5.08  | 117.11      | 109.50   |
| 3   | C     | 155  | GLY  | N-CA-C      | 5.08  | 120.40      | 111.57   |
| 5   | E     | 103  | GLY  | N-CA-C      | -5.07 | 105.83      | 112.82   |
| 12  | L     | 30   | ALA  | N-CA-C      | -5.05 | 102.70      | 110.07   |
| 1   | A     | 1479 | A    | C4'-C3'-O3' | 5.04  | 116.96      | 109.40   |
| 1   | A     | 108  | G    | O4'-C1'-C2' | 5.04  | 110.84      | 105.80   |
| 1   | A     | 1007 | C    | C3'-C2'-O2' | 5.04  | 118.26      | 110.70   |
| 1   | A     | 514  | U    | C4'-C3'-O3' | 5.04  | 116.96      | 109.40   |
| 1   | A     | 704  | G    | N9-C1'-C2'  | 5.03  | 121.55      | 114.00   |
| 1   | A     | 800  | C    | C4'-C3'-C2' | 5.03  | 107.63      | 102.60   |
| 1   | A     | 1067 | U    | C2'-C3'-O3' | 5.02  | 117.04      | 109.50   |
| 16  | P     | 20   | VAL  | N-CA-C      | 5.02  | 116.83      | 108.99   |
| 1   | A     | 850  | A    | O4'-C1'-C2' | 5.02  | 110.82      | 105.80   |

There are no chirality outliers.

All (42) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1003 | U    | Sidechain |
| 1   | A     | 1006 | C    | Sidechain |
| 1   | A     | 1036 | C    | Sidechain |
| 1   | A     | 1047 | U    | Sidechain |
| 1   | A     | 1049 | A    | Sidechain |
| 1   | A     | 1067 | U    | Sidechain |
| 1   | A     | 1098 | C    | Sidechain |
| 1   | A     | 1113 | G    | Sidechain |
| 1   | A     | 1177 | U    | Sidechain |
| 1   | A     | 1205 | G    | Sidechain |
| 1   | A     | 1207 | C    | Sidechain |
| 1   | A     | 1262 | U    | Sidechain |
| 1   | A     | 1300 | A    | Sidechain |
| 1   | A     | 1387 | G    | Sidechain |
| 1   | A     | 1430 | U    | Sidechain |
| 1   | A     | 1434 | G    | Sidechain |
| 1   | A     | 1509 | U    | Sidechain |
| 1   | A     | 203  | A    | Sidechain |
| 1   | A     | 208  | U    | Sidechain |
| 1   | A     | 211  | G    | Sidechain |
| 1   | A     | 239  | U    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 246 | G    | Sidechain |
| 1   | A     | 357 | G    | Sidechain |
| 1   | A     | 382 | U    | Sidechain |
| 1   | A     | 47  | C    | Sidechain |
| 1   | A     | 515 | A    | Sidechain |
| 1   | A     | 543 | U    | Sidechain |
| 1   | A     | 544 | U    | Sidechain |
| 1   | A     | 549 | G    | Sidechain |
| 1   | A     | 556 | A    | Sidechain |
| 1   | A     | 558 | G    | Sidechain |
| 1   | A     | 617 | C    | Sidechain |
| 1   | A     | 710 | G    | Sidechain |
| 1   | A     | 79  | U    | Sidechain |
| 1   | A     | 800 | C    | Sidechain |
| 1   | A     | 851 | G    | Sidechain |
| 1   | A     | 856 | C    | Sidechain |
| 1   | A     | 875 | G    | Sidechain |
| 1   | A     | 923 | A    | Sidechain |
| 1   | A     | 951 | A    | Sidechain |
| 1   | A     | 952 | A    | Sidechain |
| 1   | A     | 980 | G    | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32515 | 0        | 16410    | 1006    | 0            |
| 2   | B     | 1900  | 0        | 1951     | 191     | 0            |
| 3   | C     | 1612  | 0        | 1677     | 165     | 0            |
| 4   | D     | 1703  | 0        | 1765     | 112     | 0            |
| 5   | E     | 1146  | 0        | 1207     | 66      | 0            |
| 6   | F     | 843   | 0        | 857      | 57      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 76      | 0            |
| 8   | H     | 1116  | 0        | 1177     | 62      | 0            |
| 9   | I     | 1011  | 0        | 1043     | 102     | 0            |
| 10  | J     | 792   | 0        | 835      | 109     | 0            |
| 11  | K     | 885   | 0        | 904      | 54      | 0            |
| 12  | L     | 970   | 0        | 1057     | 105     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13  | M     | 997   | 0        | 1072     | 96      | 0            |
| 14  | N     | 492   | 0        | 529      | 48      | 0            |
| 15  | O     | 734   | 0        | 771      | 32      | 0            |
| 16  | P     | 700   | 0        | 720      | 32      | 0            |
| 17  | Q     | 857   | 0        | 930      | 47      | 0            |
| 18  | R     | 597   | 0        | 668      | 40      | 0            |
| 19  | S     | 647   | 0        | 673      | 68      | 0            |
| 20  | T     | 762   | 0        | 859      | 58      | 0            |
| 21  | V     | 208   | 0        | 221      | 12      | 0            |
| 22  | W     | 68    | 0        | 34       | 12      | 0            |
| 23  | X     | 247   | 0        | 130      | 18      | 0            |
| 24  | A     | 185   | 0        | 0        | 0       | 0            |
| 24  | B     | 1     | 0        | 0        | 0       | 0            |
| 25  | A     | 42    | 0        | 45       | 4       | 0            |
| 26  | D     | 1     | 0        | 0        | 0       | 0            |
| 26  | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 52289 | 0        | 36831    | 2347    | 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 26.

All (2347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:50:A:H3'     | 1:A:50:A:P       | 1.73                     | 1.29              |
| 1:A:1236:G:N2    | 1:A:1263:C:O2    | 1.78                     | 1.16              |
| 1:A:1425:G:H5''  | 1:A:1426:A:C5'   | 1.74                     | 1.15              |
| 1:A:1425:G:C5'   | 1:A:1426:A:H5'   | 1.76                     | 1.15              |
| 1:A:669:U:H1'    | 11:K:42:TRP:HE1  | 1.09                     | 1.14              |
| 19:S:33:THR:HG22 | 19:S:35:SER:H    | 1.09                     | 1.13              |
| 1:A:1236:G:N2    | 1:A:1263:C:C2    | 2.18                     | 1.11              |
| 1:A:1237:A:H2'   | 1:A:1238:U:C4'   | 1.79                     | 1.11              |
| 1:A:1035:G:H4'   | 1:A:1036:C:H5'   | 1.25                     | 1.11              |
| 10:J:8:LEU:HB2   | 10:J:70:ARG:HB2  | 1.34                     | 1.09              |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:HD2  | 1.34                     | 1.07              |
| 12:L:41:ARG:HG2  | 12:L:42:THR:H    | 1.18                     | 1.07              |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:CD   | 1.82                     | 1.06              |
| 1:A:1237:A:C2'   | 1:A:1238:U:H4'   | 1.85                     | 1.05              |
| 1:A:48:C:O2'     | 1:A:49:U:OP1     | 1.74                     | 1.05              |
| 12:L:41:ARG:HB3  | 12:L:41:ARG:HH11 | 1.19                     | 1.04              |
| 12:L:41:ARG:HB3  | 12:L:41:ARG:NH1  | 1.73                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:802:A:H5'     | 1:A:802:A:H8      | 1.23                     | 1.04              |
| 1:A:1133:A:O2'    | 1:A:1134:A:H5'    | 1.56                     | 1.03              |
| 10:J:6:ILE:HG22   | 10:J:98:ILE:HG22  | 1.33                     | 1.03              |
| 1:A:50:A:H3'      | 1:A:50:A:OP1      | 1.55                     | 1.02              |
| 10:J:90:LEU:H     | 10:J:91:PRO:HD2   | 1.22                     | 1.02              |
| 5:E:81:GLU:HG2    | 5:E:90:VAL:HG22   | 1.42                     | 1.01              |
| 1:A:1036:C:H3'    | 1:A:1036:C:C6     | 1.97                     | 0.99              |
| 3:C:119:ARG:HE    | 3:C:140:ARG:HH12  | 0.97                     | 0.97              |
| 13:M:3:ARG:HA     | 13:M:8:GLU:O      | 1.65                     | 0.97              |
| 2:B:80:ILE:HD12   | 2:B:80:ILE:H      | 1.27                     | 0.96              |
| 1:A:1219:A:H5'    | 1:A:1317:C:H41    | 1.30                     | 0.96              |
| 23:X:30:G:H2'     | 23:X:31:A:H8      | 1.32                     | 0.94              |
| 1:A:367:C:H5''    | 1:A:368:A:OP1     | 1.67                     | 0.94              |
| 1:A:50:A:P        | 1:A:50:A:C3'      | 2.55                     | 0.94              |
| 1:A:647:G:H22     | 1:A:724:G:H1      | 1.11                     | 0.94              |
| 25:A:1786:PAR:O52 | 25:A:1786:PAR:H11 | 1.63                     | 0.94              |
| 1:A:821:G:H22     | 1:A:825:C:H42     | 1.13                     | 0.94              |
| 1:A:1349:C:H5'    | 10:J:60:ARG:HH12  | 1.29                     | 0.93              |
| 4:D:162:LEU:HD22  | 4:D:181:MET:HE2   | 1.51                     | 0.93              |
| 1:A:406:A:H62     | 1:A:408:G:H21     | 1.08                     | 0.93              |
| 1:A:238:A:H4'     | 1:A:239:U:H5'     | 1.50                     | 0.93              |
| 1:A:1133:A:HO2'   | 1:A:1134:A:H8     | 0.93                     | 0.93              |
| 4:D:187:ARG:HD2   | 4:D:188:LEU:H     | 1.32                     | 0.92              |
| 1:A:49:U:O3'      | 1:A:50:A:H3'      | 1.68                     | 0.92              |
| 1:A:1083:A:H4'    | 1:A:1084:A:O5'    | 1.67                     | 0.92              |
| 1:A:952:A:H4'     | 1:A:953:G:C5'     | 2.00                     | 0.91              |
| 1:A:1106:G:H4'    | 1:A:1107:U:OP1    | 1.69                     | 0.91              |
| 19:S:62:ILE:HD12  | 19:S:66:MET:HG3   | 1.50                     | 0.91              |
| 1:A:562:G:H5'     | 1:A:711:A:H1'     | 1.53                     | 0.91              |
| 1:A:636:A:H5'     | 8:H:56:LYS:HE3    | 1.50                     | 0.91              |
| 3:C:70:VAL:HG21   | 3:C:76:VAL:HG21   | 1.53                     | 0.90              |
| 1:A:802:A:H5'     | 1:A:802:A:C8      | 2.06                     | 0.90              |
| 1:A:1236:G:N2     | 1:A:1263:C:N3     | 2.15                     | 0.90              |
| 1:A:1121:G:H5'    | 1:A:1122:C:OP1    | 1.71                     | 0.90              |
| 9:I:8:GLY:HA2     | 9:I:79:LEU:HD12   | 1.53                     | 0.90              |
| 6:F:2:ARG:HE      | 6:F:69:GLU:HG2    | 1.37                     | 0.90              |
| 14:N:12:ARG:CZ    | 14:N:12:ARG:HA    | 2.01                     | 0.90              |
| 7:G:50:ILE:O      | 7:G:54:THR:HG22   | 1.73                     | 0.89              |
| 1:A:339:A:H4'     | 1:A:340:C:OP2     | 1.68                     | 0.89              |
| 12:L:59:ARG:HD3   | 12:L:65:GLU:HG3   | 1.55                     | 0.89              |
| 19:S:13:ASP:HA    | 19:S:16:LEU:HB3   | 1.55                     | 0.89              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1479:A:H2     | 1:A:1482:G:H1    | 1.16                     | 0.88              |
| 3:C:14:ILE:HD13   | 3:C:14:ILE:H     | 1.36                     | 0.88              |
| 1:A:246:G:H4'     | 1:A:247:U:O5'    | 1.71                     | 0.88              |
| 13:M:65:LYS:HE3   | 13:M:69:GLU:HG2  | 1.55                     | 0.88              |
| 17:Q:97:SER:HB3   | 17:Q:105:ALA:HB3 | 1.55                     | 0.87              |
| 20:T:39:LYS:HD2   | 20:T:55:ILE:HD13 | 1.56                     | 0.87              |
| 1:A:408:G:H2'     | 1:A:423:G:N2     | 1.88                     | 0.87              |
| 12:L:42:THR:HG21  | 12:L:52:LEU:HD22 | 1.56                     | 0.87              |
| 1:A:545:C:O2'     | 12:L:15:ARG:HB3  | 1.73                     | 0.86              |
| 1:A:123:G:N3      | 1:A:189:U:H5'    | 1.90                     | 0.86              |
| 1:A:485:G:OP1     | 12:L:118:SER:HB3 | 1.74                     | 0.86              |
| 13:M:117:VAL:HG12 | 13:M:118:ALA:H   | 1.39                     | 0.86              |
| 1:A:50:A:N6       | 1:A:356:G:H4'    | 1.89                     | 0.86              |
| 9:I:15:ALA:HB2    | 9:I:65:VAL:HG13  | 1.55                     | 0.86              |
| 5:E:80:ILE:HD12   | 5:E:138:ALA:HB1  | 1.55                     | 0.86              |
| 11:K:54:ARG:O     | 11:K:57:THR:HG22 | 1.74                     | 0.86              |
| 1:A:346:G:H4'     | 1:A:347:C:OP1    | 1.76                     | 0.86              |
| 19:S:15:LEU:HD23  | 19:S:15:LEU:H    | 1.40                     | 0.86              |
| 1:A:1004:G:H1     | 1:A:1018:G:H22   | 1.22                     | 0.85              |
| 13:M:10:PRO:HB2   | 13:M:18:ALA:HB1  | 1.58                     | 0.85              |
| 2:B:21:ARG:HD3    | 2:B:21:ARG:H     | 1.40                     | 0.85              |
| 1:A:1266:A:H4'    | 1:A:1267:A:O5'   | 1.74                     | 0.85              |
| 2:B:80:ILE:HD11   | 2:B:208:ILE:HG23 | 1.58                     | 0.85              |
| 2:B:230:VAL:HG12  | 2:B:231:GLU:H    | 1.42                     | 0.85              |
| 2:B:102:LEU:HD21  | 2:B:162:ILE:HD11 | 1.58                     | 0.85              |
| 1:A:1516:C:H5     | 7:G:82:GLY:HA2   | 1.40                     | 0.85              |
| 14:N:22:THR:HB    | 14:N:33:VAL:HG21 | 1.57                     | 0.84              |
| 2:B:209:ARG:NH2   | 2:B:239:VAL:HG23 | 1.92                     | 0.84              |
| 1:A:1303:C:H4'    | 1:A:1304:G:OP1   | 1.77                     | 0.84              |
| 1:A:1406:C:H2'    | 1:A:1407:U:H5'   | 1.59                     | 0.84              |
| 1:A:446:A:H5'     | 16:P:72:ARG:NH2  | 1.93                     | 0.84              |
| 3:C:64:VAL:HG21   | 3:C:95:THR:HG21  | 1.59                     | 0.84              |
| 6:F:101:ALA:HB2   | 18:R:28:GLU:HA   | 1.58                     | 0.84              |
| 13:M:120:LYS:NZ   | 13:M:123:ALA:HB3 | 1.93                     | 0.84              |
| 1:A:1243:C:H2'    | 1:A:1244:C:H5'   | 1.58                     | 0.84              |
| 15:O:17:ARG:HG3   | 15:O:17:ARG:HH11 | 1.43                     | 0.84              |
| 1:A:1133:A:H4'    | 1:A:1134:A:OP1   | 1.76                     | 0.84              |
| 1:A:634:C:H5''    | 1:A:635:U:OP2    | 1.77                     | 0.84              |
| 10:J:24:VAL:HG13  | 10:J:34:VAL:HG11 | 1.56                     | 0.84              |
| 2:B:16:HIS:NE2    | 2:B:213:LEU:HD13 | 1.92                     | 0.83              |
| 10:J:9:ARG:O      | 10:J:16:LEU:HD21 | 1.79                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:997:C:H2'    | 1:A:998:U:H5'    | 1.60                     | 0.83              |
| 3:C:58:GLU:HB3   | 10:J:92:THR:HG21 | 1.60                     | 0.83              |
| 1:A:49:U:H4'     | 1:A:50:A:OP2     | 1.78                     | 0.83              |
| 1:A:849:A:H4'    | 1:A:850:A:OP1    | 1.76                     | 0.83              |
| 12:L:59:ARG:NH1  | 12:L:65:GLU:HB3  | 1.94                     | 0.83              |
| 2:B:95:GLN:O     | 2:B:96:ARG:HD2   | 1.79                     | 0.83              |
| 5:E:64:ARG:HG2   | 5:E:64:ARG:HH11  | 1.43                     | 0.82              |
| 8:H:86:ILE:HD11  | 8:H:136:GLU:HB2  | 1.61                     | 0.82              |
| 1:A:936:A:H3'    | 1:A:937:U:H5''   | 1.59                     | 0.82              |
| 2:B:55:PHE:HE1   | 2:B:218:ALA:HA   | 1.43                     | 0.82              |
| 2:B:209:ARG:HH21 | 2:B:239:VAL:HG23 | 1.44                     | 0.81              |
| 12:L:25:PRO:C    | 12:L:27:LEU:H    | 1.88                     | 0.81              |
| 1:A:916:G:H5''   | 7:G:102:ARG:HH22 | 1.44                     | 0.81              |
| 1:A:1005:C:H2'   | 1:A:1006:C:C5    | 2.14                     | 0.81              |
| 1:A:106:G:H1'    | 1:A:349:G:H5'    | 1.62                     | 0.81              |
| 2:B:132:LYS:O    | 2:B:136:VAL:HG23 | 1.80                     | 0.81              |
| 2:B:82:ARG:HB2   | 2:B:94:ASN:ND2   | 1.95                     | 0.81              |
| 19:S:11:VAL:HG13 | 19:S:38:SER:HB2  | 1.62                     | 0.81              |
| 1:A:1221:U:OP1   | 7:G:116:ALA:HB2  | 1.80                     | 0.81              |
| 2:B:9:GLU:HG2    | 2:B:217:ARG:NH2  | 1.95                     | 0.81              |
| 18:R:19:LYS:H    | 18:R:19:LYS:HD2  | 1.45                     | 0.81              |
| 11:K:48:ILE:HD11 | 11:K:64:ALA:HA   | 1.63                     | 0.81              |
| 1:A:666:G:H21    | 11:K:38:ASN:HD22 | 1.29                     | 0.81              |
| 1:A:1004:G:H1    | 1:A:1018:G:N2    | 1.79                     | 0.81              |
| 10:J:46:ARG:HG2  | 10:J:46:ARG:HH11 | 1.46                     | 0.81              |
| 12:L:41:ARG:HG2  | 12:L:42:THR:N    | 1.95                     | 0.81              |
| 1:A:669:U:H1'    | 11:K:42:TRP:NE1  | 1.93                     | 0.81              |
| 2:B:208:ILE:H    | 2:B:208:ILE:HD12 | 1.46                     | 0.81              |
| 1:A:1192:U:H5'   | 1:A:1193:U:OP1   | 1.81                     | 0.81              |
| 1:A:406:A:N6     | 1:A:408:G:H21    | 1.79                     | 0.81              |
| 1:A:35:G:H2'     | 1:A:36:C:C6      | 2.15                     | 0.80              |
| 1:A:916:G:H5''   | 7:G:102:ARG:NH2  | 1.96                     | 0.80              |
| 1:A:1521:U:O3'   | 22:W:1:A:OP3     | 1.99                     | 0.80              |
| 3:C:119:ARG:NE   | 3:C:140:ARG:HH12 | 1.79                     | 0.80              |
| 1:A:1036:C:C6    | 1:A:1036:C:C3'   | 2.63                     | 0.80              |
| 1:A:1121:G:N2    | 1:A:1125:G:H21   | 1.80                     | 0.80              |
| 14:N:29:ARG:HG2  | 14:N:29:ARG:HH11 | 1.45                     | 0.80              |
| 18:R:37:VAL:O    | 18:R:41:LYS:HG3  | 1.80                     | 0.80              |
| 11:K:54:ARG:HB3  | 11:K:54:ARG:HH11 | 1.45                     | 0.80              |
| 18:R:88:LYS:HB3  | 18:R:88:LYS:NZ   | 1.97                     | 0.80              |
| 1:A:388:A:H2'    | 1:A:389:G:C5'    | 2.13                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1237:A:H2'   | 1:A:1238:U:H4'   | 0.90                     | 0.79              |
| 2:B:71:VAL:O     | 2:B:165:VAL:HG23 | 1.82                     | 0.79              |
| 1:A:196:U:O2     | 20:T:105:SER:HB2 | 1.82                     | 0.79              |
| 13:M:49:THR:HB   | 13:M:52:GLU:HG3  | 1.64                     | 0.79              |
| 18:R:54:ARG:HD3  | 18:R:55:ARG:HG2  | 1.63                     | 0.79              |
| 18:R:86:VAL:O    | 18:R:87:ARG:HB2  | 1.82                     | 0.79              |
| 6:F:2:ARG:NE     | 6:F:69:GLU:HG2   | 1.97                     | 0.79              |
| 1:A:424:U:H4'    | 1:A:425:A:O5'    | 1.80                     | 0.79              |
| 1:A:1231:A:H4'   | 9:I:68:GLY:H     | 1.46                     | 0.79              |
| 1:A:1261:A:O2'   | 1:A:1262:U:OP1   | 2.01                     | 0.79              |
| 1:A:1479:A:H2    | 1:A:1482:G:N1    | 1.81                     | 0.79              |
| 1:A:543:U:H4'    | 1:A:544:U:H5''   | 1.65                     | 0.78              |
| 4:D:151:LYS:N    | 4:D:151:LYS:HD2  | 1.98                     | 0.78              |
| 13:M:120:LYS:HZ2 | 13:M:123:ALA:HB3 | 1.46                     | 0.78              |
| 18:R:38:GLU:HA   | 18:R:41:LYS:HE2  | 1.64                     | 0.78              |
| 1:A:637:G:C6     | 1:A:638:A:C5     | 2.71                     | 0.78              |
| 1:A:50:A:OP1     | 1:A:50:A:C3'     | 2.31                     | 0.78              |
| 1:A:201:A:H4'    | 20:T:68:LYS:HE2  | 1.65                     | 0.78              |
| 2:B:87:ARG:HD2   | 2:B:233:SER:HB3  | 1.66                     | 0.78              |
| 2:B:178:ARG:HH11 | 2:B:178:ARG:HG3  | 1.48                     | 0.77              |
| 19:S:33:THR:HG22 | 19:S:35:SER:N    | 1.95                     | 0.77              |
| 12:L:26:ALA:O    | 12:L:27:LEU:O    | 2.02                     | 0.77              |
| 1:A:1139:A:H5'   | 1:A:1140:C:C6    | 2.19                     | 0.77              |
| 1:A:60:A:H4'     | 1:A:61:G:O5'     | 1.84                     | 0.77              |
| 1:A:203:A:H4'    | 1:A:204:G:O5'    | 1.83                     | 0.77              |
| 5:E:12:LEU:HD23  | 5:E:31:LEU:HB2   | 1.66                     | 0.77              |
| 2:B:51:LEU:HD13  | 2:B:201:ILE:HG23 | 1.66                     | 0.77              |
| 13:M:59:TYR:O    | 13:M:63:THR:HG22 | 1.85                     | 0.77              |
| 1:A:984:C:H42    | 1:A:1002:G:H21   | 1.31                     | 0.77              |
| 1:A:1133:A:O2'   | 1:A:1134:A:H8    | 1.66                     | 0.77              |
| 2:B:114:ARG:HH11 | 2:B:118:LEU:HD11 | 1.48                     | 0.76              |
| 1:A:952:A:H4'    | 1:A:953:G:H5''   | 1.66                     | 0.76              |
| 1:A:1237:A:OP2   | 1:A:1260:A:N6    | 2.18                     | 0.76              |
| 3:C:101:LEU:HD23 | 3:C:102:ASN:N    | 2.01                     | 0.76              |
| 1:A:238:A:H4'    | 1:A:239:U:C5'    | 2.15                     | 0.76              |
| 6:F:22:GLU:OE2   | 6:F:82:ARG:HD3   | 1.84                     | 0.76              |
| 10:J:79:ARG:O    | 10:J:83:GLU:HG3  | 1.85                     | 0.76              |
| 1:A:1035:G:H4'   | 1:A:1036:C:C5'   | 2.12                     | 0.76              |
| 6:F:99:ALA:C     | 6:F:101:ALA:H    | 1.93                     | 0.76              |
| 1:A:944:C:H4'    | 9:I:128:ARG:HG3  | 1.68                     | 0.76              |
| 2:B:78:GLN:HE22  | 2:B:96:ARG:HH12  | 1.34                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1035:G:H2'   | 1:A:1180:U:H5    | 1.48                     | 0.76              |
| 1:A:1093:A:N1    | 3:C:177:THR:HG22 | 2.01                     | 0.76              |
| 1:A:1068:U:H3    | 1:A:1081:G:H22   | 1.33                     | 0.76              |
| 9:I:65:VAL:HG11  | 9:I:73:GLN:HB3   | 1.68                     | 0.76              |
| 5:E:51:VAL:HB    | 5:E:52:PRO:HD3   | 1.68                     | 0.76              |
| 22:W:3:G:H22     | 23:X:34:70U:HN3  | 1.32                     | 0.76              |
| 1:A:388:A:H2'    | 1:A:389:G:H5'    | 1.69                     | 0.75              |
| 1:A:407:A:N1     | 4:D:35:ARG:HB3   | 2.00                     | 0.75              |
| 3:C:52:LEU:HD23  | 3:C:52:LEU:H     | 1.50                     | 0.75              |
| 4:D:162:LEU:HD22 | 4:D:181:MET:CE   | 2.16                     | 0.75              |
| 10:J:26:ALA:HB1  | 10:J:81:THR:HG23 | 1.68                     | 0.75              |
| 1:A:238:A:C4'    | 1:A:239:U:H5'    | 2.16                     | 0.75              |
| 20:T:45:GLN:HG2  | 20:T:91:LEU:HD22 | 1.69                     | 0.75              |
| 3:C:64:VAL:HB    | 3:C:99:VAL:HG12  | 1.68                     | 0.75              |
| 12:L:53:ARG:HG3  | 12:L:93:LEU:HD21 | 1.68                     | 0.75              |
| 1:A:49:U:C4      | 1:A:359:A:C6     | 2.74                     | 0.75              |
| 1:A:361:C:O2'    | 1:A:389:G:N2     | 2.20                     | 0.75              |
| 1:A:986:C:H42    | 1:A:999:G:H1     | 1.32                     | 0.75              |
| 2:B:211:ILE:O    | 2:B:215:LEU:HB2  | 1.87                     | 0.75              |
| 12:L:74:GLY:O    | 12:L:102:ARG:NH2 | 2.15                     | 0.75              |
| 17:Q:68:ARG:HH11 | 17:Q:68:ARG:HG3  | 1.51                     | 0.75              |
| 1:A:49:U:O3'     | 1:A:50:A:C3'     | 2.35                     | 0.74              |
| 3:C:12:LEU:HD21  | 14:N:51:GLY:HA2  | 1.67                     | 0.74              |
| 8:H:4:ASP:OD2    | 8:H:7:ALA:HB2    | 1.87                     | 0.74              |
| 5:E:79:GLU:HG3   | 5:E:93:PRO:HD2   | 1.69                     | 0.74              |
| 5:E:152:ARG:HA   | 8:H:64:LYS:NZ    | 2.03                     | 0.74              |
| 13:M:9:ILE:HD12  | 13:M:9:ILE:N     | 2.02                     | 0.74              |
| 12:L:42:THR:HG21 | 12:L:52:LEU:CD2  | 2.17                     | 0.74              |
| 19:S:15:LEU:HA   | 19:S:18:LYS:HB3  | 1.69                     | 0.74              |
| 20:T:56:MET:HE3  | 20:T:88:VAL:HG11 | 1.69                     | 0.74              |
| 2:B:141:GLU:O    | 2:B:144:ARG:HG3  | 1.88                     | 0.74              |
| 1:A:705:A:O2'    | 1:A:706:U:H3'    | 1.87                     | 0.73              |
| 3:C:29:TYR:HE2   | 3:C:33:LEU:HD22  | 1.51                     | 0.73              |
| 20:T:39:LYS:HD2  | 20:T:55:ILE:CD1  | 2.19                     | 0.73              |
| 1:A:340:C:H4'    | 1:A:341:G:O5'    | 1.87                     | 0.73              |
| 3:C:3:ASN:HD22   | 3:C:3:ASN:N      | 1.84                     | 0.73              |
| 23:X:30:G:H2'    | 23:X:31:A:C8     | 2.20                     | 0.73              |
| 1:A:211:G:H2'    | 1:A:212:C:C6     | 2.23                     | 0.73              |
| 1:A:241:A:H4'    | 1:A:242:G:OP1    | 1.88                     | 0.73              |
| 1:A:1521:U:O3'   | 22:W:1:A:P       | 2.47                     | 0.73              |
| 5:E:64:ARG:O     | 5:E:65:ASN:HB3   | 1.86                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:33:TYR:HA    | 6:F:71:ARG:HH21  | 1.53                     | 0.73              |
| 8:H:113:SER:HB2  | 8:H:134:ILE:HD11 | 1.71                     | 0.73              |
| 20:T:10:LEU:HD12 | 20:T:12:ALA:HB2  | 1.71                     | 0.73              |
| 1:A:949:C:OP1    | 10:J:57:LYS:HD3  | 1.88                     | 0.73              |
| 10:J:49:VAL:O    | 10:J:60:ARG:HA   | 1.87                     | 0.73              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H    | 1.53                     | 0.73              |
| 19:S:12:ASP:H    | 19:S:38:SER:HB3  | 1.52                     | 0.73              |
| 1:A:416:U:H5'    | 1:A:417:C:C5     | 2.23                     | 0.72              |
| 3:C:26:LYS:H     | 3:C:26:LYS:HD3   | 1.54                     | 0.72              |
| 1:A:530:A:H4'    | 1:A:531:G:O5'    | 1.88                     | 0.72              |
| 13:M:15:VAL:HG23 | 13:M:43:THR:O    | 1.87                     | 0.72              |
| 1:A:1110:C:H5''  | 9:I:16:ARG:HH22  | 1.52                     | 0.72              |
| 4:D:3:ARG:HA     | 4:D:3:ARG:HE     | 1.54                     | 0.72              |
| 7:G:138:LYS:HE2  | 7:G:142:GLU:OE1  | 1.90                     | 0.72              |
| 18:R:33:ASP:OD2  | 18:R:36:ASN:HB2  | 1.90                     | 0.72              |
| 2:B:80:ILE:H     | 2:B:80:ILE:CD1   | 1.98                     | 0.72              |
| 1:A:821:G:N2     | 1:A:825:C:H42    | 1.88                     | 0.72              |
| 7:G:15:ASP:OD2   | 7:G:18:TYR:N     | 2.20                     | 0.72              |
| 19:S:47:HIS:O    | 19:S:62:ILE:HG22 | 1.89                     | 0.72              |
| 1:A:689:A:H1'    | 11:K:29:ILE:HD11 | 1.70                     | 0.72              |
| 1:A:985:C:H42    | 1:A:1000:G:H1    | 1.36                     | 0.72              |
| 17:Q:69:LYS:C    | 17:Q:70:ARG:HD2  | 2.15                     | 0.72              |
| 4:D:36:ARG:N     | 4:D:37:PRO:HD3   | 2.05                     | 0.72              |
| 10:J:78:ASN:HB2  | 10:J:81:THR:HB   | 1.71                     | 0.72              |
| 15:O:39:LEU:HD13 | 15:O:56:LEU:HB2  | 1.69                     | 0.72              |
| 8:H:86:ILE:HG21  | 8:H:133:LEU:HD13 | 1.71                     | 0.71              |
| 1:A:1116:G:H1    | 1:A:1122:C:H42   | 1.36                     | 0.71              |
| 2:B:143:GLU:O    | 2:B:147:LYS:HG3  | 1.90                     | 0.71              |
| 4:D:119:GLN:HG2  | 4:D:123:HIS:CD2  | 2.24                     | 0.71              |
| 2:B:95:GLN:HG3   | 2:B:147:LYS:O    | 1.90                     | 0.71              |
| 2:B:16:HIS:CD2   | 2:B:213:LEU:HD13 | 2.25                     | 0.71              |
| 7:G:122:HIS:HA   | 7:G:125:MET:HE3  | 1.73                     | 0.71              |
| 19:S:33:THR:HG22 | 19:S:34:TRP:N    | 2.06                     | 0.71              |
| 20:T:67:ALA:HA   | 20:T:73:HIS:H    | 1.55                     | 0.71              |
| 2:B:35:GLU:HA    | 2:B:39:ILE:O     | 1.90                     | 0.71              |
| 3:C:119:ARG:HE   | 3:C:140:ARG:NH1  | 1.82                     | 0.71              |
| 5:E:137:GLU:O    | 5:E:141:GLN:HG3  | 1.90                     | 0.71              |
| 21:V:6:ARG:HD2   | 21:V:15:ARG:HH12 | 1.55                     | 0.71              |
| 13:M:8:GLU:HG3   | 13:M:22:ILE:HG12 | 1.72                     | 0.71              |
| 1:A:1207:C:H4'   | 1:A:1208:A:OP1   | 1.90                     | 0.71              |
| 1:A:1349:C:C5'   | 10:J:60:ARG:HH12 | 2.02                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1417:G:H2'   | 1:A:1418:U:C6     | 2.24                     | 0.71              |
| 1:A:589:G:H2'    | 1:A:614:G:H1      | 1.54                     | 0.71              |
| 2:B:144:ARG:HA   | 2:B:147:LYS:HD2   | 1.73                     | 0.71              |
| 2:B:235:SER:O    | 2:B:239:VAL:HG22  | 1.91                     | 0.71              |
| 1:A:637:G:C6     | 1:A:638:A:C4      | 2.79                     | 0.70              |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA    | 1.72                     | 0.70              |
| 1:A:468:G:H4'    | 1:A:469:G:O5'     | 1.91                     | 0.70              |
| 1:A:348:A:H5'    | 1:A:348:A:H8      | 1.56                     | 0.70              |
| 1:A:1036:C:C4    | 23:X:34:70U:H4'   | 2.26                     | 0.70              |
| 1:A:1288:U:H5'   | 13:M:109:THR:HG21 | 1.72                     | 0.70              |
| 2:B:95:GLN:C     | 2:B:96:ARG:HD2    | 2.16                     | 0.70              |
| 3:C:45:LYS:HE3   | 3:C:46:GLU:OE2    | 1.90                     | 0.70              |
| 1:A:8:A:H4'      | 1:A:9:G:OP1       | 1.90                     | 0.70              |
| 14:N:27:CYS:SG   | 14:N:29:ARG:HB2   | 2.32                     | 0.70              |
| 1:A:1113:G:C8    | 1:A:1113:G:H3'    | 2.27                     | 0.70              |
| 1:A:1185:A:H5'   | 1:A:1186:U:OP2    | 1.91                     | 0.70              |
| 4:D:8:VAL:HG22   | 4:D:115:ARG:NH1   | 2.06                     | 0.70              |
| 5:E:7:GLU:O      | 5:E:34:VAL:HA     | 1.91                     | 0.70              |
| 1:A:1349:C:H5'   | 10:J:60:ARG:NH1   | 2.04                     | 0.70              |
| 2:B:25:ASN:HD22  | 2:B:25:ASN:C      | 2.00                     | 0.70              |
| 12:L:46:LYS:HE3  | 12:L:47:LYS:HG3   | 1.74                     | 0.70              |
| 2:B:142:LEU:HD21 | 2:B:146:GLN:OE1   | 1.92                     | 0.70              |
| 10:J:27:ALA:HB1  | 10:J:31:GLY:H     | 1.55                     | 0.70              |
| 4:D:24:GLU:O     | 4:D:26:CYS:N      | 2.24                     | 0.70              |
| 16:P:51:VAL:O    | 16:P:52:ASP:HB3   | 1.91                     | 0.70              |
| 9:I:3:GLN:HG3    | 9:I:20:ARG:HG2    | 1.74                     | 0.70              |
| 1:A:748:G:N2     | 1:A:795:C:HO2'    | 1.90                     | 0.70              |
| 2:B:80:ILE:HD12  | 2:B:80:ILE:N      | 2.04                     | 0.70              |
| 1:A:997:C:C2'    | 1:A:998:U:H5'     | 2.21                     | 0.69              |
| 4:D:8:VAL:CG2    | 4:D:115:ARG:NH1   | 2.54                     | 0.69              |
| 1:A:1170:C:P     | 10:J:51:ARG:HH22  | 2.16                     | 0.69              |
| 1:A:701:G:H5'    | 11:K:117:ASN:ND2  | 2.08                     | 0.69              |
| 1:A:951:A:OP1    | 14:N:31:ARG:HG2   | 1.91                     | 0.69              |
| 12:L:70:ILE:HD13 | 12:L:77:LEU:HD12  | 1.73                     | 0.69              |
| 12:L:33:ARG:HD3  | 12:L:62:SER:HB3   | 1.74                     | 0.69              |
| 17:Q:45:HIS:HB3  | 17:Q:72:ARG:HG2   | 1.75                     | 0.69              |
| 10:J:90:LEU:N    | 10:J:91:PRO:HD2   | 2.02                     | 0.69              |
| 1:A:1110:C:O2'   | 1:A:1111:C:H5''   | 1.91                     | 0.69              |
| 1:A:1207:C:H5''  | 13:M:103:THR:OG1  | 1.93                     | 0.69              |
| 1:A:1287:A:N6    | 1:A:1312:G:H1'    | 2.07                     | 0.69              |
| 2:B:55:PHE:CE1   | 2:B:218:ALA:HA    | 2.27                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:3:ASN:N       | 3:C:3:ASN:ND2     | 2.37                     | 0.69              |
| 4:D:70:ILE:HD11   | 4:D:100:ARG:HD3   | 1.75                     | 0.69              |
| 9:I:70:LYS:O      | 9:I:74:ILE:HG13   | 1.93                     | 0.69              |
| 4:D:7:PRO:HB2     | 4:D:10:ARG:HG2    | 1.74                     | 0.69              |
| 22:W:2:A:H5'      | 22:W:2:A:H8       | 1.58                     | 0.69              |
| 2:B:78:GLN:NE2    | 2:B:96:ARG:HH12   | 1.90                     | 0.69              |
| 4:D:36:ARG:H      | 4:D:37:PRO:HD3    | 1.57                     | 0.69              |
| 20:T:49:ALA:HB3   | 20:T:99:LEU:HG    | 1.75                     | 0.69              |
| 1:A:636:A:H2'     | 1:A:636:A:N3      | 2.06                     | 0.68              |
| 1:A:1279:C:O2'    | 1:A:1280:A:OP2    | 2.12                     | 0.68              |
| 1:A:260:G:C2'     | 1:A:261:G:H5'     | 2.23                     | 0.68              |
| 1:A:1035:G:H2'    | 1:A:1180:U:C5     | 2.28                     | 0.68              |
| 1:A:1406:C:C2'    | 1:A:1407:U:H5'    | 2.22                     | 0.68              |
| 12:L:28:LYS:O     | 12:L:29:GLY:C     | 2.34                     | 0.68              |
| 12:L:59:ARG:HH11  | 12:L:65:GLU:HB3   | 1.58                     | 0.68              |
| 1:A:102:A:H4'     | 1:A:103:C:OP2     | 1.93                     | 0.68              |
| 1:A:1206:A:H3'    | 1:A:1207:C:C6     | 2.28                     | 0.68              |
| 4:D:8:VAL:HG22    | 4:D:115:ARG:HH12  | 1.57                     | 0.68              |
| 6:F:29:ALA:HA     | 6:F:32:ASN:OD1    | 1.93                     | 0.68              |
| 8:H:23:SER:HA     | 8:H:63:LEU:HD22   | 1.75                     | 0.68              |
| 1:A:610:G:O2'     | 1:A:611:G:H5'     | 1.92                     | 0.68              |
| 7:G:111:ARG:HB3   | 7:G:113:GLU:OE2   | 1.93                     | 0.68              |
| 9:I:127:LYS:H     | 9:I:127:LYS:HD2   | 1.59                     | 0.68              |
| 12:L:41:ARG:NH1   | 12:L:41:ARG:CB    | 2.54                     | 0.68              |
| 25:A:1786:PAR:O62 | 25:A:1786:PAR:H13 | 1.95                     | 0.68              |
| 6:F:2:ARG:HE      | 6:F:69:GLU:CG     | 2.07                     | 0.68              |
| 1:A:1114:C:H2'    | 1:A:1115:G:C8     | 2.29                     | 0.67              |
| 2:B:80:ILE:HD11   | 2:B:208:ILE:CG2   | 2.24                     | 0.67              |
| 3:C:62:ASP:O      | 3:C:97:LYS:HB3    | 1.95                     | 0.67              |
| 12:L:75:HIS:HA    | 12:L:102:ARG:NH2  | 2.10                     | 0.67              |
| 15:O:2:PRO:C      | 15:O:38:ARG:HH22  | 2.01                     | 0.67              |
| 1:A:1047:U:O2'    | 1:A:1048:C:OP2    | 2.10                     | 0.67              |
| 1:A:1243:C:H2'    | 1:A:1244:C:C5'    | 2.24                     | 0.67              |
| 1:A:1350:G:O2'    | 1:A:1351:C:H5'    | 1.94                     | 0.67              |
| 2:B:212:GLN:HE22  | 2:B:235:SER:HB2   | 1.59                     | 0.67              |
| 6:F:15:ASP:H      | 6:F:18:GLN:NE2    | 1.93                     | 0.67              |
| 7:G:125:MET:O     | 7:G:129:GLU:HG2   | 1.94                     | 0.67              |
| 10:J:6:ILE:HD11   | 10:J:72:VAL:HG11  | 1.76                     | 0.67              |
| 11:K:57:THR:HG23  | 11:K:60:ALA:H     | 1.58                     | 0.67              |
| 17:Q:59:ILE:HG22  | 17:Q:71:PHE:CD1   | 2.29                     | 0.67              |
| 1:A:1005:C:H2'    | 1:A:1006:C:C6     | 2.30                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1119:C:H4'    | 1:A:1120:G:C2    | 2.29                     | 0.67              |
| 1:A:1516:C:C5     | 7:G:82:GLY:HA2   | 2.28                     | 0.67              |
| 7:G:15:ASP:HB3    | 7:G:19:GLY:N     | 2.09                     | 0.67              |
| 10:J:4:ILE:O      | 10:J:73:ASP:HA   | 1.95                     | 0.67              |
| 1:A:170:C:OP1     | 20:T:29:LYS:NZ   | 2.27                     | 0.67              |
| 1:A:670:A:H4'     | 1:A:671:G:O5'    | 1.95                     | 0.67              |
| 6:F:15:ASP:H      | 6:F:18:GLN:HE22  | 1.42                     | 0.67              |
| 9:I:10:ARG:HD3    | 9:I:105:ASP:HB3  | 1.77                     | 0.67              |
| 1:A:1035:G:O2'    | 1:A:1036:C:OP2   | 2.06                     | 0.67              |
| 1:A:416:U:H4'     | 1:A:417:C:OP2    | 1.94                     | 0.67              |
| 1:A:433:G:H4'     | 1:A:434:A:OP1    | 1.93                     | 0.67              |
| 4:D:187:ARG:HD2   | 4:D:188:LEU:N    | 2.09                     | 0.67              |
| 19:S:77:THR:HG22  | 19:S:78:ARG:N    | 2.10                     | 0.66              |
| 1:A:79:U:H3'      | 1:A:79:U:H6      | 1.60                     | 0.66              |
| 13:M:16:ASP:OD2   | 13:M:31:LYS:HE2  | 1.95                     | 0.66              |
| 1:A:1077:U:H2'    | 1:A:1078:C:C6    | 2.30                     | 0.66              |
| 9:I:111:ARG:HG2   | 9:I:112:LYS:N    | 2.08                     | 0.66              |
| 19:S:62:ILE:CD1   | 19:S:66:MET:HG3  | 2.25                     | 0.66              |
| 1:A:120:G:HO2'    | 17:Q:2:PRO:N     | 1.94                     | 0.66              |
| 1:A:830:G:O2'     | 1:A:831:G:H5'    | 1.96                     | 0.66              |
| 1:A:1107:U:H3     | 10:J:5:ARG:HH21  | 1.43                     | 0.66              |
| 13:M:15:VAL:HG21  | 13:M:48:LEU:HD21 | 1.78                     | 0.66              |
| 1:A:358:A:H62     | 12:L:28:LYS:NZ   | 1.93                     | 0.66              |
| 16:P:18:ARG:HG3   | 16:P:35:LYS:HE3  | 1.77                     | 0.66              |
| 1:A:388:A:H2'     | 1:A:389:G:H5''   | 1.78                     | 0.66              |
| 1:A:507:G:H2'     | 1:A:508:C:C6     | 2.31                     | 0.66              |
| 1:A:1047:U:H5''   | 1:A:1171:G:N2    | 2.11                     | 0.66              |
| 1:A:982:A:N3      | 1:A:982:A:H5''   | 2.10                     | 0.65              |
| 3:C:72:LYS:O      | 3:C:75:VAL:HG22  | 1.96                     | 0.65              |
| 11:K:120:ARG:HH21 | 11:K:126:ARG:CZ  | 2.08                     | 0.65              |
| 14:N:22:THR:CB    | 14:N:33:VAL:HG21 | 2.26                     | 0.65              |
| 1:A:358:A:H62     | 12:L:28:LYS:HZ1  | 1.44                     | 0.65              |
| 1:A:760:A:H8      | 1:A:760:A:H5''   | 1.61                     | 0.65              |
| 1:A:1487:U:H2'    | 1:A:1488:G:C8    | 2.32                     | 0.65              |
| 12:L:34:ARG:O     | 12:L:61:THR:HG23 | 1.96                     | 0.65              |
| 1:A:408:G:H2'     | 1:A:423:G:H22    | 1.62                     | 0.65              |
| 1:A:803:U:H4'     | 1:A:804:G:OP2    | 1.97                     | 0.65              |
| 1:A:79:U:H3'      | 1:A:79:U:C6      | 2.32                     | 0.65              |
| 1:A:382:U:H5'     | 1:A:383:G:OP1    | 1.96                     | 0.65              |
| 19:S:30:LEU:O     | 19:S:31:ILE:HD13 | 1.96                     | 0.65              |
| 1:A:35:G:H2'      | 1:A:36:C:H6      | 1.62                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:948:G:H4'    | 1:A:949:C:OP2    | 1.95                     | 0.65              |
| 1:A:1039:G:H5''  | 3:C:154:SER:HB2  | 1.79                     | 0.65              |
| 1:A:1449:U:H2'   | 1:A:1450:A:H8    | 1.62                     | 0.65              |
| 3:C:60:ALA:O     | 3:C:62:ASP:N     | 2.29                     | 0.65              |
| 6:F:80:ARG:NH1   | 6:F:88:VAL:HB    | 2.11                     | 0.65              |
| 11:K:22:HIS:HB3  | 11:K:29:ILE:HG23 | 1.79                     | 0.65              |
| 1:A:242:G:OP2    | 17:Q:100:LYS:HE2 | 1.97                     | 0.65              |
| 1:A:379:G:H2'    | 1:A:380:C:C6     | 2.32                     | 0.65              |
| 1:A:822:U:H5'    | 1:A:823:C:H5     | 1.61                     | 0.65              |
| 1:A:1123:C:H2'   | 1:A:1124:G:H5'   | 1.79                     | 0.65              |
| 1:A:1260:A:H5''  | 1:A:1261:A:OP1   | 1.97                     | 0.65              |
| 7:G:26:PHE:CE2   | 7:G:30:ILE:HD11  | 2.32                     | 0.65              |
| 12:L:41:ARG:HH22 | 12:L:57:LYS:CE   | 2.09                     | 0.65              |
| 2:B:103:THR:HG23 | 2:B:176:GLU:OE1  | 1.97                     | 0.65              |
| 9:I:106:ALA:O    | 9:I:108:VAL:HG23 | 1.97                     | 0.65              |
| 10:J:7:LYS:HB3   | 10:J:97:GLU:HB3  | 1.78                     | 0.65              |
| 21:V:5:ASP:O     | 21:V:11:GLY:HA3  | 1.97                     | 0.65              |
| 1:A:348:A:H5'    | 1:A:348:A:C8     | 2.32                     | 0.64              |
| 1:A:660:U:H3     | 1:A:696:G:H22    | 1.44                     | 0.64              |
| 2:B:21:ARG:HD3   | 2:B:21:ARG:N     | 2.11                     | 0.64              |
| 4:D:164:ALA:O    | 4:D:168:ARG:HD3  | 1.98                     | 0.64              |
| 13:M:3:ARG:NH1   | 13:M:7:VAL:HG12  | 2.12                     | 0.64              |
| 1:A:238:A:C5'    | 1:A:239:U:H5'    | 2.27                     | 0.64              |
| 1:A:1108:U:H2'   | 1:A:1109:G:H5'   | 1.79                     | 0.64              |
| 9:I:40:LEU:O     | 9:I:42:ARG:N     | 2.30                     | 0.64              |
| 20:T:53:LEU:HB2  | 20:T:100:ILE:CG2 | 2.28                     | 0.64              |
| 1:A:124:A:O2'    | 1:A:125:C:O5'    | 2.14                     | 0.64              |
| 1:A:198:U:O4'    | 20:T:103:GLY:HA2 | 1.97                     | 0.64              |
| 1:A:982:A:N6     | 1:A:1019:C:H42   | 1.96                     | 0.64              |
| 4:D:187:ARG:CD   | 4:D:188:LEU:H    | 2.10                     | 0.64              |
| 9:I:127:LYS:HE2  | 13:M:126:LYS:CE  | 2.28                     | 0.64              |
| 15:O:45:VAL:HG12 | 15:O:46:HIS:H    | 1.63                     | 0.64              |
| 1:A:1381:C:H4'   | 1:A:1382:C:O5'   | 1.96                     | 0.64              |
| 4:D:31:CYS:C     | 4:D:33:MET:H     | 2.05                     | 0.64              |
| 7:G:145:ALA:O    | 7:G:146:GLU:C    | 2.41                     | 0.64              |
| 1:A:442:A:OP2    | 1:A:469:G:N2     | 2.22                     | 0.64              |
| 1:A:1236:G:C2    | 1:A:1263:C:N3    | 2.65                     | 0.64              |
| 2:B:25:ASN:HD22  | 2:B:26:PRO:N     | 1.96                     | 0.64              |
| 2:B:223:ILE:HG13 | 2:B:224:GLN:N    | 2.10                     | 0.64              |
| 7:G:16:LEU:H     | 7:G:16:LEU:HD22  | 1.62                     | 0.64              |
| 1:A:31:G:N1      | 1:A:48:C:H5''    | 2.13                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:825:C:O5'    | 1:A:825:C:H6     | 1.80                     | 0.64              |
| 2:B:82:ARG:O     | 2:B:86:GLU:HG3   | 1.96                     | 0.64              |
| 11:K:84:VAL:HG23 | 11:K:110:ASP:HA  | 1.79                     | 0.64              |
| 1:A:542:A:H4'    | 1:A:543:U:H5''   | 1.80                     | 0.64              |
| 1:A:1013:G:H2'   | 1:A:1014:G:H8    | 1.61                     | 0.64              |
| 1:A:1333:C:H2'   | 1:A:1334:G:C8    | 2.32                     | 0.64              |
| 1:A:1374:G:N2    | 1:A:1479:A:H8    | 1.96                     | 0.64              |
| 3:C:70:VAL:O     | 3:C:106:VAL:HG23 | 1.96                     | 0.64              |
| 1:A:1093:A:H61   | 3:C:177:THR:HG22 | 1.61                     | 0.64              |
| 2:B:80:ILE:CD1   | 2:B:208:ILE:HG23 | 2.26                     | 0.64              |
| 10:J:61:GLU:OE1  | 14:N:45:ARG:NH1  | 2.31                     | 0.64              |
| 1:A:93:C:H2'     | 1:A:94:A:C8      | 2.33                     | 0.64              |
| 2:B:230:VAL:HG12 | 2:B:231:GLU:N    | 2.11                     | 0.64              |
| 13:M:65:LYS:CE   | 13:M:69:GLU:HG2  | 2.27                     | 0.64              |
| 15:O:74:ASP:OD1  | 15:O:76:GLU:HB3  | 1.98                     | 0.64              |
| 1:A:1421:C:OP1   | 20:T:38:LYS:HE2  | 1.98                     | 0.63              |
| 1:A:402:G:H2'    | 1:A:403:A:C8     | 2.33                     | 0.63              |
| 7:G:114:ARG:HG2  | 7:G:114:ARG:HH11 | 1.63                     | 0.63              |
| 1:A:1006:C:H2'   | 1:A:1007:C:H5'   | 1.80                     | 0.63              |
| 1:A:1124:G:H2'   | 1:A:1125:G:O4'   | 1.98                     | 0.63              |
| 3:C:79:ARG:HG3   | 3:C:79:ARG:O     | 1.97                     | 0.63              |
| 6:F:4:TYR:CZ     | 6:F:72:VAL:HG21  | 2.33                     | 0.63              |
| 9:I:27:THR:HB    | 9:I:62:TYR:HD1   | 1.63                     | 0.63              |
| 12:L:47:LYS:CB   | 12:L:48:PRO:CD   | 2.68                     | 0.63              |
| 1:A:1006:C:O5'   | 1:A:1006:C:H6    | 1.81                     | 0.63              |
| 8:H:111:ILE:O    | 8:H:134:ILE:HB   | 1.98                     | 0.63              |
| 15:O:17:ARG:HG3  | 15:O:17:ARG:NH1  | 2.14                     | 0.63              |
| 22:W:3:G:N2      | 23:X:34:70U:S2   | 2.71                     | 0.63              |
| 1:A:1337:G:H2'   | 1:A:1338:A:C8    | 2.33                     | 0.63              |
| 3:C:14:ILE:HD13  | 3:C:14:ILE:N     | 2.10                     | 0.63              |
| 12:L:27:LEU:C    | 12:L:29:GLY:N    | 2.53                     | 0.63              |
| 15:O:70:LEU:HD12 | 15:O:78:TYR:CA   | 2.28                     | 0.63              |
| 1:A:209:U:H4'    | 1:A:210:U:OP1    | 1.98                     | 0.63              |
| 1:A:406:A:H62    | 1:A:408:G:N2     | 1.90                     | 0.63              |
| 1:A:1127:C:H5''  | 1:A:1128:A:OP1   | 1.97                     | 0.63              |
| 6:F:44:GLY:HA2   | 6:F:59:TYR:CE1   | 2.34                     | 0.63              |
| 1:A:79:U:H2'     | 1:A:81:U:OP2     | 1.98                     | 0.63              |
| 9:I:46:ALA:HA    | 9:I:78:LYS:HB2   | 1.80                     | 0.63              |
| 17:Q:70:ARG:HD2  | 17:Q:70:ARG:N    | 2.14                     | 0.63              |
| 18:R:36:ASN:ND2  | 18:R:38:GLU:HG2  | 2.13                     | 0.63              |
| 19:S:33:THR:CG2  | 19:S:35:SER:H    | 1.98                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:64:VAL:HG12   | 3:C:66:VAL:HG23   | 1.81                     | 0.63              |
| 6:F:100:ASN:HB2   | 18:R:23:LYS:HZ2   | 1.63                     | 0.63              |
| 1:A:1262:U:H5'    | 1:A:1263:C:H5     | 1.64                     | 0.63              |
| 1:A:1509:U:H2'    | 1:A:1510:C:C5'    | 2.28                     | 0.63              |
| 2:B:77:ALA:HB2    | 2:B:211:ILE:HD13  | 1.81                     | 0.63              |
| 14:N:12:ARG:O     | 14:N:13:THR:C     | 2.42                     | 0.63              |
| 1:A:823:C:H3'     | 1:A:823:C:OP2     | 1.99                     | 0.62              |
| 6:F:99:ALA:O      | 6:F:101:ALA:N     | 2.32                     | 0.62              |
| 12:L:59:ARG:HH11  | 12:L:65:GLU:CB    | 2.11                     | 0.62              |
| 15:O:70:LEU:HD12  | 15:O:78:TYR:HA    | 1.80                     | 0.62              |
| 1:A:1203:G:OP1    | 19:S:77:THR:HG21  | 1.98                     | 0.62              |
| 4:D:62:GLN:HE22   | 4:D:65:ARG:NH1    | 1.97                     | 0.62              |
| 12:L:41:ARG:HD2   | 12:L:42:THR:O     | 1.99                     | 0.62              |
| 12:L:89:ARG:HH21  | 12:L:97:ARG:HH21  | 1.47                     | 0.62              |
| 1:A:1259:U:H5''   | 1:A:1260:A:H5'    | 1.80                     | 0.62              |
| 1:A:1307:C:OP1    | 21:V:12:LYS:NZ    | 2.31                     | 0.62              |
| 5:E:57:LYS:HG2    | 5:E:61:TYR:CE2    | 2.34                     | 0.62              |
| 11:K:101:SER:C    | 11:K:103:LEU:H    | 2.07                     | 0.62              |
| 12:L:41:ARG:HH22  | 12:L:57:LYS:NZ    | 1.96                     | 0.62              |
| 12:L:47:LYS:CB    | 12:L:48:PRO:HD2   | 2.22                     | 0.62              |
| 16:P:28:ARG:HG3   | 16:P:29:ASP:OD2   | 1.99                     | 0.62              |
| 1:A:506:A:H61     | 12:L:92:ASP:HB2   | 1.62                     | 0.62              |
| 1:A:686:G:O2'     | 1:A:687:A:OP2     | 2.16                     | 0.62              |
| 25:A:1786:PAR:O44 | 25:A:1786:PAR:N64 | 2.30                     | 0.62              |
| 3:C:179:ARG:O     | 3:C:179:ARG:HG2   | 1.96                     | 0.62              |
| 6:F:8:ILE:HD11    | 6:F:79:LEU:HD13   | 1.80                     | 0.62              |
| 1:A:1286:G:N2     | 1:A:1312:G:O2'    | 2.33                     | 0.62              |
| 12:L:27:LEU:O     | 12:L:29:GLY:N     | 2.32                     | 0.62              |
| 1:A:1110:C:C5'    | 9:I:16:ARG:HH22   | 2.12                     | 0.62              |
| 1:A:1286:G:N2     | 1:A:1312:G:C2'    | 2.62                     | 0.62              |
| 1:A:542:A:H4'     | 1:A:543:U:C5'     | 2.30                     | 0.62              |
| 1:A:867:G:O2'     | 1:A:868:U:OP2     | 2.18                     | 0.62              |
| 1:A:1110:C:H5''   | 9:I:16:ARG:NH2    | 2.14                     | 0.62              |
| 12:L:46:LYS:CE    | 12:L:47:LYS:HG3   | 2.28                     | 0.62              |
| 15:O:26:GLU:OE1   | 15:O:77:ARG:HD2   | 1.99                     | 0.62              |
| 18:R:88:LYS:HB3   | 18:R:88:LYS:HZ3   | 1.63                     | 0.62              |
| 1:A:774:G:H2'     | 1:A:775:A:H5'     | 1.82                     | 0.62              |
| 1:A:923:A:H2'     | 1:A:924:G:C8      | 2.34                     | 0.62              |
| 1:A:1171:G:OP1    | 3:C:4:LYS:HA      | 2.00                     | 0.62              |
| 9:I:9:ARG:HG2     | 9:I:14:VAL:HG22   | 1.82                     | 0.62              |
| 17:Q:63:ARG:O     | 17:Q:65:ILE:HD12  | 2.00                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:36:ARG:HG2    | 4:D:36:ARG:HH11   | 1.65                     | 0.62              |
| 6:F:21:LEU:O      | 6:F:25:ILE:HG13   | 2.00                     | 0.62              |
| 14:N:8:GLU:O      | 14:N:11:LYS:HB2   | 2.00                     | 0.62              |
| 1:A:726:U:H2'     | 1:A:727:C:C6      | 2.35                     | 0.62              |
| 1:A:997:C:H2'     | 1:A:998:U:C5'     | 2.30                     | 0.62              |
| 2:B:178:ARG:HG3   | 2:B:178:ARG:NH1   | 2.13                     | 0.61              |
| 7:G:137:LYS:O     | 7:G:141:VAL:HG23  | 2.00                     | 0.61              |
| 4:D:28:SER:O      | 4:D:30:LYS:N      | 2.32                     | 0.61              |
| 10:J:26:ALA:HA    | 10:J:84:GLN:HE22  | 1.65                     | 0.61              |
| 12:L:59:ARG:HH11  | 12:L:65:GLU:CG    | 2.12                     | 0.61              |
| 20:T:57:ARG:HH22  | 20:T:100:ILE:HG12 | 1.65                     | 0.61              |
| 4:D:98:GLU:HG2    | 4:D:189:PRO:HG3   | 1.83                     | 0.61              |
| 10:J:49:VAL:HG22  | 14:N:41:ARG:HB2   | 1.82                     | 0.61              |
| 1:A:705:A:H1'     | 1:A:706:U:H6      | 1.65                     | 0.61              |
| 1:A:984:C:H3'     | 1:A:984:C:H6      | 1.65                     | 0.61              |
| 1:A:1121:G:H21    | 1:A:1125:G:H21    | 1.46                     | 0.61              |
| 1:A:260:G:H2'     | 1:A:261:G:H5'     | 1.82                     | 0.61              |
| 1:A:328:G:H4'     | 20:T:16:HIS:CE1   | 2.35                     | 0.61              |
| 1:A:1267:A:C8     | 1:A:1268:A:H4'    | 2.36                     | 0.61              |
| 3:C:3:ASN:ND2     | 3:C:3:ASN:H       | 1.97                     | 0.61              |
| 3:C:139:GLN:HA    | 3:C:139:GLN:NE2   | 2.15                     | 0.61              |
| 8:H:91:ARG:HG3    | 12:L:7:ILE:HG13   | 1.83                     | 0.61              |
| 1:A:1209:C:H4'    | 13:M:116:THR:HA   | 1.82                     | 0.61              |
| 18:R:53:ARG:HG2   | 18:R:63:GLN:OE1   | 2.00                     | 0.61              |
| 2:B:17:PHE:HA     | 2:B:44:LEU:HD21   | 1.82                     | 0.61              |
| 2:B:169:LYS:O     | 2:B:169:LYS:HD3   | 2.00                     | 0.61              |
| 13:M:125:ARG:HH12 | 13:M:126:LYS:CG   | 2.13                     | 0.61              |
| 2:B:41:ILE:HD12   | 2:B:41:ILE:N      | 2.15                     | 0.61              |
| 1:A:1267:A:C2     | 21:V:18:TYR:OH    | 2.54                     | 0.61              |
| 3:C:64:VAL:CB     | 3:C:99:VAL:HG12   | 2.30                     | 0.61              |
| 7:G:79:ARG:NH1    | 7:G:83:ALA:HA     | 2.15                     | 0.61              |
| 13:M:108:ARG:NH2  | 13:M:114:ARG:HA   | 2.16                     | 0.61              |
| 1:A:367:C:C5'     | 1:A:368:A:OP1     | 2.45                     | 0.60              |
| 1:A:1134:A:H2'    | 1:A:1135:C:O4'    | 2.01                     | 0.60              |
| 1:A:1203:G:P      | 19:S:77:THR:HG21  | 2.41                     | 0.60              |
| 4:D:19:LEU:O      | 4:D:20:TYR:C      | 2.44                     | 0.60              |
| 4:D:104:VAL:HG21  | 4:D:140:VAL:HG21  | 1.83                     | 0.60              |
| 1:A:323:C:O2      | 1:A:323:C:H2'     | 2.02                     | 0.60              |
| 1:A:563:U:H2'     | 1:A:564:G:O4'     | 2.01                     | 0.60              |
| 1:A:1080:C:H2'    | 1:A:1081:G:C8     | 2.35                     | 0.60              |
| 2:B:226:ARG:HG2   | 2:B:226:ARG:HH11  | 1.66                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:105:VAL:HB    | 5:E:106:PRO:HD3  | 1.82                     | 0.60              |
| 13:M:22:ILE:HD12  | 13:M:25:ILE:HD12 | 1.83                     | 0.60              |
| 1:A:814:U:H2'     | 1:A:815:C:H6     | 1.66                     | 0.60              |
| 2:B:87:ARG:HD2    | 2:B:233:SER:CB   | 2.30                     | 0.60              |
| 3:C:76:VAL:O      | 3:C:83:ARG:HG2   | 2.01                     | 0.60              |
| 6:F:99:ALA:C      | 6:F:101:ALA:N    | 2.58                     | 0.60              |
| 13:M:122:LYS:HG2  | 23:X:40:C:H5'    | 1.84                     | 0.60              |
| 1:A:1077:U:H5''   | 1:A:1091:C:O2    | 2.01                     | 0.60              |
| 4:D:32:ALA:C      | 4:D:34:GLU:H     | 2.07                     | 0.60              |
| 10:J:6:ILE:HG22   | 10:J:98:ILE:CG2  | 2.20                     | 0.60              |
| 1:A:1118:U:H5''   | 1:A:1119:C:OP2   | 2.01                     | 0.60              |
| 7:G:29:LYS:HE2    | 7:G:29:LYS:HA    | 1.84                     | 0.60              |
| 10:J:40:LEU:HD11  | 10:J:71:LEU:HD23 | 1.83                     | 0.60              |
| 13:M:125:ARG:HH12 | 13:M:126:LYS:HG2 | 1.65                     | 0.60              |
| 21:V:24:ARG:O     | 21:V:25:LYS:HB2  | 2.01                     | 0.60              |
| 1:A:636:A:C5'     | 8:H:56:LYS:HE3   | 2.27                     | 0.60              |
| 1:A:242:G:OP2     | 17:Q:100:LYS:HB3 | 2.02                     | 0.60              |
| 1:A:930:G:H5'     | 1:A:942:A:H61    | 1.67                     | 0.60              |
| 3:C:135:LYS:NZ    | 5:E:50:GLU:HG2   | 2.17                     | 0.60              |
| 7:G:75:VAL:HG21   | 7:G:144:MET:HE3  | 1.84                     | 0.60              |
| 10:J:75:ILE:O     | 10:J:76:ASN:HB2  | 2.02                     | 0.60              |
| 1:A:388:A:C2'     | 1:A:389:G:H5''   | 2.31                     | 0.60              |
| 1:A:1113:G:H3'    | 1:A:1113:G:H8    | 1.67                     | 0.60              |
| 3:C:58:GLU:H      | 3:C:65:ALA:HB3   | 1.67                     | 0.60              |
| 9:I:33:PHE:C      | 9:I:35:GLU:H     | 2.10                     | 0.60              |
| 1:A:52:G:C5       | 1:A:355:A:C2     | 2.90                     | 0.60              |
| 3:C:155:GLY:HA3   | 3:C:163:ALA:HB1  | 1.84                     | 0.60              |
| 11:K:121:PRO:HG2  | 11:K:126:ARG:CG  | 2.32                     | 0.60              |
| 14:N:29:ARG:HG2   | 14:N:29:ARG:NH1  | 2.15                     | 0.60              |
| 16:P:81:ARG:NH1   | 16:P:83:GLU:HG3  | 2.16                     | 0.60              |
| 1:A:325:C:H6      | 1:A:325:C:H5''   | 1.66                     | 0.59              |
| 1:A:520:G:OP1     | 12:L:113:ARG:NH2 | 2.34                     | 0.59              |
| 1:A:680:U:H2'     | 1:A:681:G:H5'    | 1.83                     | 0.59              |
| 1:A:701:G:C5'     | 11:K:117:ASN:ND2 | 2.64                     | 0.59              |
| 1:A:1406:C:H2'    | 1:A:1407:U:C5'   | 2.31                     | 0.59              |
| 1:A:1509:U:H2'    | 1:A:1510:C:H5'   | 1.84                     | 0.59              |
| 11:K:48:ILE:O     | 11:K:48:ILE:HG22 | 2.00                     | 0.59              |
| 3:C:3:ASN:O       | 3:C:4:LYS:HB2    | 2.02                     | 0.59              |
| 3:C:12:LEU:HD21   | 14:N:51:GLY:CA   | 2.32                     | 0.59              |
| 10:J:78:ASN:HB2   | 10:J:81:THR:CB   | 2.32                     | 0.59              |
| 14:N:9:LYS:HD3    | 14:N:9:LYS:C     | 2.26                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:S:4:SER:O     | 19:S:5:LEU:HD23  | 2.02                     | 0.59              |
| 1:A:49:U:O4      | 1:A:359:A:C5     | 2.55                     | 0.59              |
| 1:A:1425:G:H5''  | 1:A:1426:A:H5'   | 0.81                     | 0.59              |
| 2:B:36:ARG:H     | 2:B:41:ILE:CD1   | 2.15                     | 0.59              |
| 2:B:142:LEU:O    | 2:B:146:GLN:HG3  | 2.02                     | 0.59              |
| 14:N:14:PRO:O    | 14:N:15:LYS:HB2  | 2.02                     | 0.59              |
| 18:R:38:GLU:H    | 18:R:38:GLU:CD   | 2.10                     | 0.59              |
| 19:S:15:LEU:HD23 | 19:S:15:LEU:N    | 2.14                     | 0.59              |
| 1:A:339:A:C4'    | 1:A:340:C:OP2    | 2.48                     | 0.59              |
| 13:M:3:ARG:HG2   | 13:M:9:ILE:HG13  | 1.85                     | 0.59              |
| 1:A:501:C:O2'    | 12:L:50:SER:HB3  | 2.02                     | 0.59              |
| 1:A:731:C:H5'    | 1:A:732:C:OP1    | 2.03                     | 0.59              |
| 1:A:959:U:H4'    | 1:A:960:A:O5'    | 2.01                     | 0.59              |
| 1:A:1373:U:H2'   | 1:A:1374:G:C8    | 2.37                     | 0.59              |
| 1:A:1426:A:H4'   | 1:A:1427:G:OP1   | 2.02                     | 0.59              |
| 3:C:76:VAL:O     | 3:C:83:ARG:HB3   | 2.02                     | 0.59              |
| 4:D:11:LEU:O     | 4:D:15:GLU:HG2   | 2.01                     | 0.59              |
| 6:F:23:LYS:NZ    | 6:F:42:GLU:OE2   | 2.33                     | 0.59              |
| 12:L:60:LEU:HB2  | 12:L:64:TYR:O    | 2.02                     | 0.59              |
| 1:A:645:G:H2'    | 1:A:646:A:C8     | 2.37                     | 0.59              |
| 1:A:937:U:O2'    | 1:A:1204:C:H4'   | 2.02                     | 0.59              |
| 1:A:1237:A:H1'   | 1:A:1239:G:O4'   | 2.02                     | 0.59              |
| 6:F:82:ARG:HA    | 6:F:82:ARG:HE    | 1.66                     | 0.59              |
| 7:G:65:ALA:O     | 7:G:69:VAL:HG23  | 2.03                     | 0.59              |
| 9:I:11:LYS:O     | 9:I:11:LYS:HG2   | 2.03                     | 0.59              |
| 12:L:24:VAL:HG23 | 12:L:24:VAL:O    | 2.02                     | 0.59              |
| 1:A:1108:U:H2'   | 1:A:1109:G:C5'   | 2.33                     | 0.59              |
| 1:A:1231:A:H4'   | 9:I:68:GLY:N     | 2.17                     | 0.59              |
| 3:C:132:ARG:O    | 3:C:136:GLN:HG3  | 2.01                     | 0.59              |
| 4:D:146:ILE:N    | 4:D:146:ILE:HD12 | 2.17                     | 0.59              |
| 19:S:49:ILE:N    | 19:S:49:ILE:HD12 | 2.18                     | 0.59              |
| 1:A:402:G:H2'    | 1:A:403:A:H8     | 1.66                     | 0.59              |
| 1:A:1262:U:H4'   | 1:A:1263:C:OP2   | 2.03                     | 0.59              |
| 1:A:274:A:H5''   | 1:A:275:C:H3'    | 1.82                     | 0.59              |
| 1:A:1035:G:C4'   | 1:A:1036:C:H5'   | 2.16                     | 0.59              |
| 7:G:141:VAL:O    | 7:G:144:MET:HB2  | 2.03                     | 0.59              |
| 1:A:260:G:O2'    | 1:A:261:G:H5'    | 2.02                     | 0.59              |
| 1:A:821:G:H22    | 1:A:825:C:N4     | 1.92                     | 0.59              |
| 1:A:1039:G:H5''  | 3:C:154:SER:CB   | 2.33                     | 0.59              |
| 1:A:1206:A:H5'   | 13:M:103:THR:OG1 | 2.03                     | 0.59              |
| 5:E:152:ARG:HA   | 8:H:64:LYS:HZ3   | 1.67                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:17:ASP:C    | 10:J:19:SER:H     | 2.11                     | 0.59              |
| 20:T:10:LEU:HD12 | 20:T:12:ALA:CB    | 2.33                     | 0.59              |
| 9:I:127:LYS:HE2  | 13:M:126:LYS:HE2  | 1.85                     | 0.58              |
| 10:J:80:LYS:HA   | 10:J:83:GLU:OE1   | 2.03                     | 0.58              |
| 1:A:701:G:H4'    | 11:K:117:ASN:HD21 | 1.68                     | 0.58              |
| 1:A:1243:C:H42   | 1:A:1254:G:H1     | 1.48                     | 0.58              |
| 2:B:178:ARG:HH21 | 2:B:196:LEU:C     | 2.12                     | 0.58              |
| 3:C:15:THR:O     | 3:C:16:ARG:HB2    | 2.03                     | 0.58              |
| 3:C:189:ALA:O    | 3:C:191:THR:HG23  | 2.03                     | 0.58              |
| 4:D:63:LYS:HD2   | 4:D:198:VAL:HG12  | 1.86                     | 0.58              |
| 11:K:34:ASP:O    | 11:K:36:ASP:N     | 2.36                     | 0.58              |
| 13:M:52:GLU:HG2  | 13:M:55:ARG:HH21  | 1.68                     | 0.58              |
| 19:S:12:ASP:HB2  | 19:S:35:SER:OG    | 2.03                     | 0.58              |
| 1:A:238:A:H5''   | 1:A:239:U:H5'     | 1.85                     | 0.58              |
| 1:A:350:C:O4'    | 1:A:383:G:O2'     | 2.20                     | 0.58              |
| 1:A:48:C:C2'     | 1:A:49:U:OP1      | 2.52                     | 0.58              |
| 1:A:562:G:C5'    | 1:A:711:A:H1'     | 2.32                     | 0.58              |
| 1:A:1206:A:H5''  | 1:A:1207:C:C5     | 2.38                     | 0.58              |
| 2:B:102:LEU:HD21 | 2:B:162:ILE:CD1   | 2.32                     | 0.58              |
| 2:B:124:SER:O    | 2:B:127:ILE:HG13  | 2.03                     | 0.58              |
| 3:C:19:GLU:O     | 3:C:40:ARG:NH2    | 2.36                     | 0.58              |
| 10:J:24:VAL:HG12 | 10:J:24:VAL:O     | 2.04                     | 0.58              |
| 10:J:71:LEU:O    | 10:J:72:VAL:HB    | 2.03                     | 0.58              |
| 1:A:406:A:C4     | 1:A:408:G:H1'     | 2.37                     | 0.58              |
| 1:A:1316:C:O2'   | 1:A:1317:C:OP2    | 2.18                     | 0.58              |
| 2:B:91:PRO:HG2   | 2:B:155:LEU:HD23  | 1.86                     | 0.58              |
| 12:L:115:LYS:O   | 12:L:117:ARG:N    | 2.32                     | 0.58              |
| 1:A:388:A:C2'    | 1:A:389:G:C5'     | 2.82                     | 0.58              |
| 1:A:656:G:H2'    | 1:A:657:G:C8      | 2.38                     | 0.58              |
| 1:A:1237:A:H2'   | 1:A:1238:U:C5'    | 2.32                     | 0.58              |
| 2:B:82:ARG:HB2   | 2:B:94:ASN:HD22   | 1.69                     | 0.58              |
| 2:B:209:ARG:HH21 | 2:B:239:VAL:CG2   | 2.15                     | 0.58              |
| 10:J:78:ASN:O    | 10:J:82:ILE:HG13  | 2.04                     | 0.58              |
| 6:F:10:LEU:HD12  | 6:F:59:TYR:O      | 2.02                     | 0.58              |
| 15:O:45:VAL:O    | 15:O:46:HIS:C     | 2.47                     | 0.58              |
| 16:P:11:SER:OG   | 16:P:14:ASN:HB3   | 2.03                     | 0.58              |
| 3:C:139:GLN:CA   | 3:C:139:GLN:HE21  | 2.15                     | 0.58              |
| 3:C:148:GLY:HA3  | 3:C:172:ARG:O     | 2.03                     | 0.58              |
| 4:D:32:ALA:O     | 4:D:36:ARG:HB3    | 2.02                     | 0.58              |
| 8:H:10:LEU:HD12  | 8:H:85:ARG:HG2    | 1.84                     | 0.58              |
| 10:J:4:ILE:HG13  | 10:J:74:ILE:O     | 2.03                     | 0.58              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 14:N:9:LYS:HG3  | 14:N:22:THR:O    | 2.04                     | 0.58              |
| 1:A:446:A:HO2'  | 1:A:447:A:C5'    | 2.15                     | 0.58              |
| 1:A:1105:A:H2   | 10:J:39:PRO:HG3  | 1.69                     | 0.58              |
| 1:A:1351:C:H2'  | 1:A:1352:G:C8    | 2.39                     | 0.58              |
| 1:A:211:G:H2'   | 1:A:212:C:H6     | 1.68                     | 0.58              |
| 2:B:10:LEU:O    | 2:B:12:GLU:N     | 2.32                     | 0.58              |
| 2:B:108:ILE:O   | 2:B:108:ILE:HG22 | 2.04                     | 0.58              |
| 3:C:155:GLY:O   | 3:C:156:ARG:HB2  | 2.03                     | 0.58              |
| 7:G:59:LEU:HG   | 7:G:63:LYS:HE2   | 1.85                     | 0.58              |
| 12:L:40:VAL:O   | 12:L:40:VAL:HG12 | 2.03                     | 0.58              |
| 15:O:56:LEU:HA  | 15:O:59:MET:HE2  | 1.86                     | 0.58              |
| 1:A:208:U:OP2   | 1:A:209:U:OP2    | 2.22                     | 0.57              |
| 1:A:413:C:H2'   | 1:A:414:C:C6     | 2.39                     | 0.57              |
| 1:A:542:A:OP1   | 5:E:126:ARG:NH2  | 2.37                     | 0.57              |
| 1:A:1054:G:H2'  | 1:A:1055:U:C6    | 2.39                     | 0.57              |
| 9:I:46:ALA:O    | 9:I:49:PRO:HD2   | 2.04                     | 0.57              |
| 10:J:20:ALA:HB1 | 10:J:37:PRO:HG3  | 1.86                     | 0.57              |
| 1:A:264:C:H2'   | 1:A:265:A:C8     | 2.38                     | 0.57              |
| 1:A:504:G:OP1   | 12:L:73:GLU:O    | 2.22                     | 0.57              |
| 1:A:981:G:H2'   | 1:A:982:A:O4'    | 2.04                     | 0.57              |
| 1:A:1157:A:H2'  | 1:A:1158:G:C8    | 2.38                     | 0.57              |
| 3:C:6:HIS:HD2   | 3:C:8:ILE:H      | 1.51                     | 0.57              |
| 10:J:6:ILE:CG2  | 10:J:98:ILE:HG22 | 2.22                     | 0.57              |
| 13:M:8:GLU:C    | 13:M:9:ILE:HD12  | 2.29                     | 0.57              |
| 1:A:1449:U:H2'  | 1:A:1450:A:C8    | 2.39                     | 0.57              |
| 2:B:114:ARG:NH1 | 2:B:118:LEU:HD21 | 2.20                     | 0.57              |
| 7:G:69:VAL:HG21 | 7:G:104:LEU:HD21 | 1.86                     | 0.57              |
| 11:K:12:ARG:N   | 11:K:12:ARG:HD2  | 2.19                     | 0.57              |
| 1:A:446:A:O2'   | 1:A:447:A:O5'    | 2.22                     | 0.57              |
| 3:C:34:LEU:O    | 3:C:38:ARG:HG2   | 2.04                     | 0.57              |
| 6:F:2:ARG:HH21  | 6:F:69:GLU:HG2   | 1.69                     | 0.57              |
| 8:H:64:LYS:HG2  | 8:H:79:VAL:HG21  | 1.87                     | 0.57              |
| 9:I:4:TYR:CD2   | 9:I:88:TYR:HA    | 2.39                     | 0.57              |
| 17:Q:92:ARG:HG3 | 17:Q:92:ARG:HH11 | 1.70                     | 0.57              |
| 19:S:28:LYS:HD3 | 19:S:29:ARG:N    | 2.18                     | 0.57              |
| 1:A:1447:G:O2'  | 1:A:1448:G:H5'   | 2.04                     | 0.57              |
| 3:C:8:ILE:HG23  | 3:C:16:ARG:HG2   | 1.87                     | 0.57              |
| 1:A:416:U:H5'   | 1:A:417:C:H5     | 1.69                     | 0.57              |
| 1:A:1036:C:H6   | 1:A:1036:C:H5"   | 1.70                     | 0.57              |
| 1:A:1221:U:O2'  | 1:A:1222:G:OP1   | 2.21                     | 0.57              |
| 5:E:92:LYS:HB3  | 5:E:119:LEU:HB2  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:113:GLU:HG2  | 7:G:119:ARG:HG2  | 1.87                     | 0.57              |
| 20:T:36:LEU:HD12 | 20:T:62:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:269:A:O2'    | 1:A:270:G:H8     | 1.88                     | 0.57              |
| 1:A:450:C:H2'    | 1:A:451:C:H6     | 1.70                     | 0.57              |
| 1:A:484:C:H2'    | 1:A:485:G:C8     | 2.40                     | 0.57              |
| 1:A:984:C:H3'    | 1:A:984:C:C6     | 2.39                     | 0.57              |
| 7:G:46:ALA:O     | 7:G:50:ILE:HG13  | 2.04                     | 0.57              |
| 20:T:53:LEU:HD13 | 20:T:102:GLY:H   | 1.70                     | 0.57              |
| 1:A:748:G:H22    | 1:A:795:C:HO2'   | 1.50                     | 0.57              |
| 1:A:774:G:C2'    | 1:A:775:A:H5'    | 2.34                     | 0.57              |
| 2:B:81:VAL:HG22  | 2:B:215:LEU:HD11 | 1.85                     | 0.57              |
| 4:D:151:LYS:HD2  | 4:D:151:LYS:H    | 1.68                     | 0.57              |
| 6:F:22:GLU:OE2   | 6:F:25:ILE:HD12  | 2.05                     | 0.57              |
| 7:G:155:ARG:NH1  | 7:G:155:ARG:HA   | 2.19                     | 0.57              |
| 1:A:589:G:H2'    | 1:A:614:G:N1     | 2.18                     | 0.57              |
| 1:A:952:A:H5'    | 1:A:952:A:H8     | 1.68                     | 0.57              |
| 3:C:19:GLU:HA    | 3:C:54:ARG:HH21  | 1.69                     | 0.57              |
| 6:F:91:VAL:HG12  | 6:F:92:LYS:N     | 2.18                     | 0.57              |
| 1:A:198:U:C1'    | 20:T:103:GLY:HA2 | 2.35                     | 0.56              |
| 1:A:705:A:H1'    | 1:A:706:U:C6     | 2.40                     | 0.56              |
| 1:A:1509:U:H2'   | 1:A:1510:C:O5'   | 2.04                     | 0.56              |
| 4:D:64:LEU:HD21  | 4:D:97:LEU:HD13  | 1.87                     | 0.56              |
| 6:F:37:VAL:HA    | 6:F:65:VAL:HG12  | 1.87                     | 0.56              |
| 10:J:90:LEU:H    | 10:J:91:PRO:CD   | 2.06                     | 0.56              |
| 11:K:27:ASN:OD1  | 11:K:55:LYS:HB3  | 2.05                     | 0.56              |
| 1:A:404:G:H5''   | 4:D:24:GLU:HB2   | 1.88                     | 0.56              |
| 1:A:637:G:C5     | 1:A:638:A:C8     | 2.93                     | 0.56              |
| 1:A:1219:A:C5'   | 1:A:1317:C:H41   | 2.10                     | 0.56              |
| 2:B:119:GLU:HG2  | 2:B:142:LEU:HD11 | 1.86                     | 0.56              |
| 3:C:154:SER:O    | 3:C:164:ARG:O    | 2.22                     | 0.56              |
| 4:D:98:GLU:HA    | 4:D:103:ASN:ND2  | 2.21                     | 0.56              |
| 6:F:2:ARG:CZ     | 6:F:69:GLU:HG2   | 2.35                     | 0.56              |
| 6:F:2:ARG:NH2    | 6:F:69:GLU:HG2   | 2.19                     | 0.56              |
| 13:M:88:ARG:HH11 | 19:S:3:ARG:NH2   | 2.02                     | 0.56              |
| 19:S:17:GLU:O    | 19:S:21:GLU:HG3  | 2.05                     | 0.56              |
| 19:S:27:GLU:O    | 19:S:28:LYS:HB2  | 2.05                     | 0.56              |
| 1:A:125:C:H2'    | 1:A:126:C:C6     | 2.41                     | 0.56              |
| 1:A:188:U:O2'    | 1:A:189:U:O5'    | 2.19                     | 0.56              |
| 1:A:347:C:H4'    | 1:A:349:G:OP1    | 2.04                     | 0.56              |
| 1:A:501:C:HO2'   | 12:L:50:SER:HB3  | 1.70                     | 0.56              |
| 1:A:685:A:H4'    | 1:A:686:G:OP2    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:821:G:H2'    | 1:A:822:U:H5''   | 1.87                     | 0.56              |
| 1:A:931:G:H21    | 1:A:1208:A:H62   | 1.52                     | 0.56              |
| 1:A:1218:C:H3'   | 1:A:1219:A:H5'   | 1.88                     | 0.56              |
| 3:C:107:GLN:O    | 3:C:108:ASN:HB3  | 2.05                     | 0.56              |
| 4:D:112:VAL:HG22 | 4:D:116:GLN:OE1  | 2.05                     | 0.56              |
| 4:D:150:GLU:HA   | 4:D:153:ARG:HG3  | 1.87                     | 0.56              |
| 7:G:23:VAL:O     | 7:G:27:ILE:HG13  | 2.05                     | 0.56              |
| 8:H:10:LEU:HD22  | 8:H:83:ILE:HD11  | 1.87                     | 0.56              |
| 12:L:45:PRO:HD3  | 12:L:51:ALA:O    | 2.06                     | 0.56              |
| 19:S:33:THR:CG2  | 19:S:34:TRP:N    | 2.68                     | 0.56              |
| 1:A:602:U:O2     | 4:D:133:VAL:HA   | 2.05                     | 0.56              |
| 2:B:140:HIS:O    | 2:B:143:GLU:HB2  | 2.05                     | 0.56              |
| 9:I:58:ARG:HG2   | 9:I:58:ARG:HH11  | 1.70                     | 0.56              |
| 16:P:4:ILE:HG13  | 16:P:64:ALA:HB1  | 1.88                     | 0.56              |
| 1:A:49:U:C4      | 1:A:359:A:C5     | 2.93                     | 0.56              |
| 1:A:678:A:OP1    | 11:K:52:GLY:HA3  | 2.05                     | 0.56              |
| 2:B:36:ARG:H     | 2:B:41:ILE:HD11  | 1.69                     | 0.56              |
| 1:A:1345:A:H1'   | 1:A:1347:G:N7    | 2.20                     | 0.56              |
| 3:C:34:LEU:O     | 3:C:34:LEU:HD12  | 2.06                     | 0.56              |
| 4:D:92:VAL:O     | 4:D:96:LEU:HD13  | 2.06                     | 0.56              |
| 4:D:152:SER:HB3  | 4:D:155:LEU:HD12 | 1.88                     | 0.56              |
| 5:E:57:LYS:HG2   | 5:E:61:TYR:HE2   | 1.67                     | 0.56              |
| 1:A:1107:U:OP1   | 10:J:38:ILE:HD11 | 2.06                     | 0.56              |
| 1:A:1206:A:H5''  | 1:A:1207:C:H5    | 1.71                     | 0.56              |
| 1:A:1253:G:C2'   | 1:A:1254:G:H5'   | 2.36                     | 0.56              |
| 1:A:1253:G:H2'   | 1:A:1254:G:H5'   | 1.86                     | 0.56              |
| 5:E:36:ASP:CG    | 5:E:40:ARG:HB2   | 2.31                     | 0.56              |
| 9:I:11:LYS:O     | 9:I:12:GLU:CB    | 2.54                     | 0.56              |
| 9:I:125:TYR:HE1  | 9:I:128:ARG:HB3  | 1.70                     | 0.56              |
| 17:Q:68:ARG:HG3  | 17:Q:68:ARG:NH1  | 2.19                     | 0.56              |
| 1:A:1113:G:H2'   | 1:A:1114:C:O4'   | 2.06                     | 0.56              |
| 1:A:1215:C:H5'   | 1:A:1347:G:OP1   | 2.06                     | 0.56              |
| 19:S:13:ASP:O    | 19:S:17:GLU:HG2  | 2.05                     | 0.56              |
| 1:A:1193:U:H3'   | 1:A:1193:U:C6    | 2.40                     | 0.56              |
| 2:B:47:THR:HA    | 2:B:202:PRO:HG2  | 1.88                     | 0.56              |
| 2:B:60:ASP:OD1   | 2:B:64:ARG:NH2   | 2.39                     | 0.56              |
| 3:C:5:ILE:O      | 3:C:5:ILE:HD12   | 2.06                     | 0.56              |
| 6:F:101:ALA:HB2  | 18:R:28:GLU:CA   | 2.32                     | 0.56              |
| 10:J:26:ALA:CB   | 10:J:81:THR:HG23 | 2.35                     | 0.56              |
| 13:M:23:TYR:CB   | 13:M:67:GLU:HA   | 2.36                     | 0.56              |
| 20:T:96:GLY:O    | 20:T:97:ALA:HB3  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:124:A:H1'    | 1:A:258:A:O2'    | 2.06                     | 0.56              |
| 1:A:494:C:HO2'   | 1:A:495:U:C5'    | 2.18                     | 0.56              |
| 1:A:1042:C:C5    | 3:C:2:GLY:HA2    | 2.41                     | 0.56              |
| 8:H:4:ASP:CG     | 8:H:85:ARG:HH11  | 2.14                     | 0.56              |
| 13:M:6:GLY:O     | 13:M:8:GLU:HG2   | 2.05                     | 0.56              |
| 1:A:736:A:H4'    | 1:A:737:C:O5'    | 2.06                     | 0.55              |
| 12:L:27:LEU:C    | 12:L:29:GLY:H    | 2.13                     | 0.55              |
| 16:P:34:GLU:OE2  | 16:P:55:ARG:HD3  | 2.06                     | 0.55              |
| 22:W:1:A:H2'     | 22:W:2:A:H5'     | 1.87                     | 0.55              |
| 1:A:951:A:OP2    | 14:N:41:ARG:NH1  | 2.38                     | 0.55              |
| 12:L:119:LYS:O   | 12:L:120:TYR:HB2 | 2.07                     | 0.55              |
| 14:N:12:ARG:HA   | 14:N:12:ARG:NH1  | 2.21                     | 0.55              |
| 21:V:6:ARG:CD    | 21:V:15:ARG:HH12 | 2.19                     | 0.55              |
| 1:A:408:G:H2'    | 1:A:423:G:H21    | 1.71                     | 0.55              |
| 1:A:701:G:C4'    | 11:K:117:ASN:ND2 | 2.68                     | 0.55              |
| 1:A:1278:C:H1'   | 1:A:1279:C:H5    | 1.71                     | 0.55              |
| 2:B:111:ARG:HB3  | 2:B:149:LEU:HD11 | 1.87                     | 0.55              |
| 9:I:23:ASN:O     | 9:I:57:GLY:HA2   | 2.07                     | 0.55              |
| 10:J:95:GLU:C    | 10:J:96:ILE:HD12 | 2.31                     | 0.55              |
| 1:A:51:A:OP2     | 1:A:52:G:H8      | 1.90                     | 0.55              |
| 1:A:106:G:C1'    | 1:A:349:G:H5'    | 2.36                     | 0.55              |
| 10:J:8:LEU:CB    | 10:J:70:ARG:HB2  | 2.24                     | 0.55              |
| 10:J:26:ALA:HB2  | 10:J:85:LEU:HD21 | 1.88                     | 0.55              |
| 17:Q:100:LYS:HD2 | 17:Q:101:ARG:HE  | 1.71                     | 0.55              |
| 1:A:123:G:O2'    | 1:A:189:U:H5''   | 2.06                     | 0.55              |
| 1:A:1126:G:H8    | 1:A:1126:G:H3'   | 1.72                     | 0.55              |
| 1:A:1204:C:OP1   | 1:A:1205:G:H3'   | 2.06                     | 0.55              |
| 1:A:1209:C:OP1   | 13:M:115:LYS:HE3 | 2.06                     | 0.55              |
| 1:A:1379:C:H4'   | 1:A:1380:A:OP2   | 2.05                     | 0.55              |
| 1:A:1499:U:O2'   | 1:A:1500:G:H5'   | 2.06                     | 0.55              |
| 2:B:114:ARG:NH1  | 2:B:118:LEU:HD11 | 2.20                     | 0.55              |
| 3:C:154:SER:OG   | 3:C:155:GLY:N    | 2.33                     | 0.55              |
| 5:E:101:ILE:HD12 | 5:E:119:LEU:HD23 | 1.88                     | 0.55              |
| 9:I:127:LYS:HD2  | 9:I:127:LYS:N    | 2.22                     | 0.55              |
| 20:T:43:LEU:HD13 | 20:T:51:GLU:HG3  | 1.88                     | 0.55              |
| 1:A:603:C:C1'    | 4:D:135:LEU:HD13 | 2.37                     | 0.55              |
| 1:A:952:A:C4'    | 1:A:953:G:H5''   | 2.36                     | 0.55              |
| 1:A:1093:A:N6    | 3:C:177:THR:HG22 | 2.22                     | 0.55              |
| 1:A:1202:G:O3'   | 19:S:77:THR:HG21 | 2.07                     | 0.55              |
| 1:A:1294:U:H5    | 19:S:4:SER:HB2   | 1.70                     | 0.55              |
| 3:C:188:LEU:O    | 3:C:189:ALA:HB2  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:46:ARG:HG2  | 10:J:46:ARG:NH1  | 2.19                     | 0.55              |
| 14:N:3:ARG:NH1   | 14:N:6:LEU:HD11  | 2.21                     | 0.55              |
| 15:O:71:GLN:HB2  | 15:O:78:TYR:CD1  | 2.42                     | 0.55              |
| 1:A:353:U:H2'    | 1:A:354:U:H6     | 1.72                     | 0.55              |
| 1:A:408:G:C2'    | 1:A:423:G:N2     | 2.67                     | 0.55              |
| 1:A:542:A:O2'    | 1:A:543:U:OP2    | 2.19                     | 0.55              |
| 1:A:1013:G:H2'   | 1:A:1014:G:C8    | 2.42                     | 0.55              |
| 1:A:1123:C:C2'   | 1:A:1124:G:H5'   | 2.37                     | 0.55              |
| 6:F:42:GLU:HG3   | 6:F:61:LEU:HD23  | 1.88                     | 0.55              |
| 18:R:87:ARG:O    | 18:R:88:LYS:HB2  | 2.06                     | 0.55              |
| 4:D:8:VAL:HG21   | 4:D:115:ARG:NH1  | 2.21                     | 0.55              |
| 7:G:23:VAL:HG13  | 7:G:43:PHE:CE2   | 2.42                     | 0.55              |
| 7:G:38:LEU:HD12  | 7:G:38:LEU:O     | 2.06                     | 0.55              |
| 9:I:11:LYS:O     | 9:I:12:GLU:HB3   | 2.06                     | 0.55              |
| 1:A:930:G:C5'    | 1:A:942:A:H61    | 2.20                     | 0.55              |
| 1:A:1113:G:C8    | 1:A:1113:G:C3'   | 2.89                     | 0.55              |
| 1:A:1119:C:H5'   | 1:A:1120:G:C6    | 2.42                     | 0.55              |
| 1:A:1259:U:C5'   | 1:A:1260:A:H5'   | 2.36                     | 0.55              |
| 2:B:118:LEU:CB   | 2:B:142:LEU:HD12 | 2.37                     | 0.55              |
| 2:B:189:ASP:HB3  | 2:B:203:GLY:O    | 2.07                     | 0.55              |
| 3:C:134:ILE:HD11 | 3:C:153:VAL:CG2  | 2.36                     | 0.55              |
| 13:M:81:LEU:O    | 13:M:86:CYS:HB3  | 2.07                     | 0.55              |
| 1:A:275:C:H4'    | 1:A:276:G:OP2    | 2.05                     | 0.55              |
| 1:A:1042:C:C6    | 3:C:2:GLY:HA2    | 2.41                     | 0.55              |
| 1:A:1267:A:H8    | 1:A:1268:A:H4'   | 1.71                     | 0.55              |
| 2:B:17:PHE:CD1   | 2:B:18:GLY:N     | 2.75                     | 0.55              |
| 7:G:13:GLN:NE2   | 7:G:14:PRO:HD2   | 2.21                     | 0.55              |
| 13:M:6:GLY:O     | 13:M:7:VAL:C     | 2.49                     | 0.55              |
| 1:A:776:U:H4'    | 1:A:777:A:OP2    | 2.07                     | 0.54              |
| 1:A:984:C:N4     | 1:A:1002:G:H21   | 2.01                     | 0.54              |
| 1:A:1036:C:H2'   | 1:A:1037:A:H5''  | 1.89                     | 0.54              |
| 5:E:64:ARG:HG2   | 5:E:64:ARG:NH1   | 2.17                     | 0.54              |
| 9:I:118:LYS:O    | 9:I:119:ALA:HB3  | 2.07                     | 0.54              |
| 10:J:45:ARG:O    | 10:J:64:GLU:HA   | 2.07                     | 0.54              |
| 11:K:12:ARG:O    | 11:K:13:GLN:C    | 2.50                     | 0.54              |
| 12:L:111:LYS:HG2 | 12:L:112:ASP:N   | 2.21                     | 0.54              |
| 1:A:1296:U:OP2   | 19:S:6:LYS:NZ    | 2.39                     | 0.54              |
| 4:D:158:ILE:HG22 | 4:D:181:MET:HE1  | 1.87                     | 0.54              |
| 6:F:69:GLU:HA    | 6:F:72:VAL:HG23  | 1.89                     | 0.54              |
| 11:K:11:LYS:C    | 11:K:12:ARG:HD2  | 2.32                     | 0.54              |
| 1:A:48:C:HO2'    | 1:A:49:U:P       | 2.19                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:500:G:O2'    | 1:A:501:C:OP2     | 2.19                     | 0.54              |
| 1:A:775:A:O2'    | 1:A:777:A:N7      | 2.39                     | 0.54              |
| 4:D:199:ASN:ND2  | 4:D:201:GLN:H     | 2.05                     | 0.54              |
| 20:T:100:ILE:O   | 20:T:101:GLY:C    | 2.51                     | 0.54              |
| 1:A:245:A:H4'    | 1:A:246:G:O5'     | 2.07                     | 0.54              |
| 1:A:415:U:O2'    | 1:A:416:U:H5''    | 2.07                     | 0.54              |
| 1:A:418:G:H2'    | 1:A:419:G:O4'     | 2.08                     | 0.54              |
| 1:A:1023:A:H2'   | 1:A:1024:G:C8     | 2.41                     | 0.54              |
| 1:A:1121:G:N2    | 1:A:1126:G:H22    | 2.06                     | 0.54              |
| 1:A:1348:C:H2'   | 1:A:1349:C:H6     | 1.72                     | 0.54              |
| 3:C:111:LEU:HD11 | 3:C:144:SER:O     | 2.07                     | 0.54              |
| 5:E:35:GLY:HA2   | 5:E:40:ARG:O      | 2.07                     | 0.54              |
| 7:G:120:ILE:H    | 7:G:120:ILE:HD12  | 1.72                     | 0.54              |
| 1:A:475:G:O2'    | 1:A:476:G:H5'     | 2.08                     | 0.54              |
| 1:A:611:G:H2'    | 1:A:612:G:C8      | 2.42                     | 0.54              |
| 1:A:1261:A:O4'   | 10:J:41:PRO:HG3   | 2.08                     | 0.54              |
| 2:B:59:GLU:O     | 2:B:63:MET:HG2    | 2.07                     | 0.54              |
| 9:I:43:ALA:O     | 9:I:45:ALA:N      | 2.41                     | 0.54              |
| 13:M:115:LYS:O   | 13:M:117:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:56:U:H2'     | 1:A:57:G:C8       | 2.43                     | 0.54              |
| 1:A:437:C:H2'    | 1:A:438:C:H6      | 1.73                     | 0.54              |
| 1:A:1046:G:O2'   | 1:A:1171:G:N2     | 2.39                     | 0.54              |
| 5:E:143:ARG:HH12 | 8:H:77:GLU:CD     | 2.15                     | 0.54              |
| 18:R:25:THR:HG22 | 18:R:42:ARG:HH12  | 1.72                     | 0.54              |
| 1:A:637:G:O6     | 1:A:638:A:C6      | 2.61                     | 0.54              |
| 6:F:10:LEU:HD12  | 6:F:10:LEU:N      | 2.22                     | 0.54              |
| 10:J:51:ARG:HG3  | 10:J:59:SER:OG    | 2.07                     | 0.54              |
| 17:Q:45:HIS:NE2  | 17:Q:47:PRO:HG3   | 2.22                     | 0.54              |
| 1:A:1036:C:N3    | 23:X:34:70U:H4'   | 2.22                     | 0.54              |
| 1:A:1123:C:H2'   | 1:A:1124:G:C5'    | 2.37                     | 0.54              |
| 7:G:16:LEU:HD22  | 7:G:16:LEU:N      | 2.23                     | 0.54              |
| 1:A:1197:G:O2'   | 1:A:1198:C:H5'    | 2.08                     | 0.54              |
| 1:A:1220:A:H4'   | 1:A:1221:U:O5'    | 2.08                     | 0.54              |
| 19:S:7:LYS:O     | 19:S:7:LYS:CD     | 2.56                     | 0.54              |
| 1:A:316:A:H4'    | 1:A:1417:G:O2'    | 2.08                     | 0.54              |
| 1:A:352:G:O2'    | 1:A:353:U:H5'     | 2.08                     | 0.54              |
| 1:A:455:C:O2'    | 1:A:456:G:OP1     | 2.23                     | 0.54              |
| 1:A:500:G:H5'    | 1:A:502:C:C2      | 2.43                     | 0.54              |
| 1:A:748:G:H1     | 1:A:795:C:HO2'    | 1.55                     | 0.54              |
| 1:A:1304:G:H2'   | 1:A:1305:A:C8     | 2.43                     | 0.54              |
| 2:B:17:PHE:HA    | 2:B:44:LEU:CD2    | 2.38                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:69:LEU:HD12  | 2:B:155:LEU:HD11 | 1.89                     | 0.54              |
| 2:B:142:LEU:C    | 2:B:142:LEU:HD23 | 2.33                     | 0.54              |
| 3:C:167:TRP:O    | 3:C:168:ALA:HB3  | 2.08                     | 0.54              |
| 6:F:98:LEU:HD22  | 6:F:101:ALA:HB3  | 1.90                     | 0.54              |
| 7:G:144:MET:O    | 7:G:147:ALA:HB3  | 2.08                     | 0.54              |
| 10:J:60:ARG:HG2  | 10:J:60:ARG:HH11 | 1.73                     | 0.54              |
| 11:K:69:ALA:O    | 11:K:73:MET:HG2  | 2.08                     | 0.54              |
| 13:M:23:TYR:O    | 13:M:25:ILE:N    | 2.41                     | 0.54              |
| 13:M:34:LEU:CD1  | 13:M:41:PRO:HA   | 2.37                     | 0.54              |
| 1:A:636:A:H5'    | 8:H:56:LYS:CE    | 2.33                     | 0.53              |
| 1:A:670:A:N6     | 1:A:686:G:H1'    | 2.23                     | 0.53              |
| 1:A:1062:A:H5''  | 5:E:16:THR:HG21  | 1.89                     | 0.53              |
| 1:A:1254:G:H2'   | 1:A:1255:G:O4'   | 2.08                     | 0.53              |
| 1:A:1281:G:O2'   | 1:A:1282:U:P     | 2.66                     | 0.53              |
| 2:B:9:GLU:HG2    | 2:B:217:ARG:CZ   | 2.37                     | 0.53              |
| 2:B:213:LEU:O    | 2:B:217:ARG:HG2  | 2.07                     | 0.53              |
| 15:O:6:GLU:H     | 15:O:6:GLU:CD    | 2.15                     | 0.53              |
| 15:O:78:TYR:CZ   | 15:O:82:ILE:HD11 | 2.42                     | 0.53              |
| 1:A:396:C:H1'    | 1:A:605:A:H1'    | 1.90                     | 0.53              |
| 1:A:1236:G:H1    | 1:A:1263:C:N4    | 2.05                     | 0.53              |
| 5:E:148:VAL:O    | 5:E:152:ARG:HG3  | 2.08                     | 0.53              |
| 20:T:57:ARG:NH2  | 20:T:102:GLY:HA2 | 2.23                     | 0.53              |
| 1:A:201:A:H4'    | 20:T:68:LYS:CE   | 2.36                     | 0.53              |
| 1:A:637:G:C4     | 1:A:638:A:C8     | 2.97                     | 0.53              |
| 1:A:1014:G:H2'   | 1:A:1015:G:H5'   | 1.90                     | 0.53              |
| 1:A:1236:G:H1    | 1:A:1263:C:H42   | 1.56                     | 0.53              |
| 2:B:84:GLU:HB3   | 2:B:219:VAL:HG21 | 1.90                     | 0.53              |
| 4:D:199:ASN:HD21 | 4:D:201:GLN:HB3  | 1.72                     | 0.53              |
| 5:E:101:ILE:O    | 5:E:120:THR:HB   | 2.08                     | 0.53              |
| 7:G:120:ILE:HD12 | 7:G:120:ILE:N    | 2.24                     | 0.53              |
| 17:Q:67:LYS:O    | 17:Q:69:LYS:N    | 2.39                     | 0.53              |
| 19:S:44:MET:O    | 19:S:62:ILE:HG21 | 2.07                     | 0.53              |
| 2:B:108:ILE:O    | 2:B:108:ILE:CG2  | 2.56                     | 0.53              |
| 2:B:144:ARG:HA   | 2:B:147:LYS:CD   | 2.37                     | 0.53              |
| 5:E:99:GLY:O     | 5:E:117:ASP:HA   | 2.09                     | 0.53              |
| 5:E:144:THR:O    | 5:E:148:VAL:HG23 | 2.08                     | 0.53              |
| 6:F:30:LEU:HB3   | 6:F:35:ALA:HB3   | 1.91                     | 0.53              |
| 7:G:113:GLU:CG   | 7:G:119:ARG:HG2  | 2.38                     | 0.53              |
| 10:J:12:ASP:O    | 10:J:15:THR:HG22 | 2.09                     | 0.53              |
| 12:L:33:ARG:HG2  | 12:L:60:LEU:HG   | 1.91                     | 0.53              |
| 1:A:79:U:C6      | 1:A:79:U:C3'     | 2.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:738:G:OP2    | 15:O:65:ARG:HG2   | 2.08                     | 0.53              |
| 1:A:1063:G:H5'   | 5:E:18:ARG:HG3    | 1.90                     | 0.53              |
| 2:B:212:GLN:HE22 | 2:B:235:SER:CB    | 2.20                     | 0.53              |
| 5:E:87:SER:HB3   | 5:E:131:ILE:HD13  | 1.90                     | 0.53              |
| 7:G:146:GLU:HA   | 7:G:149:ARG:HG2   | 1.90                     | 0.53              |
| 18:R:87:ARG:HD2  | 18:R:88:LYS:H     | 1.74                     | 0.53              |
| 20:T:50:GLU:H    | 20:T:99:LEU:HD12  | 1.73                     | 0.53              |
| 1:A:377:A:H2'    | 1:A:378:A:C8      | 2.43                     | 0.53              |
| 1:A:484:C:H2'    | 1:A:485:G:H8      | 1.73                     | 0.53              |
| 1:A:600:G:H5'    | 16:P:45:THR:HG22  | 1.89                     | 0.53              |
| 1:A:648:A:N3     | 1:A:715:C:H2'     | 2.24                     | 0.53              |
| 2:B:28:PHE:HE2   | 2:B:42:ILE:HD12   | 1.72                     | 0.53              |
| 10:J:47:PHE:HD2  | 14:N:34:TYR:CD2   | 2.26                     | 0.53              |
| 15:O:60:VAL:O    | 15:O:64:ARG:HG2   | 2.08                     | 0.53              |
| 1:A:811:A:H2'    | 1:A:812:G:O4'     | 2.08                     | 0.53              |
| 1:A:1004:G:H2'   | 1:A:1005:C:H5'    | 1.90                     | 0.53              |
| 1:A:1238:U:OP2   | 3:C:27:LYS:HE3    | 2.08                     | 0.53              |
| 1:A:1288:U:H2'   | 1:A:1289:U:C6     | 2.44                     | 0.53              |
| 3:C:58:GLU:O     | 3:C:59:ARG:HG2    | 2.09                     | 0.53              |
| 4:D:31:CYS:O     | 4:D:33:MET:N      | 2.35                     | 0.53              |
| 4:D:64:LEU:HD22  | 4:D:75:PHE:HE1    | 1.73                     | 0.53              |
| 8:H:9:MET:HG3    | 8:H:26:VAL:HG21   | 1.91                     | 0.53              |
| 11:K:101:SER:O   | 11:K:103:LEU:N    | 2.42                     | 0.53              |
| 12:L:59:ARG:HH11 | 12:L:65:GLU:HG3   | 1.73                     | 0.53              |
| 20:T:69:GLY:O    | 20:T:73:HIS:CD2   | 2.62                     | 0.53              |
| 20:T:86:ARG:HH11 | 20:T:86:ARG:HG2   | 1.72                     | 0.53              |
| 1:A:17:U:H1'     | 1:A:1062:A:N3     | 2.24                     | 0.53              |
| 1:A:50:A:N6      | 1:A:356:G:C4'     | 2.67                     | 0.53              |
| 3:C:99:VAL:HG23  | 3:C:99:VAL:O      | 2.09                     | 0.53              |
| 4:D:52:SER:O     | 4:D:53:ASP:C      | 2.51                     | 0.53              |
| 4:D:121:VAL:O    | 4:D:134:ASP:HA    | 2.09                     | 0.53              |
| 9:I:10:ARG:HG2   | 9:I:75:ASP:HB2    | 1.89                     | 0.53              |
| 12:L:78:GLN:C    | 12:L:80:HIS:H     | 2.17                     | 0.53              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N     | 2.24                     | 0.53              |
| 1:A:125:C:H2'    | 1:A:126:C:H6      | 1.73                     | 0.53              |
| 4:D:199:ASN:HD21 | 4:D:201:GLN:CB    | 2.22                     | 0.53              |
| 12:L:42:THR:HG21 | 12:L:52:LEU:HB3   | 1.91                     | 0.53              |
| 18:R:25:THR:CG2  | 18:R:42:ARG:HH12  | 2.23                     | 0.53              |
| 20:T:67:ALA:O    | 20:T:73:HIS:ND1   | 2.42                     | 0.53              |
| 1:A:925:C:OP1    | 13:M:109:THR:HG22 | 2.09                     | 0.52              |
| 1:A:1125:G:H8    | 1:A:1125:G:O5'    | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1170:C:OP1   | 10:J:51:ARG:NH2  | 2.42                     | 0.52              |
| 1:A:1262:U:H5'   | 1:A:1263:C:C5    | 2.42                     | 0.52              |
| 3:C:13:GLY:HA3   | 14:N:57:ARG:HH21 | 1.74                     | 0.52              |
| 3:C:156:ARG:H    | 3:C:163:ALA:HA   | 1.73                     | 0.52              |
| 17:Q:96:GLN:HB2  | 17:Q:105:ALA:HB2 | 1.91                     | 0.52              |
| 1:A:425:A:H2'    | 1:A:426:A:H5'    | 1.91                     | 0.52              |
| 7:G:75:VAL:CG2   | 7:G:144:MET:HE3  | 2.39                     | 0.52              |
| 8:H:68:ARG:HG2   | 8:H:68:ARG:HH11  | 1.73                     | 0.52              |
| 9:I:5:TYR:CG     | 9:I:6:GLY:N      | 2.77                     | 0.52              |
| 18:R:19:LYS:HE2  | 18:R:54:ARG:CZ   | 2.39                     | 0.52              |
| 1:A:1286:G:H22   | 1:A:1312:G:H2'   | 1.74                     | 0.52              |
| 2:B:25:ASN:ND2   | 2:B:27:LYS:H     | 2.07                     | 0.52              |
| 3:C:84:ILE:HG13  | 3:C:88:ARG:NH1   | 2.23                     | 0.52              |
| 4:D:70:ILE:HG22  | 4:D:71:SER:O     | 2.10                     | 0.52              |
| 4:D:122:ARG:NH2  | 4:D:134:ASP:OD2  | 2.42                     | 0.52              |
| 12:L:87:GLY:HA2  | 12:L:98:TYR:HA   | 1.90                     | 0.52              |
| 1:A:353:U:H2'    | 1:A:354:U:C6     | 2.44                     | 0.52              |
| 1:A:472:C:O5'    | 1:A:472:C:H6     | 1.92                     | 0.52              |
| 1:A:1084:A:H2'   | 1:A:1085:C:C6    | 2.45                     | 0.52              |
| 2:B:84:GLU:OE1   | 2:B:216:SER:HA   | 2.09                     | 0.52              |
| 2:B:92:TYR:HH    | 2:B:150:SER:HG   | 1.57                     | 0.52              |
| 4:D:199:ASN:HD22 | 4:D:199:ASN:C    | 2.16                     | 0.52              |
| 6:F:91:VAL:CG1   | 6:F:92:LYS:N     | 2.72                     | 0.52              |
| 8:H:13:ILE:O     | 8:H:17:THR:HG23  | 2.08                     | 0.52              |
| 18:R:88:LYS:HB3  | 18:R:88:LYS:HZ2  | 1.74                     | 0.52              |
| 1:A:1110:C:C5'   | 9:I:16:ARG:NH2   | 2.72                     | 0.52              |
| 2:B:71:VAL:CG2   | 2:B:164:VAL:HG22 | 2.39                     | 0.52              |
| 2:B:91:PRO:HG3   | 2:B:154:LEU:HB2  | 1.91                     | 0.52              |
| 3:C:23:TYR:CD2   | 3:C:24:ALA:N     | 2.77                     | 0.52              |
| 4:D:32:ALA:C     | 4:D:34:GLU:N     | 2.63                     | 0.52              |
| 9:I:95:LYS:O     | 9:I:98:PRO:HD2   | 2.08                     | 0.52              |
| 18:R:86:VAL:O    | 18:R:87:ARG:CB   | 2.57                     | 0.52              |
| 1:A:310:A:O2'    | 1:A:311:G:OP2    | 2.22                     | 0.52              |
| 1:A:1311:U:OP1   | 13:M:23:TYR:O    | 2.26                     | 0.52              |
| 3:C:193:TYR:HE1  | 3:C:196:LEU:HD11 | 1.73                     | 0.52              |
| 5:E:52:PRO:O     | 5:E:56:GLN:HG3   | 2.09                     | 0.52              |
| 16:P:51:VAL:O    | 16:P:52:ASP:CB   | 2.58                     | 0.52              |
| 17:Q:51:TYR:C    | 17:Q:52:LYS:HD2  | 2.35                     | 0.52              |
| 1:A:952:A:C5'    | 1:A:953:G:H5''   | 2.40                     | 0.52              |
| 1:A:1014:G:C2'   | 1:A:1015:G:H5'   | 2.40                     | 0.52              |
| 8:H:121:ASP:O    | 8:H:125:ARG:HB2  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:I:40:LEU:C      | 9:I:42:ARG:H     | 2.17                     | 0.52              |
| 18:R:22:VAL:O     | 18:R:26:LEU:HD13 | 2.09                     | 0.52              |
| 19:S:55:LYS:C     | 19:S:56:GLN:HG3  | 2.35                     | 0.52              |
| 2:B:239:VAL:HG23  | 2:B:239:VAL:O    | 2.10                     | 0.52              |
| 6:F:82:ARG:HB2    | 6:F:85:VAL:CG2   | 2.40                     | 0.52              |
| 13:M:23:TYR:C     | 13:M:25:ILE:H    | 2.18                     | 0.52              |
| 1:A:816:U:H2'     | 1:A:817:C:H6     | 1.75                     | 0.52              |
| 1:A:926:A:N7      | 13:M:106:ASN:ND2 | 2.57                     | 0.52              |
| 1:A:1112:A:P      | 1:A:1113:G:OP2   | 2.68                     | 0.52              |
| 10:J:60:ARG:NH1   | 10:J:60:ARG:HG2  | 2.25                     | 0.52              |
| 20:T:67:ALA:HB2   | 20:T:77:ALA:HB2  | 1.92                     | 0.52              |
| 1:A:603:C:N1      | 4:D:135:LEU:HD13 | 2.24                     | 0.52              |
| 1:A:1035:G:OP1    | 1:A:1036:C:H5    | 1.93                     | 0.52              |
| 3:C:110:ASN:C     | 3:C:111:LEU:HD12 | 2.35                     | 0.52              |
| 4:D:31:CYS:C      | 4:D:33:MET:N     | 2.67                     | 0.52              |
| 13:M:117:VAL:HG12 | 13:M:118:ALA:N   | 2.18                     | 0.52              |
| 16:P:74:LEU:O     | 16:P:79:VAL:HG23 | 2.09                     | 0.52              |
| 20:T:54:LYS:HA    | 20:T:57:ARG:NH1  | 2.25                     | 0.52              |
| 1:A:1193:U:H3'    | 1:A:1193:U:H6    | 1.75                     | 0.51              |
| 2:B:17:PHE:HD1    | 2:B:18:GLY:H     | 1.58                     | 0.51              |
| 2:B:78:GLN:NE2    | 2:B:96:ARG:NH1   | 2.56                     | 0.51              |
| 2:B:211:ILE:HG22  | 2:B:215:LEU:HD12 | 1.92                     | 0.51              |
| 12:L:55:VAL:HG12  | 12:L:56:ALA:N    | 2.25                     | 0.51              |
| 13:M:40:ASN:C     | 13:M:40:ASN:HD22 | 2.18                     | 0.51              |
| 16:P:36:ILE:O     | 16:P:51:VAL:O    | 2.28                     | 0.51              |
| 1:A:392:A:N7      | 1:A:530:A:O2'    | 2.35                     | 0.51              |
| 1:A:453:G:H3'     | 1:A:454:A:C5'    | 2.40                     | 0.51              |
| 1:A:916:G:H2'     | 1:A:917:C:C6     | 2.45                     | 0.51              |
| 3:C:38:ARG:HG3    | 3:C:38:ARG:NH1   | 2.25                     | 0.51              |
| 4:D:25:ARG:C      | 4:D:27:TYR:H     | 2.18                     | 0.51              |
| 12:L:109:GLY:HA3  | 12:L:121:GLY:O   | 2.10                     | 0.51              |
| 14:N:8:GLU:OE1    | 14:N:8:GLU:C     | 2.54                     | 0.51              |
| 1:A:31:G:H4'      | 1:A:32:A:OP2     | 2.10                     | 0.51              |
| 1:A:108:G:H1'     | 1:A:109:A:N7     | 2.26                     | 0.51              |
| 1:A:167:U:H5''    | 1:A:203:A:O4'    | 2.10                     | 0.51              |
| 1:A:798:A:H5''    | 1:A:800:C:N4     | 2.26                     | 0.51              |
| 1:A:1027:C:H2'    | 1:A:1028:A:O5'   | 2.10                     | 0.51              |
| 1:A:1130:U:H2'    | 1:A:1131:C:O4'   | 2.10                     | 0.51              |
| 1:A:1236:G:H2'    | 1:A:1260:A:H62   | 1.76                     | 0.51              |
| 1:A:1293:G:N7     | 19:S:3:ARG:O     | 2.43                     | 0.51              |
| 1:A:1303:C:C4'    | 1:A:1304:G:OP1   | 2.56                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:118:LEU:HB3  | 2:B:142:LEU:HD12 | 1.92                     | 0.51              |
| 3:C:70:VAL:HG21  | 3:C:76:VAL:CG2   | 2.34                     | 0.51              |
| 5:E:8:GLU:HA     | 5:E:33:VAL:O     | 2.10                     | 0.51              |
| 10:J:16:LEU:HD23 | 10:J:94:VAL:HG22 | 1.93                     | 0.51              |
| 10:J:80:LYS:HD3  | 10:J:83:GLU:OE1  | 2.10                     | 0.51              |
| 10:J:96:ILE:HD12 | 10:J:96:ILE:N    | 2.25                     | 0.51              |
| 16:P:45:THR:HB   | 16:P:46:PRO:HD2  | 1.91                     | 0.51              |
| 1:A:66:G:OP1     | 1:A:66:G:C8      | 2.64                     | 0.51              |
| 1:A:988:G:N2     | 1:A:998:U:H1'    | 2.25                     | 0.51              |
| 1:A:1015:G:H2'   | 1:A:1016:G:C8    | 2.45                     | 0.51              |
| 1:A:1073:U:O2    | 1:A:1075:A:C8    | 2.63                     | 0.51              |
| 1:A:1469:A:H1'   | 22:W:2:A:O2'     | 2.10                     | 0.51              |
| 5:E:103:GLY:O    | 5:E:106:PRO:HD2  | 2.11                     | 0.51              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:N    | 2.22                     | 0.51              |
| 1:A:512:G:O6     | 12:L:49:ASN:HA   | 2.11                     | 0.51              |
| 1:A:982:A:H62    | 1:A:1019:C:H42   | 1.58                     | 0.51              |
| 1:A:1348:C:H2'   | 1:A:1349:C:C6    | 2.45                     | 0.51              |
| 2:B:222:ILE:O    | 2:B:226:ARG:HG3  | 2.11                     | 0.51              |
| 6:F:50:TYR:CE1   | 18:R:77:GLY:HA2  | 2.46                     | 0.51              |
| 1:A:49:U:N3      | 1:A:359:A:N6     | 2.59                     | 0.51              |
| 1:A:239:U:H4'    | 1:A:240:C:O5'    | 2.10                     | 0.51              |
| 1:A:379:G:H2'    | 1:A:380:C:H6     | 1.75                     | 0.51              |
| 1:A:383:G:O2'    | 1:A:384:A:P      | 2.69                     | 0.51              |
| 1:A:961:C:H2'    | 1:A:962:C:H6     | 1.75                     | 0.51              |
| 1:A:1145:C:H2'   | 1:A:1146:G:H8    | 1.76                     | 0.51              |
| 1:A:1164:A:O2'   | 1:A:1165:G:OP1   | 2.24                     | 0.51              |
| 1:A:1295:C:O2'   | 1:A:1296:U:H5'   | 2.11                     | 0.51              |
| 2:B:15:VAL:HG21  | 2:B:209:ARG:HB3  | 1.91                     | 0.51              |
| 2:B:48:MET:O     | 2:B:52:GLU:HB2   | 2.11                     | 0.51              |
| 3:C:11:ARG:O     | 3:C:12:LEU:C     | 2.53                     | 0.51              |
| 4:D:64:LEU:HD23  | 4:D:64:LEU:C     | 2.36                     | 0.51              |
| 6:F:100:ASN:OD1  | 18:R:23:LYS:O    | 2.28                     | 0.51              |
| 12:L:25:PRO:C    | 12:L:27:LEU:N    | 2.59                     | 0.51              |
| 13:M:22:ILE:CD1  | 13:M:25:ILE:HD12 | 2.40                     | 0.51              |
| 1:A:969:U:O2'    | 1:A:970:G:OP2    | 2.23                     | 0.51              |
| 1:A:1108:U:C2'   | 1:A:1109:G:H5'   | 2.40                     | 0.51              |
| 2:B:91:PRO:HG3   | 2:B:154:LEU:CB   | 2.40                     | 0.51              |
| 2:B:97:TRP:CH2   | 2:B:176:GLU:OE2  | 2.64                     | 0.51              |
| 6:F:19:LEU:C     | 6:F:19:LEU:HD23  | 2.36                     | 0.51              |
| 7:G:15:ASP:HB3   | 7:G:19:GLY:H     | 1.75                     | 0.51              |
| 1:A:385:C:H2'    | 1:A:386:G:C8     | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1206:A:H2'   | 1:A:1206:A:N3    | 2.26                     | 0.51              |
| 1:A:1238:U:OP2   | 3:C:27:LYS:CE    | 2.58                     | 0.51              |
| 2:B:98:LEU:O     | 2:B:101:MET:HG3  | 2.10                     | 0.51              |
| 2:B:218:ALA:O    | 2:B:222:ILE:HG13 | 2.11                     | 0.51              |
| 5:E:47:LYS:N     | 5:E:47:LYS:HD3   | 2.25                     | 0.51              |
| 5:E:74:GLY:HA3   | 5:E:116:THR:HG22 | 1.91                     | 0.51              |
| 13:M:23:TYR:HB2  | 13:M:67:GLU:CD   | 2.36                     | 0.51              |
| 1:A:190:G:H4'    | 1:A:191:G:OP2    | 2.11                     | 0.51              |
| 1:A:701:G:H4'    | 11:K:117:ASN:ND2 | 2.25                     | 0.51              |
| 1:A:705:A:H5''   | 1:A:706:U:OP1    | 2.10                     | 0.51              |
| 1:A:1182:A:H4'   | 1:A:1183:G:O5'   | 2.11                     | 0.51              |
| 4:D:194:LEU:HD22 | 4:D:194:LEU:N    | 2.25                     | 0.51              |
| 7:G:69:VAL:HG12  | 7:G:69:VAL:O     | 2.11                     | 0.51              |
| 12:L:65:GLU:CD   | 12:L:65:GLU:N    | 2.69                     | 0.51              |
| 1:A:49:U:N3      | 1:A:359:A:C6     | 2.78                     | 0.51              |
| 1:A:980:G:C8     | 1:A:980:G:H3'    | 2.45                     | 0.51              |
| 1:A:984:C:C6     | 1:A:984:C:C3'    | 2.93                     | 0.51              |
| 1:A:1126:G:H3'   | 1:A:1126:G:C8    | 2.46                     | 0.51              |
| 2:B:223:ILE:HD12 | 2:B:230:VAL:H    | 1.75                     | 0.51              |
| 3:C:83:ARG:C     | 3:C:85:ARG:H     | 2.19                     | 0.51              |
| 4:D:175:SER:OG   | 4:D:184:LYS:HB3  | 2.09                     | 0.51              |
| 5:E:50:GLU:HB2   | 5:E:53:LEU:HD12  | 1.93                     | 0.51              |
| 5:E:144:THR:H    | 5:E:147:ASP:HB2  | 1.76                     | 0.51              |
| 12:L:57:LYS:HG2  | 12:L:67:THR:HG22 | 1.92                     | 0.51              |
| 18:R:53:ARG:NH1  | 18:R:59:SER:HA   | 2.26                     | 0.51              |
| 19:S:15:LEU:O    | 19:S:19:VAL:N    | 2.39                     | 0.51              |
| 19:S:55:LYS:O    | 19:S:56:GLN:HG3  | 2.11                     | 0.51              |
| 20:T:50:GLU:HB2  | 20:T:99:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:123:G:C2     | 1:A:189:U:H5'    | 2.46                     | 0.50              |
| 1:A:669:U:O4     | 1:A:686:G:O2'    | 2.29                     | 0.50              |
| 1:A:690:C:H2'    | 1:A:691:C:C6     | 2.46                     | 0.50              |
| 1:A:858:G:P      | 12:L:12:ARG:HH22 | 2.33                     | 0.50              |
| 1:A:983:A:H5'    | 1:A:984:C:C2     | 2.45                     | 0.50              |
| 1:A:1376:A:O5'   | 1:A:1376:A:H8    | 1.93                     | 0.50              |
| 2:B:223:ILE:HG13 | 2:B:224:GLN:H    | 1.76                     | 0.50              |
| 3:C:157:ILE:HG21 | 3:C:164:ARG:NH2  | 2.26                     | 0.50              |
| 3:C:179:ARG:O    | 3:C:179:ARG:CG   | 2.56                     | 0.50              |
| 4:D:189:PRO:HB2  | 4:D:194:LEU:HD21 | 1.93                     | 0.50              |
| 11:K:126:ARG:O   | 11:K:127:LYS:C   | 2.53                     | 0.50              |
| 1:A:1093:A:C6    | 3:C:177:THR:HG22 | 2.46                     | 0.50              |
| 3:C:38:ARG:HG3   | 3:C:38:ARG:HH11  | 1.76                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:64:VAL:CG2   | 3:C:99:VAL:HG12   | 2.40                     | 0.50              |
| 3:C:91:LEU:HB3   | 3:C:99:VAL:HG21   | 1.92                     | 0.50              |
| 11:K:18:ARG:NH1  | 11:K:36:ASP:HA    | 2.26                     | 0.50              |
| 15:O:53:HIS:CE1  | 15:O:57:LEU:HD11  | 2.47                     | 0.50              |
| 20:T:53:LEU:HB2  | 20:T:100:ILE:HG22 | 1.93                     | 0.50              |
| 1:A:330:C:H2'    | 1:A:331:C:C6      | 2.46                     | 0.50              |
| 1:A:423:G:H4'    | 1:A:424:U:O5'     | 2.11                     | 0.50              |
| 1:A:699:A:H2'    | 1:A:700:C:O4'     | 2.11                     | 0.50              |
| 1:A:961:C:H2'    | 1:A:962:C:C6      | 2.46                     | 0.50              |
| 2:B:21:ARG:NE    | 2:B:23:ARG:HD2    | 2.26                     | 0.50              |
| 2:B:213:LEU:HD23 | 2:B:213:LEU:C     | 2.36                     | 0.50              |
| 7:G:78:ARG:HH11  | 7:G:154:TYR:HB3   | 1.76                     | 0.50              |
| 12:L:33:ARG:CD   | 12:L:62:SER:HB3   | 2.40                     | 0.50              |
| 1:A:334:C:H2'    | 1:A:335:U:C6      | 2.47                     | 0.50              |
| 1:A:635:U:H6     | 1:A:635:U:O5'     | 1.94                     | 0.50              |
| 1:A:1011:G:O2'   | 1:A:1012:A:H5'    | 2.12                     | 0.50              |
| 3:C:29:TYR:C     | 3:C:29:TYR:CD2    | 2.89                     | 0.50              |
| 3:C:46:GLU:HB3   | 3:C:83:ARG:HH21   | 1.77                     | 0.50              |
| 17:Q:92:ARG:HG3  | 17:Q:92:ARG:NH1   | 2.27                     | 0.50              |
| 1:A:269:A:HO2'   | 1:A:270:G:H8      | 1.59                     | 0.50              |
| 1:A:685:A:HO2'   | 1:A:686:G:P       | 2.34                     | 0.50              |
| 1:A:895:A:H2'    | 1:A:896:A:C8      | 2.47                     | 0.50              |
| 1:A:1193:U:C6    | 1:A:1193:U:C3'    | 2.95                     | 0.50              |
| 1:A:1253:G:H2'   | 1:A:1254:G:C5'    | 2.41                     | 0.50              |
| 1:A:1286:G:N2    | 1:A:1312:G:H2'    | 2.27                     | 0.50              |
| 3:C:86:VAL:O     | 3:C:89:GLU:HB3    | 2.12                     | 0.50              |
| 16:P:43:LYS:HA   | 16:P:48:TRP:HB3   | 1.94                     | 0.50              |
| 1:A:249:G:OP1    | 17:Q:67:LYS:O     | 2.29                     | 0.50              |
| 1:A:994:A:H2'    | 1:A:995:G:O4'     | 2.12                     | 0.50              |
| 3:C:14:ILE:H     | 3:C:14:ILE:CD1    | 2.17                     | 0.50              |
| 5:E:61:TYR:O     | 5:E:64:ARG:O      | 2.30                     | 0.50              |
| 13:M:81:LEU:HD11 | 13:M:88:ARG:NH2   | 2.26                     | 0.50              |
| 20:T:43:LEU:HD11 | 20:T:55:ILE:HD12  | 1.92                     | 0.50              |
| 21:V:3:LYS:HG2   | 21:V:14:TRP:CD1   | 2.47                     | 0.50              |
| 1:A:8:A:C6       | 4:D:209:ARG:HA    | 2.47                     | 0.50              |
| 1:A:49:U:O2'     | 1:A:50:A:OP1      | 2.30                     | 0.50              |
| 1:A:52:G:C6      | 1:A:355:A:C4      | 3.00                     | 0.50              |
| 1:A:514:U:H4'    | 1:A:515:A:OP1     | 2.11                     | 0.50              |
| 1:A:637:G:C5     | 1:A:638:A:N7      | 2.80                     | 0.50              |
| 1:A:1210:A:H2'   | 1:A:1211:C:C6     | 2.47                     | 0.50              |
| 4:D:64:LEU:HD22  | 4:D:75:PHE:CE1    | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:65:U:O2'     | 1:A:66:G:OP2     | 2.26                     | 0.50              |
| 1:A:684:C:H5''   | 1:A:686:G:O4'    | 2.11                     | 0.50              |
| 1:A:685:A:O2'    | 1:A:686:G:OP1    | 2.29                     | 0.50              |
| 1:A:1328:G:O2'   | 1:A:1329:U:OP2   | 2.30                     | 0.50              |
| 1:A:1403:G:H1    | 1:A:1456:C:H42   | 1.60                     | 0.50              |
| 3:C:34:LEU:HD11  | 3:C:38:ARG:HD3   | 1.94                     | 0.50              |
| 4:D:6:GLY:O      | 4:D:7:PRO:C      | 2.55                     | 0.50              |
| 9:I:46:ALA:HB1   | 9:I:77:ILE:HG22  | 1.93                     | 0.50              |
| 9:I:127:LYS:HG2  | 13:M:126:LYS:HZ1 | 1.76                     | 0.50              |
| 13:M:5:ALA:O     | 13:M:6:GLY:C     | 2.53                     | 0.50              |
| 1:A:5:U:H4'      | 1:A:6:G:O5'      | 2.11                     | 0.50              |
| 1:A:100:G:H2'    | 1:A:101:G:H5'    | 1.94                     | 0.50              |
| 1:A:249:G:OP1    | 17:Q:68:ARG:HB2  | 2.12                     | 0.50              |
| 1:A:842:A:H5'    | 1:A:1060:U:O4    | 2.12                     | 0.50              |
| 1:A:1051:C:O2'   | 1:A:1173:C:H1'   | 2.12                     | 0.50              |
| 1:A:1326:U:O2'   | 1:A:1327:A:OP2   | 2.24                     | 0.50              |
| 18:R:53:ARG:HH11 | 18:R:59:SER:HA   | 1.77                     | 0.50              |
| 1:A:123:G:O2'    | 1:A:189:U:H3'    | 2.12                     | 0.49              |
| 1:A:227:G:H1'    | 1:A:257:A:N1     | 2.27                     | 0.49              |
| 1:A:936:A:C3'    | 1:A:937:U:H5''   | 2.37                     | 0.49              |
| 1:A:1295:C:C6    | 19:S:6:LYS:HE2   | 2.47                     | 0.49              |
| 1:A:1334:G:H2'   | 1:A:1335:C:C6    | 2.46                     | 0.49              |
| 1:A:1461:C:H6    | 1:A:1461:C:O5'   | 1.95                     | 0.49              |
| 1:A:1463:G:H2'   | 1:A:1464:G:O4'   | 2.12                     | 0.49              |
| 4:D:152:SER:O    | 4:D:158:ILE:HD12 | 2.12                     | 0.49              |
| 9:I:49:PRO:O     | 9:I:52:ALA:HB3   | 2.12                     | 0.49              |
| 11:K:121:PRO:HG2 | 11:K:126:ARG:HG2 | 1.92                     | 0.49              |
| 12:L:102:ARG:HG3 | 12:L:109:GLY:HA2 | 1.94                     | 0.49              |
| 17:Q:80:GLY:O    | 17:Q:81:ARG:HB3  | 2.12                     | 0.49              |
| 1:A:578:G:O2'    | 1:A:579:C:OP2    | 2.23                     | 0.49              |
| 1:A:816:U:H2'    | 1:A:817:C:C6     | 2.47                     | 0.49              |
| 1:A:1475:U:H2'   | 1:A:1520:C:OP1   | 2.12                     | 0.49              |
| 6:F:97:PHE:HE2   | 18:R:62:GLU:HG2  | 1.76                     | 0.49              |
| 14:N:23:ARG:HG2  | 14:N:23:ARG:HH11 | 1.76                     | 0.49              |
| 16:P:18:ARG:O    | 16:P:20:VAL:HG13 | 2.13                     | 0.49              |
| 1:A:959:U:O2'    | 1:A:960:A:OP2    | 2.28                     | 0.49              |
| 1:A:982:A:N3     | 1:A:982:A:C5'    | 2.75                     | 0.49              |
| 1:A:1049:A:H4'   | 1:A:1050:G:O5'   | 2.12                     | 0.49              |
| 1:A:1297:G:N2    | 1:A:1299:A:H3'   | 2.27                     | 0.49              |
| 2:B:52:GLU:O     | 2:B:56:ARG:HG3   | 2.12                     | 0.49              |
| 3:C:132:ARG:HH11 | 3:C:132:ARG:HG2  | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:4:LYS:HD2   | 17:Q:6:LEU:HD21  | 1.94                     | 0.49              |
| 18:R:36:ASN:HD21 | 18:R:38:GLU:HG2  | 1.74                     | 0.49              |
| 18:R:47:THR:HG22 | 18:R:48:GLY:N    | 2.27                     | 0.49              |
| 1:A:377:A:C2     | 1:A:378:A:C4     | 3.01                     | 0.49              |
| 1:A:697:G:N2     | 1:A:760:A:H1'    | 2.27                     | 0.49              |
| 1:A:1257:G:H8    | 1:A:1257:G:O5'   | 1.95                     | 0.49              |
| 1:A:1282:U:O2'   | 1:A:1283:U:OP1   | 2.25                     | 0.49              |
| 1:A:1383:G:C2    | 1:A:1384:C:H1'   | 2.48                     | 0.49              |
| 2:B:7:VAL:HG23   | 2:B:8:LYS:HG3    | 1.93                     | 0.49              |
| 2:B:21:ARG:HE    | 2:B:23:ARG:CD    | 2.24                     | 0.49              |
| 2:B:55:PHE:CD1   | 2:B:221:LEU:HD22 | 2.48                     | 0.49              |
| 8:H:4:ASP:OD1    | 8:H:85:ARG:NH1   | 2.46                     | 0.49              |
| 19:S:18:LYS:HA   | 19:S:21:GLU:OE2  | 2.12                     | 0.49              |
| 1:A:49:U:O3'     | 1:A:50:A:O3'     | 2.30                     | 0.49              |
| 1:A:50:A:C6      | 1:A:356:G:C4'    | 2.94                     | 0.49              |
| 1:A:75:G:O2'     | 1:A:76:G:H5'     | 2.13                     | 0.49              |
| 1:A:570:G:N2     | 1:A:737:C:OP2    | 2.43                     | 0.49              |
| 1:A:704:G:H4'    | 1:A:705:A:O5'    | 2.11                     | 0.49              |
| 1:A:942:A:H4'    | 1:A:943:G:O5'    | 2.13                     | 0.49              |
| 1:A:1294:U:C5    | 19:S:4:SER:HB2   | 2.48                     | 0.49              |
| 1:A:1434:G:O2'   | 1:A:1435:G:H5'   | 2.13                     | 0.49              |
| 4:D:18:LYS:HG3   | 4:D:33:MET:HG3   | 1.93                     | 0.49              |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:CD1  | 2.43                     | 0.49              |
| 5:E:82:VAL:HG11  | 5:E:137:GLU:HB3  | 1.94                     | 0.49              |
| 14:N:11:LYS:O    | 14:N:11:LYS:HG2  | 2.11                     | 0.49              |
| 1:A:340:C:O2'    | 1:A:341:G:OP2    | 2.29                     | 0.49              |
| 1:A:382:U:H5'    | 1:A:383:G:P      | 2.53                     | 0.49              |
| 1:A:413:C:H6     | 1:A:413:C:O5'    | 1.95                     | 0.49              |
| 1:A:465:G:C5'    | 1:A:466:A:OP1    | 2.61                     | 0.49              |
| 1:A:495:U:H1'    | 4:D:42:GLN:HE22  | 1.78                     | 0.49              |
| 1:A:1139:A:O2'   | 1:A:1140:C:OP2   | 2.24                     | 0.49              |
| 1:A:1210:A:C2    | 1:A:1211:C:C4    | 3.01                     | 0.49              |
| 1:A:1295:C:C5    | 19:S:6:LYS:HE2   | 2.47                     | 0.49              |
| 1:A:1407:U:H2'   | 1:A:1408:C:C6    | 2.48                     | 0.49              |
| 2:B:12:GLU:HA    | 2:B:12:GLU:OE2   | 2.11                     | 0.49              |
| 2:B:101:MET:N    | 2:B:108:ILE:HD12 | 2.27                     | 0.49              |
| 3:C:20:SER:O     | 14:N:54:PRO:HB3  | 2.12                     | 0.49              |
| 3:C:130:VAL:HG12 | 3:C:134:ILE:HD12 | 1.93                     | 0.49              |
| 7:G:79:ARG:HH11  | 7:G:83:ALA:HA    | 1.77                     | 0.49              |
| 9:I:48:GLU:N     | 9:I:49:PRO:HD2   | 2.27                     | 0.49              |
| 12:L:46:LYS:CD   | 12:L:47:LYS:HG3  | 2.41                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:100:LYS:HD2 | 17:Q:100:LYS:C   | 2.37                     | 0.49              |
| 1:A:264:C:H2'    | 1:A:265:A:H8     | 1.76                     | 0.49              |
| 1:A:669:U:H2'    | 1:A:670:A:O5'    | 2.13                     | 0.49              |
| 1:A:911:C:H4'    | 1:A:912:A:OP1    | 2.11                     | 0.49              |
| 1:A:1121:G:C5'   | 1:A:1122:C:OP1   | 2.55                     | 0.49              |
| 1:A:1278:C:O2'   | 1:A:1279:C:OP2   | 2.25                     | 0.49              |
| 5:E:120:THR:CG2  | 5:E:121:LYS:N    | 2.73                     | 0.49              |
| 12:L:27:LEU:O    | 12:L:28:LYS:C    | 2.55                     | 0.49              |
| 12:L:28:LYS:O    | 12:L:30:ALA:N    | 2.46                     | 0.49              |
| 19:S:33:THR:CG2  | 19:S:34:TRP:H    | 2.26                     | 0.49              |
| 1:A:41:G:H2'     | 1:A:42:G:C8      | 2.48                     | 0.49              |
| 1:A:521:G:OP2    | 12:L:115:LYS:HG3 | 2.13                     | 0.49              |
| 1:A:670:A:O2'    | 1:A:671:G:OP2    | 2.29                     | 0.49              |
| 1:A:1085:C:H5''  | 2:B:98:LEU:HD22  | 1.95                     | 0.49              |
| 4:D:153:ARG:HH12 | 4:D:180:GLY:HA2  | 1.78                     | 0.49              |
| 7:G:115:ARG:HB2  | 7:G:118:VAL:HG23 | 1.94                     | 0.49              |
| 12:L:24:VAL:O    | 12:L:26:ALA:N    | 2.38                     | 0.49              |
| 16:P:10:GLY:HA3  | 16:P:14:ASN:O    | 2.13                     | 0.49              |
| 23:X:32:C:H6     | 23:X:32:C:H5''   | 1.77                     | 0.49              |
| 1:A:294:G:H2'    | 1:A:295:A:C8     | 2.48                     | 0.49              |
| 1:A:417:C:O2'    | 1:A:418:G:OP2    | 2.28                     | 0.49              |
| 1:A:763:A:O2'    | 1:A:764:A:H5''   | 2.13                     | 0.49              |
| 1:A:795:C:O2'    | 1:A:796:U:OP2    | 2.30                     | 0.49              |
| 1:A:992:A:C2     | 1:A:1200:U:H1'   | 2.48                     | 0.49              |
| 1:A:1197:G:H5''  | 14:N:5:ALA:HB2   | 1.95                     | 0.49              |
| 4:D:36:ARG:N     | 4:D:37:PRO:CD    | 2.75                     | 0.49              |
| 13:M:54:VAL:O    | 13:M:58:GLU:HG2  | 2.13                     | 0.49              |
| 1:A:670:A:HO2'   | 1:A:671:G:P      | 2.35                     | 0.49              |
| 1:A:1281:G:H1'   | 1:A:1282:U:H5    | 1.76                     | 0.49              |
| 1:A:1479:A:H2'   | 1:A:1479:A:N3    | 2.27                     | 0.49              |
| 4:D:63:LYS:O     | 4:D:67:ILE:HG13  | 2.13                     | 0.49              |
| 8:H:22:GLU:OE2   | 8:H:22:GLU:HA    | 2.12                     | 0.49              |
| 11:K:48:ILE:CD1  | 11:K:64:ALA:HA   | 2.40                     | 0.49              |
| 13:M:90:LEU:HD23 | 13:M:93:ARG:NH1  | 2.27                     | 0.49              |
| 22:W:3:G:H1      | 23:X:34:70U:HN3  | 1.58                     | 0.49              |
| 1:A:30:U:O2'     | 1:A:31:G:OP1     | 2.24                     | 0.48              |
| 1:A:385:C:O3'    | 16:P:28:ARG:NH2  | 2.46                     | 0.48              |
| 1:A:1135:C:OP1   | 10:J:13:HIS:HE1  | 1.96                     | 0.48              |
| 1:A:1206:A:H4'   | 1:A:1207:C:OP2   | 2.12                     | 0.48              |
| 4:D:29:PRO:O     | 4:D:30:LYS:HG3   | 2.13                     | 0.48              |
| 4:D:58:LEU:O     | 4:D:58:LEU:HD22  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:88:PRO:HB3   | 7:G:145:ALA:HB1  | 1.95                     | 0.48              |
| 9:I:43:ALA:C     | 9:I:45:ALA:N     | 2.69                     | 0.48              |
| 10:J:46:ARG:HH11 | 10:J:46:ARG:CG   | 2.21                     | 0.48              |
| 12:L:46:LYS:HD2  | 12:L:47:LYS:HG3  | 1.94                     | 0.48              |
| 1:A:99:C:O2      | 1:A:374:C:H4'    | 2.13                     | 0.48              |
| 1:A:262:C:H2'    | 1:A:263:C:C6     | 2.48                     | 0.48              |
| 1:A:417:C:H4'    | 1:A:418:G:O5'    | 2.12                     | 0.48              |
| 1:A:516:A:O2'    | 1:A:518:A:OP2    | 2.31                     | 0.48              |
| 1:A:705:A:H3'    | 1:A:705:A:N3     | 2.28                     | 0.48              |
| 11:K:121:PRO:HG2 | 11:K:126:ARG:HG3 | 1.95                     | 0.48              |
| 12:L:78:GLN:O    | 12:L:80:HIS:N    | 2.38                     | 0.48              |
| 17:Q:89:LEU:O    | 17:Q:92:ARG:HB3  | 2.13                     | 0.48              |
| 17:Q:100:LYS:HD2 | 17:Q:101:ARG:NE  | 2.27                     | 0.48              |
| 1:A:636:A:N3     | 1:A:636:A:C2'    | 2.73                     | 0.48              |
| 1:A:637:G:N1     | 1:A:638:A:C4     | 2.81                     | 0.48              |
| 1:A:1106:G:O5'   | 10:J:35:SER:O    | 2.31                     | 0.48              |
| 1:A:1349:C:C5'   | 10:J:60:ARG:NH1  | 2.72                     | 0.48              |
| 1:A:1521:U:HO3'  | 22:W:1:A:P       | 2.31                     | 0.48              |
| 2:B:47:THR:O     | 2:B:51:LEU:HB2   | 2.13                     | 0.48              |
| 2:B:97:TRP:CZ3   | 2:B:176:GLU:OE2  | 2.66                     | 0.48              |
| 2:B:195:ASP:O    | 8:H:74:PRO:HG3   | 2.13                     | 0.48              |
| 3:C:14:ILE:N     | 3:C:14:ILE:CD1   | 2.75                     | 0.48              |
| 4:D:17:VAL:HG11  | 4:D:197:PRO:HB2  | 1.96                     | 0.48              |
| 4:D:126:ILE:HG22 | 4:D:127:THR:N    | 2.28                     | 0.48              |
| 10:J:32:ALA:HB1  | 10:J:75:ILE:O    | 2.14                     | 0.48              |
| 14:N:22:THR:O    | 14:N:23:ARG:HB2  | 2.12                     | 0.48              |
| 1:A:775:A:O2'    | 1:A:776:U:OP2    | 2.29                     | 0.48              |
| 1:A:1139:A:H4'   | 1:A:1140:C:O5'   | 2.13                     | 0.48              |
| 1:A:1293:G:O2'   | 1:A:1294:U:H5'   | 2.14                     | 0.48              |
| 2:B:91:PRO:HG2   | 2:B:155:LEU:CD2  | 2.43                     | 0.48              |
| 2:B:115:LEU:HD11 | 2:B:146:GLN:HG2  | 1.94                     | 0.48              |
| 2:B:132:LYS:HD2  | 2:B:135:GLN:HB2  | 1.96                     | 0.48              |
| 2:B:220:ASP:O    | 2:B:224:GLN:HG3  | 2.13                     | 0.48              |
| 4:D:36:ARG:HG2   | 4:D:36:ARG:NH1   | 2.28                     | 0.48              |
| 8:H:107:LEU:HD23 | 8:H:107:LEU:N    | 2.29                     | 0.48              |
| 17:Q:27:PHE:HB2  | 17:Q:28:PRO:HD2  | 1.94                     | 0.48              |
| 1:A:207:C:H6     | 1:A:207:C:OP2    | 1.96                     | 0.48              |
| 1:A:927:U:C5     | 13:M:102:ARG:NE  | 2.82                     | 0.48              |
| 1:A:953:G:O2'    | 1:A:954:A:P      | 2.71                     | 0.48              |
| 1:A:1136:G:H2'   | 1:A:1137:G:H8    | 1.79                     | 0.48              |
| 2:B:27:LYS:HD3   | 2:B:195:ASP:OD2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:50:ILE:HG22  | 7:G:54:THR:HG22   | 1.96                     | 0.48              |
| 8:H:88:LYS:HB2   | 8:H:89:PRO:HD2    | 1.95                     | 0.48              |
| 9:I:33:PHE:C     | 9:I:35:GLU:N      | 2.70                     | 0.48              |
| 10:J:54:PHE:CD2  | 10:J:55:LYS:HG2   | 2.49                     | 0.48              |
| 12:L:53:ARG:CG   | 12:L:93:LEU:HD21  | 2.41                     | 0.48              |
| 13:M:3:ARG:HD3   | 13:M:7:VAL:HA     | 1.95                     | 0.48              |
| 14:N:57:ARG:HG2  | 14:N:58:LYS:H     | 1.79                     | 0.48              |
| 18:R:55:ARG:HH11 | 18:R:55:ARG:HA    | 1.78                     | 0.48              |
| 1:A:323:C:O2'    | 1:A:324:A:OP2     | 2.29                     | 0.48              |
| 1:A:1182:A:O2'   | 1:A:1183:G:OP2    | 2.27                     | 0.48              |
| 8:H:10:LEU:HD12  | 8:H:85:ARG:CG     | 2.43                     | 0.48              |
| 10:J:86:MET:HA   | 10:J:86:MET:HE3   | 1.94                     | 0.48              |
| 18:R:44:LEU:HD22 | 18:R:48:GLY:O     | 2.14                     | 0.48              |
| 19:S:63:THR:HG22 | 19:S:64:GLU:N     | 2.26                     | 0.48              |
| 1:A:705:A:H4'    | 1:A:706:U:O5'     | 2.12                     | 0.48              |
| 1:A:983:A:OP2    | 1:A:984:C:C5      | 2.67                     | 0.48              |
| 1:A:1267:A:H2    | 21:V:18:TYR:OH    | 1.96                     | 0.48              |
| 4:D:62:GLN:NE2   | 4:D:65:ARG:NH1    | 2.62                     | 0.48              |
| 9:I:125:TYR:CE1  | 9:I:128:ARG:HB3   | 2.47                     | 0.48              |
| 10:J:20:ALA:CB   | 10:J:37:PRO:HG3   | 2.44                     | 0.48              |
| 10:J:82:ILE:O    | 10:J:86:MET:HB2   | 2.14                     | 0.48              |
| 11:K:54:ARG:HB3  | 11:K:54:ARG:NH1   | 2.22                     | 0.48              |
| 19:S:19:VAL:HG13 | 19:S:20:LEU:N     | 2.28                     | 0.48              |
| 1:A:44:G:OP2     | 16:P:12:LYS:HB2   | 2.14                     | 0.48              |
| 1:A:332:C:H2'    | 1:A:333:A:C8      | 2.49                     | 0.48              |
| 1:A:647:G:OP1    | 18:R:64:ARG:HD2   | 2.13                     | 0.48              |
| 1:A:927:U:OP2    | 13:M:102:ARG:HG2  | 2.14                     | 0.48              |
| 1:A:981:G:H2'    | 1:A:982:A:O5'     | 2.14                     | 0.48              |
| 3:C:147:LYS:NZ   | 3:C:206:GLU:HB2   | 2.29                     | 0.48              |
| 9:I:12:GLU:HG3   | 9:I:12:GLU:O      | 2.14                     | 0.48              |
| 11:K:54:ARG:O    | 11:K:57:THR:CG2   | 2.55                     | 0.48              |
| 16:P:42:ARG:C    | 16:P:43:LYS:HG3   | 2.38                     | 0.48              |
| 20:T:10:LEU:O    | 20:T:13:LEU:HG    | 2.14                     | 0.48              |
| 1:A:83:A:H2'     | 1:A:84:C:O4'      | 2.14                     | 0.48              |
| 1:A:322:A:H4'    | 1:A:323:C:OP1     | 2.13                     | 0.48              |
| 1:A:525:G:H2'    | 1:A:526:C:H6      | 1.78                     | 0.48              |
| 1:A:701:G:C5'    | 11:K:117:ASN:HD22 | 2.27                     | 0.48              |
| 3:C:44:GLU:HA    | 3:C:52:LEU:HD11   | 1.95                     | 0.48              |
| 3:C:162:GLN:OE1  | 3:C:163:ALA:O     | 2.32                     | 0.48              |
| 16:P:75:ARG:HH11 | 16:P:75:ARG:HG3   | 1.78                     | 0.48              |
| 23:X:34:70U:H2'  | 23:X:35:U:C6      | 2.48                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:66:G:OP1     | 1:A:66:G:H8       | 1.97                     | 0.48              |
| 1:A:931:G:H2'    | 1:A:932:U:C6      | 2.49                     | 0.48              |
| 1:A:1294:U:OP2   | 19:S:6:LYS:HA     | 2.14                     | 0.48              |
| 7:G:95:ARG:HG3   | 7:G:95:ARG:HH11   | 1.79                     | 0.48              |
| 8:H:72:PRO:O     | 8:H:73:ASP:HB3    | 2.14                     | 0.48              |
| 9:I:97:LYS:HB3   | 9:I:98:PRO:HD3    | 1.95                     | 0.48              |
| 10:J:8:LEU:CD2   | 10:J:96:ILE:HG13  | 2.43                     | 0.48              |
| 12:L:65:GLU:N    | 12:L:65:GLU:OE1   | 2.47                     | 0.48              |
| 1:A:155:A:C2'    | 1:A:156:A:O5'     | 2.62                     | 0.47              |
| 1:A:170:C:H2'    | 1:A:171:C:H6      | 1.79                     | 0.47              |
| 1:A:330:C:H2'    | 1:A:331:C:H6      | 1.77                     | 0.47              |
| 2:B:15:VAL:C     | 2:B:16:HIS:CG     | 2.91                     | 0.47              |
| 2:B:134:GLU:C    | 2:B:136:VAL:H     | 2.22                     | 0.47              |
| 3:C:5:ILE:HD13   | 3:C:10:PHE:HB2    | 1.96                     | 0.47              |
| 6:F:11:ASN:OD1   | 6:F:13:ASN:N      | 2.44                     | 0.47              |
| 8:H:23:SER:HA    | 8:H:63:LEU:CD2    | 2.41                     | 0.47              |
| 10:J:84:GLN:C    | 10:J:86:MET:H     | 2.21                     | 0.47              |
| 12:L:70:ILE:CD1  | 12:L:77:LEU:HD12  | 2.40                     | 0.47              |
| 19:S:15:LEU:O    | 19:S:19:VAL:HG12  | 2.14                     | 0.47              |
| 1:A:1253:G:O2'   | 1:A:1254:G:H5'    | 2.14                     | 0.47              |
| 1:A:1259:U:H4'   | 1:A:1260:A:O4'    | 2.14                     | 0.47              |
| 1:A:1354:U:OP1   | 9:I:71:SER:HB3    | 2.13                     | 0.47              |
| 2:B:17:PHE:HD1   | 2:B:18:GLY:N      | 2.11                     | 0.47              |
| 2:B:21:ARG:HE    | 2:B:23:ARG:HD2    | 1.79                     | 0.47              |
| 3:C:46:GLU:C     | 3:C:48:TYR:H      | 2.23                     | 0.47              |
| 3:C:58:GLU:HB2   | 3:C:65:ALA:HB2    | 1.96                     | 0.47              |
| 3:C:83:ARG:C     | 3:C:85:ARG:N      | 2.71                     | 0.47              |
| 7:G:145:ALA:C    | 7:G:147:ALA:N     | 2.68                     | 0.47              |
| 9:I:5:TYR:O      | 9:I:84:ALA:HA     | 2.13                     | 0.47              |
| 11:K:34:ASP:OD1  | 11:K:38:ASN:HB2   | 2.14                     | 0.47              |
| 11:K:80:VAL:HG13 | 11:K:103:LEU:HD22 | 1.96                     | 0.47              |
| 14:N:23:ARG:NH1  | 14:N:30:ALA:HB2   | 2.30                     | 0.47              |
| 15:O:4:THR:HB    | 15:O:6:GLU:OE2    | 2.14                     | 0.47              |
| 1:A:760:A:H5''   | 1:A:760:A:C8      | 2.47                     | 0.47              |
| 1:A:942:A:C2     | 1:A:946:A:C2      | 3.02                     | 0.47              |
| 1:A:1192:U:H4'   | 1:A:1193:U:H4'    | 1.97                     | 0.47              |
| 1:A:1374:G:N2    | 1:A:1479:A:C8     | 2.80                     | 0.47              |
| 1:A:1461:C:H2'   | 1:A:1462:U:O4'    | 2.14                     | 0.47              |
| 1:A:1509:U:O2    | 1:A:1510:C:H4'    | 2.14                     | 0.47              |
| 2:B:230:VAL:CG1  | 2:B:231:GLU:H     | 2.20                     | 0.47              |
| 4:D:24:GLU:C     | 4:D:26:CYS:H      | 2.18                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:143:ARG:NH1  | 8:H:77:GLU:OE2   | 2.47                     | 0.47              |
| 9:I:69:GLY:O     | 9:I:73:GLN:HG3   | 2.14                     | 0.47              |
| 9:I:100:GLY:O    | 9:I:102:LEU:N    | 2.47                     | 0.47              |
| 19:S:19:VAL:HG23 | 19:S:47:HIS:CD2  | 2.49                     | 0.47              |
| 1:A:446:A:O2'    | 1:A:447:A:P      | 2.71                     | 0.47              |
| 1:A:482:A:O2'    | 1:A:483:G:C8     | 2.68                     | 0.47              |
| 1:A:1339:U:H2'   | 1:A:1340:C:O4'   | 2.15                     | 0.47              |
| 2:B:25:ASN:C     | 2:B:25:ASN:ND2   | 2.70                     | 0.47              |
| 2:B:62:ALA:O     | 2:B:64:ARG:N     | 2.38                     | 0.47              |
| 2:B:124:SER:C    | 2:B:126:GLU:H    | 2.22                     | 0.47              |
| 3:C:12:LEU:HD11  | 14:N:51:GLY:HA3  | 1.96                     | 0.47              |
| 3:C:193:TYR:CE1  | 3:C:196:LEU:HD11 | 2.49                     | 0.47              |
| 10:J:42:THR:HB   | 10:J:67:THR:O    | 2.15                     | 0.47              |
| 17:Q:65:ILE:HD12 | 17:Q:65:ILE:N    | 2.29                     | 0.47              |
| 1:A:1420:G:H2'   | 1:A:1421:C:C6    | 2.50                     | 0.47              |
| 9:I:17:VAL:HG21  | 9:I:80:GLY:HA3   | 1.96                     | 0.47              |
| 10:J:19:SER:O    | 10:J:23:ILE:HG13 | 2.14                     | 0.47              |
| 12:L:42:THR:HG22 | 12:L:43:VAL:N    | 2.29                     | 0.47              |
| 15:O:16:ALA:HB1  | 15:O:21:ASP:HB3  | 1.96                     | 0.47              |
| 17:Q:12:SER:HB3  | 17:Q:20:THR:OG1  | 2.14                     | 0.47              |
| 1:A:408:G:C2'    | 1:A:423:G:H22    | 2.27                     | 0.47              |
| 1:A:942:A:O2'    | 1:A:943:G:OP2    | 2.32                     | 0.47              |
| 1:A:1125:G:O5'   | 1:A:1125:G:C8    | 2.67                     | 0.47              |
| 1:A:1170:C:C5'   | 1:A:1171:G:OP2   | 2.63                     | 0.47              |
| 3:C:172:ARG:NH2  | 3:C:203:PHE:CZ   | 2.82                     | 0.47              |
| 10:J:69:ASN:O    | 10:J:70:ARG:HD3  | 2.14                     | 0.47              |
| 20:T:97:ALA:O    | 20:T:99:LEU:N    | 2.47                     | 0.47              |
| 1:A:50:A:C6      | 1:A:356:G:H4'    | 2.47                     | 0.47              |
| 1:A:50:A:H5''    | 1:A:51:A:O3'     | 2.14                     | 0.47              |
| 1:A:141:G:O2'    | 1:A:142:G:H5'    | 2.15                     | 0.47              |
| 1:A:545:C:O2'    | 12:L:15:ARG:CB   | 2.55                     | 0.47              |
| 1:A:866:A:H4'    | 1:A:867:G:O5'    | 2.14                     | 0.47              |
| 1:A:1068:U:H3    | 1:A:1081:G:N2    | 2.08                     | 0.47              |
| 1:A:1100:C:H1'   | 1:A:1160:A:C4    | 2.49                     | 0.47              |
| 1:A:1109:G:O2'   | 1:A:1129:C:N3    | 2.47                     | 0.47              |
| 1:A:1311:U:H2'   | 1:A:1312:G:H5'   | 1.96                     | 0.47              |
| 1:A:1378:A:H4'   | 1:A:1379:C:H5''  | 1.97                     | 0.47              |
| 2:B:15:VAL:CG2   | 2:B:209:ARG:HB3  | 2.44                     | 0.47              |
| 2:B:71:VAL:HG21  | 2:B:164:VAL:HG22 | 1.96                     | 0.47              |
| 2:B:74:LYS:HG2   | 2:B:76:GLN:H     | 1.80                     | 0.47              |
| 5:E:82:VAL:HG21  | 5:E:138:ALA:HA   | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:82:ARG:HB2   | 6:F:85:VAL:HG23  | 1.96                     | 0.47              |
| 7:G:37:ASN:OD1   | 9:I:41:VAL:HG22  | 2.15                     | 0.47              |
| 9:I:42:ARG:HG2   | 9:I:42:ARG:HH11  | 1.80                     | 0.47              |
| 10:J:5:ARG:HA    | 10:J:73:ASP:OD1  | 2.14                     | 0.47              |
| 10:J:23:ILE:HA   | 10:J:85:LEU:HD22 | 1.96                     | 0.47              |
| 11:K:101:SER:C   | 11:K:103:LEU:N   | 2.72                     | 0.47              |
| 12:L:18:VAL:HG12 | 12:L:19:ARG:N    | 2.30                     | 0.47              |
| 12:L:50:SER:O    | 12:L:51:ALA:HB2  | 2.14                     | 0.47              |
| 13:M:15:VAL:CG2  | 13:M:48:LEU:HD21 | 2.43                     | 0.47              |
| 13:M:37:THR:CG2  | 13:M:55:ARG:HB3  | 2.45                     | 0.47              |
| 17:Q:59:ILE:HD13 | 17:Q:73:VAL:HA   | 1.96                     | 0.47              |
| 19:S:33:THR:HG22 | 19:S:34:TRP:H    | 1.78                     | 0.47              |
| 21:V:2:GLY:C     | 21:V:4:GLY:H     | 2.23                     | 0.47              |
| 1:A:518:A:H4'    | 1:A:519:C:OP1    | 2.12                     | 0.47              |
| 1:A:544:U:O2'    | 1:A:545:C:P      | 2.72                     | 0.47              |
| 1:A:953:G:N7     | 1:A:1339:U:C2    | 2.83                     | 0.47              |
| 1:A:1187:G:H1'   | 3:C:193:TYR:O    | 2.14                     | 0.47              |
| 1:A:1328:G:N2    | 1:A:1355:G:H2'   | 2.30                     | 0.47              |
| 2:B:29:ALA:C     | 2:B:31:TYR:H     | 2.22                     | 0.47              |
| 15:O:26:GLU:HG3  | 15:O:81:LEU:HG   | 1.97                     | 0.47              |
| 1:A:927:U:H5     | 13:M:102:ARG:NE  | 2.13                     | 0.47              |
| 3:C:173:VAL:O    | 3:C:173:VAL:HG12 | 2.14                     | 0.47              |
| 6:F:19:LEU:O     | 6:F:23:LYS:HG3   | 2.14                     | 0.47              |
| 9:I:83:ARG:C     | 9:I:85:LEU:N     | 2.72                     | 0.47              |
| 10:J:32:ALA:CB   | 10:J:76:ASN:HB2  | 2.45                     | 0.47              |
| 11:K:126:ARG:O   | 11:K:129:SER:C   | 2.58                     | 0.47              |
| 12:L:59:ARG:HH12 | 12:L:65:GLU:HB3  | 1.78                     | 0.47              |
| 17:Q:101:ARG:HE  | 17:Q:101:ARG:HA  | 1.79                     | 0.47              |
| 18:R:45:SER:C    | 18:R:47:THR:N    | 2.68                     | 0.47              |
| 1:A:859:C:O2'    | 1:A:860:C:H5'    | 2.15                     | 0.47              |
| 1:A:1024:G:H2'   | 1:A:1025:C:H5'   | 1.97                     | 0.47              |
| 1:A:1111:C:O2'   | 1:A:1112:A:P     | 2.73                     | 0.47              |
| 1:A:1334:G:H2'   | 1:A:1335:C:H6    | 1.80                     | 0.47              |
| 2:B:76:GLN:HG3   | 2:B:206:ASP:OD1  | 2.15                     | 0.47              |
| 7:G:145:ALA:O    | 7:G:147:ALA:N    | 2.48                     | 0.47              |
| 9:I:33:PHE:CE1   | 9:I:37:PHE:HD1   | 2.33                     | 0.47              |
| 10:J:4:ILE:HA    | 10:J:100:THR:CB  | 2.45                     | 0.47              |
| 1:A:669:U:C2'    | 1:A:670:A:O5'    | 2.62                     | 0.46              |
| 1:A:838:G:O2'    | 1:A:839:C:H5'    | 2.16                     | 0.46              |
| 1:A:1125:G:N3    | 1:A:1126:G:N1    | 2.64                     | 0.46              |
| 2:B:130:ARG:O    | 2:B:131:PRO:C    | 2.57                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:151:LEU:HD11 | 8:H:77:GLU:OE2   | 2.14                     | 0.46              |
| 9:I:32:ASP:OD2   | 9:I:33:PHE:N     | 2.49                     | 0.46              |
| 11:K:15:ALA:HA   | 11:K:76:GLY:O    | 2.15                     | 0.46              |
| 17:Q:79:SER:O    | 17:Q:80:GLY:O    | 2.34                     | 0.46              |
| 20:T:68:LYS:HA   | 20:T:68:LYS:HD2  | 1.77                     | 0.46              |
| 1:A:1006:C:C6    | 1:A:1006:C:H3'   | 2.51                     | 0.46              |
| 1:A:1134:A:H2'   | 1:A:1135:C:O5'   | 2.15                     | 0.46              |
| 1:A:1519:U:O5'   | 1:A:1519:U:H6    | 1.98                     | 0.46              |
| 2:B:61:LEU:HD11  | 2:B:160:ASP:HB3  | 1.96                     | 0.46              |
| 2:B:103:THR:HA   | 2:B:180:LEU:HD11 | 1.97                     | 0.46              |
| 4:D:148:VAL:CG1  | 4:D:158:ILE:HD13 | 2.46                     | 0.46              |
| 10:J:39:PRO:O    | 10:J:40:LEU:HB2  | 2.14                     | 0.46              |
| 13:M:88:ARG:HH11 | 19:S:3:ARG:HH21  | 1.63                     | 0.46              |
| 21:V:21:TYR:O    | 21:V:22:ARG:HB2  | 2.13                     | 0.46              |
| 23:X:32:C:H5''   | 23:X:32:C:C6     | 2.50                     | 0.46              |
| 1:A:17:U:H2'     | 1:A:18:C:C6      | 2.50                     | 0.46              |
| 1:A:49:U:C2      | 1:A:359:A:N6     | 2.84                     | 0.46              |
| 1:A:542:A:H4'    | 1:A:544:U:OP1    | 2.16                     | 0.46              |
| 1:A:794:C:H4'    | 1:A:877:A:N6     | 2.31                     | 0.46              |
| 1:A:818:U:OP1    | 18:R:64:ARG:NH2  | 2.36                     | 0.46              |
| 1:A:1222:G:H2'   | 1:A:1223:C:C6    | 2.50                     | 0.46              |
| 3:C:134:ILE:CG2  | 3:C:168:ALA:HB3  | 2.45                     | 0.46              |
| 8:H:65:TYR:HA    | 8:H:79:VAL:HG23  | 1.98                     | 0.46              |
| 8:H:80:ILE:O     | 8:H:80:ILE:HG22  | 2.14                     | 0.46              |
| 10:J:12:ASP:HB3  | 10:J:15:THR:CG2  | 2.46                     | 0.46              |
| 12:L:71:PRO:O    | 12:L:102:ARG:NH1 | 2.48                     | 0.46              |
| 13:M:9:ILE:N     | 13:M:9:ILE:CD1   | 2.73                     | 0.46              |
| 13:M:23:TYR:HB3  | 13:M:67:GLU:H    | 1.81                     | 0.46              |
| 17:Q:4:LYS:HD2   | 17:Q:6:LEU:CD2   | 2.46                     | 0.46              |
| 1:A:208:U:H5''   | 1:A:209:U:OP2    | 2.14                     | 0.46              |
| 1:A:577:G:C2'    | 1:A:578:G:H5'    | 2.45                     | 0.46              |
| 3:C:186:PHE:CZ   | 3:C:188:LEU:HD23 | 2.50                     | 0.46              |
| 4:D:16:GLY:C     | 4:D:33:MET:HE1   | 2.40                     | 0.46              |
| 12:L:42:THR:CG2  | 12:L:52:LEU:HB3  | 2.45                     | 0.46              |
| 19:S:7:LYS:O     | 19:S:7:LYS:HD2   | 2.15                     | 0.46              |
| 1:A:485:G:H2'    | 1:A:486:C:O4'    | 2.15                     | 0.46              |
| 1:A:534:U:H2'    | 1:A:535:U:C6     | 2.50                     | 0.46              |
| 1:A:613:G:H2'    | 1:A:614:G:H5'    | 1.98                     | 0.46              |
| 1:A:795:C:H4'    | 1:A:796:U:O5'    | 2.14                     | 0.46              |
| 1:A:953:G:O2'    | 1:A:954:A:OP2    | 2.33                     | 0.46              |
| 1:A:988:G:H2'    | 1:A:989:G:C8     | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:58:LEU:O     | 4:D:62:GLN:HG2   | 2.16                     | 0.46              |
| 7:G:15:ASP:O     | 7:G:19:GLY:HA2   | 2.14                     | 0.46              |
| 7:G:148:ASN:C    | 7:G:150:ALA:N    | 2.73                     | 0.46              |
| 10:J:34:VAL:HA   | 10:J:74:ILE:HG23 | 1.96                     | 0.46              |
| 20:T:54:LYS:HA   | 20:T:57:ARG:HH12 | 1.81                     | 0.46              |
| 1:A:666:G:H21    | 11:K:38:ASN:ND2  | 2.07                     | 0.46              |
| 1:A:855:G:OP1    | 8:H:88:LYS:HG3   | 2.16                     | 0.46              |
| 1:A:1207:C:H5''  | 13:M:103:THR:HG1 | 1.80                     | 0.46              |
| 1:A:1413:C:H2'   | 1:A:1414:G:H5'   | 1.97                     | 0.46              |
| 2:B:92:TYR:OH    | 2:B:150:SER:OG   | 2.30                     | 0.46              |
| 2:B:100:GLY:C    | 2:B:108:ILE:HD12 | 2.40                     | 0.46              |
| 2:B:178:ARG:HH22 | 8:H:68:ARG:NH2   | 2.13                     | 0.46              |
| 2:B:178:ARG:O    | 8:H:71:GLY:HA2   | 2.14                     | 0.46              |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:HB   | 1.98                     | 0.46              |
| 5:E:126:ARG:HG3  | 5:E:126:ARG:HH11 | 1.81                     | 0.46              |
| 7:G:78:ARG:NH1   | 7:G:154:TYR:HB3  | 2.31                     | 0.46              |
| 11:K:51:LYS:O    | 11:K:55:LYS:HE2  | 2.16                     | 0.46              |
| 16:P:48:TRP:CD1  | 16:P:48:TRP:H    | 2.33                     | 0.46              |
| 20:T:45:GLN:HG2  | 20:T:91:LEU:CD2  | 2.41                     | 0.46              |
| 1:A:100:G:C2'    | 1:A:101:G:H5'    | 2.46                     | 0.46              |
| 1:A:241:A:C4'    | 1:A:242:G:OP1    | 2.62                     | 0.46              |
| 3:C:20:SER:HB3   | 3:C:40:ARG:HH22  | 1.80                     | 0.46              |
| 3:C:139:GLN:HA   | 3:C:139:GLN:HE21 | 1.76                     | 0.46              |
| 4:D:199:ASN:ND2  | 4:D:199:ASN:C    | 2.73                     | 0.46              |
| 6:F:2:ARG:HH21   | 6:F:69:GLU:CG    | 2.28                     | 0.46              |
| 8:H:10:LEU:CD1   | 8:H:85:ARG:HG2   | 2.45                     | 0.46              |
| 8:H:24:THR:HG22  | 8:H:63:LEU:HD21  | 1.98                     | 0.46              |
| 9:I:127:LYS:H    | 9:I:127:LYS:CD   | 2.28                     | 0.46              |
| 10:J:48:THR:HG23 | 10:J:62:HIS:CD2  | 2.50                     | 0.46              |
| 20:T:57:ARG:CZ   | 20:T:102:GLY:HA2 | 2.46                     | 0.46              |
| 22:W:3:G:N2      | 23:X:34:70U:HN3  | 2.05                     | 0.46              |
| 23:X:31:A:C2'    | 23:X:32:C:OP1    | 2.64                     | 0.46              |
| 1:A:94:A:O2'     | 1:A:95:G:H5'     | 2.16                     | 0.46              |
| 1:A:855:G:OP1    | 8:H:89:PRO:O     | 2.34                     | 0.46              |
| 1:A:949:C:OP1    | 10:J:57:LYS:CD   | 2.61                     | 0.46              |
| 1:A:1088:G:H5''  | 3:C:172:ARG:HG2  | 1.97                     | 0.46              |
| 1:A:1302:C:H2'   | 1:A:1303:C:C5    | 2.51                     | 0.46              |
| 2:B:169:LYS:HD3  | 2:B:169:LYS:C    | 2.41                     | 0.46              |
| 3:C:167:TRP:HB3  | 3:C:168:ALA:H    | 1.39                     | 0.46              |
| 7:G:122:HIS:HD2  | 7:G:125:MET:CE   | 2.28                     | 0.46              |
| 7:G:143:ARG:O    | 7:G:147:ALA:HB2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:83:ILE:HG23  | 8:H:83:ILE:O     | 2.16                     | 0.46              |
| 10:J:48:THR:OG1  | 10:J:62:HIS:CD2  | 2.68                     | 0.46              |
| 1:A:269:A:O2'    | 1:A:270:G:C8     | 2.69                     | 0.46              |
| 1:A:424:U:H1'    | 1:A:425:A:H5''   | 1.97                     | 0.46              |
| 1:A:469:G:O2'    | 1:A:470:U:OP2    | 2.29                     | 0.46              |
| 1:A:627:G:O2'    | 1:A:628:C:H5'    | 2.16                     | 0.46              |
| 1:A:695:A:H2'    | 1:A:696:G:O4'    | 2.16                     | 0.46              |
| 2:B:60:ASP:OD1   | 2:B:64:ARG:CZ    | 2.64                     | 0.46              |
| 2:B:231:GLU:HG3  | 2:B:232:PRO:HD2  | 1.98                     | 0.46              |
| 3:C:84:ILE:HG13  | 3:C:88:ARG:HH12  | 1.80                     | 0.46              |
| 5:E:143:ARG:HA   | 5:E:143:ARG:HD3  | 1.58                     | 0.46              |
| 10:J:6:ILE:HA    | 10:J:97:GLU:O    | 2.16                     | 0.46              |
| 14:N:45:ARG:HH11 | 14:N:45:ARG:HG3  | 1.81                     | 0.46              |
| 23:X:31:A:H2'    | 23:X:31:A:N3     | 2.31                     | 0.46              |
| 1:A:697:G:H21    | 1:A:760:A:H1'    | 1.79                     | 0.46              |
| 1:A:949:C:P      | 10:J:57:LYS:HD3  | 2.56                     | 0.46              |
| 1:A:1355:G:H8    | 1:A:1355:G:O5'   | 1.98                     | 0.46              |
| 3:C:139:GLN:NE2  | 3:C:139:GLN:CA   | 2.73                     | 0.46              |
| 5:E:116:THR:HG23 | 5:E:117:ASP:OD2  | 2.16                     | 0.46              |
| 6:F:76:ALA:O     | 6:F:80:ARG:HG3   | 2.16                     | 0.46              |
| 11:K:82:VAL:C    | 11:K:83:ILE:HG13 | 2.41                     | 0.46              |
| 12:L:111:LYS:HE3 | 12:L:112:ASP:OD1 | 2.15                     | 0.46              |
| 19:S:28:LYS:HD3  | 19:S:29:ARG:H    | 1.80                     | 0.46              |
| 1:A:544:U:H4'    | 1:A:545:C:OP2    | 2.16                     | 0.45              |
| 1:A:825:C:H2'    | 1:A:826:C:O5'    | 2.16                     | 0.45              |
| 1:A:929:U:O2'    | 1:A:930:G:H5'    | 2.16                     | 0.45              |
| 1:A:1219:A:H5'   | 1:A:1317:C:N4    | 2.13                     | 0.45              |
| 1:A:1450:A:O2'   | 1:A:1451:G:H5'   | 2.16                     | 0.45              |
| 1:A:1481:G:H3'   | 1:A:1481:G:OP2   | 2.16                     | 0.45              |
| 2:B:135:GLN:O    | 2:B:139:LYS:HB3  | 2.16                     | 0.45              |
| 11:K:18:ARG:HH12 | 11:K:36:ASP:HA   | 1.81                     | 0.45              |
| 16:P:26:ARG:HD2  | 16:P:31:LYS:O    | 2.16                     | 0.45              |
| 20:T:36:LEU:HD13 | 20:T:58:LYS:HG3  | 1.97                     | 0.45              |
| 1:A:1106:G:H5'   | 10:J:35:SER:OG   | 2.16                     | 0.45              |
| 1:A:1294:U:O4    | 19:S:4:SER:OG    | 2.29                     | 0.45              |
| 3:C:107:GLN:O    | 3:C:108:ASN:CB   | 2.64                     | 0.45              |
| 4:D:151:LYS:N    | 4:D:151:LYS:CD   | 2.71                     | 0.45              |
| 7:G:115:ARG:HB2  | 7:G:118:VAL:CG2  | 2.46                     | 0.45              |
| 10:J:33:GLN:O    | 10:J:34:VAL:HB   | 2.17                     | 0.45              |
| 15:O:34:LEU:O    | 15:O:34:LEU:HD23 | 2.16                     | 0.45              |
| 19:S:69:HIS:HB3  | 19:S:74:PHE:HE1  | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:10:LEU:HD13 | 20:T:11:SER:N    | 2.30                     | 0.45              |
| 1:A:1110:C:O2'   | 1:A:1112:A:N7    | 2.49                     | 0.45              |
| 1:A:1266:A:O2'   | 1:A:1267:A:OP2   | 2.32                     | 0.45              |
| 1:A:1347:G:C6    | 1:A:1348:C:C4    | 3.05                     | 0.45              |
| 3:C:68:VAL:HG12  | 3:C:70:VAL:HG13  | 1.98                     | 0.45              |
| 3:C:135:LYS:CE   | 5:E:50:GLU:HG2   | 2.47                     | 0.45              |
| 3:C:139:GLN:O    | 3:C:143:GLU:N    | 2.48                     | 0.45              |
| 12:L:56:ALA:O    | 12:L:67:THR:HA   | 2.16                     | 0.45              |
| 16:P:43:LYS:HA   | 16:P:48:TRP:CB   | 2.46                     | 0.45              |
| 16:P:81:ARG:HH11 | 16:P:83:GLU:CG   | 2.29                     | 0.45              |
| 1:A:332:C:H2'    | 1:A:333:A:H8     | 1.82                     | 0.45              |
| 1:A:407:A:C2     | 4:D:35:ARG:HB3   | 2.52                     | 0.45              |
| 1:A:613:G:C2'    | 1:A:614:G:H5'    | 2.46                     | 0.45              |
| 1:A:680:U:C2'    | 1:A:681:G:H5'    | 2.46                     | 0.45              |
| 1:A:726:U:H2'    | 1:A:727:C:H6     | 1.80                     | 0.45              |
| 2:B:208:ILE:HG21 | 2:B:239:VAL:HB   | 1.97                     | 0.45              |
| 4:D:21:LEU:HD21  | 4:D:114:ARG:HB2  | 1.97                     | 0.45              |
| 10:J:50:ILE:HA   | 10:J:60:ARG:HD2  | 1.98                     | 0.45              |
| 12:L:88:GLY:H    | 12:L:98:TYR:HA   | 1.81                     | 0.45              |
| 19:S:22:LEU:O    | 19:S:26:GLY:O    | 2.35                     | 0.45              |
| 1:A:1345:A:O2'   | 1:A:1346:U:OP2   | 2.26                     | 0.45              |
| 5:E:126:ARG:HG3  | 5:E:126:ARG:NH1  | 2.31                     | 0.45              |
| 13:M:67:GLU:O    | 13:M:70:LEU:N    | 2.44                     | 0.45              |
| 13:M:107:ALA:O   | 13:M:111:LYS:HG3 | 2.16                     | 0.45              |
| 16:P:81:ARG:HH11 | 16:P:83:GLU:HG3  | 1.80                     | 0.45              |
| 1:A:469:G:O2'    | 1:A:470:U:P      | 2.74                     | 0.45              |
| 1:A:1243:C:O5'   | 1:A:1243:C:H6    | 2.00                     | 0.45              |
| 4:D:70:ILE:HD11  | 4:D:100:ARG:CD   | 2.46                     | 0.45              |
| 12:L:60:LEU:HD21 | 12:L:85:ILE:HD11 | 1.99                     | 0.45              |
| 14:N:41:ARG:HG2  | 14:N:41:ARG:HH11 | 1.81                     | 0.45              |
| 15:O:11:VAL:HG21 | 15:O:34:LEU:HD12 | 1.99                     | 0.45              |
| 19:S:40:ILE:HB   | 19:S:67:VAL:O    | 2.16                     | 0.45              |
| 1:A:433:G:C4'    | 1:A:434:A:OP1    | 2.62                     | 0.45              |
| 1:A:581:U:H4'    | 8:H:94:TYR:CD1   | 2.51                     | 0.45              |
| 1:A:672:C:H2'    | 1:A:673:G:O4'    | 2.16                     | 0.45              |
| 1:A:798:A:O2'    | 1:A:799:A:P      | 2.75                     | 0.45              |
| 1:A:849:A:C4'    | 1:A:850:A:OP1    | 2.58                     | 0.45              |
| 1:A:915:A:C6     | 1:A:916:G:C5     | 3.05                     | 0.45              |
| 1:A:1168:G:P     | 9:I:113:LYS:NZ   | 2.90                     | 0.45              |
| 1:A:1170:C:H5'   | 1:A:1171:G:OP2   | 2.17                     | 0.45              |
| 2:B:43:ASP:OD1   | 2:B:46:LYS:HG2   | 2.17                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:106:TYR:CE1   | 4:D:113:SER:HA   | 2.52                     | 0.45              |
| 10:J:12:ASP:HB3   | 10:J:15:THR:HG22 | 1.99                     | 0.45              |
| 10:J:46:ARG:NH1   | 10:J:46:ARG:CG   | 2.78                     | 0.45              |
| 12:L:38:THR:HG21  | 12:L:59:ARG:HH21 | 1.81                     | 0.45              |
| 13:M:40:ASN:HB3   | 13:M:43:THR:HG23 | 1.99                     | 0.45              |
| 13:M:125:ARG:HH11 | 13:M:125:ARG:C   | 2.25                     | 0.45              |
| 17:Q:3:LYS:HB3    | 17:Q:61:GLU:HB3  | 1.99                     | 0.45              |
| 1:A:465:G:H2'     | 1:A:467:C:H41    | 1.82                     | 0.45              |
| 1:A:627:G:C2'     | 1:A:628:C:H5'    | 2.47                     | 0.45              |
| 1:A:1126:G:C8     | 1:A:1126:G:C3'   | 3.00                     | 0.45              |
| 3:C:58:GLU:C      | 3:C:59:ARG:HG2   | 2.41                     | 0.45              |
| 4:D:148:VAL:HG11  | 4:D:158:ILE:HD13 | 1.98                     | 0.45              |
| 9:I:3:GLN:HA      | 9:I:19:LEU:O     | 2.17                     | 0.45              |
| 9:I:4:TYR:CE2     | 9:I:88:TYR:HA    | 2.52                     | 0.45              |
| 12:L:42:THR:CG2   | 12:L:43:VAL:N    | 2.80                     | 0.45              |
| 13:M:87:TYR:C     | 13:M:89:GLY:N    | 2.73                     | 0.45              |
| 19:S:63:THR:HG21  | 19:S:65:ASN:HD21 | 1.81                     | 0.45              |
| 1:A:629:U:H2'     | 1:A:630:C:C6     | 2.52                     | 0.45              |
| 1:A:926:A:H2'     | 1:A:927:U:O4'    | 2.17                     | 0.45              |
| 1:A:963:A:H2'     | 1:A:964:G:O4'    | 2.16                     | 0.45              |
| 1:A:1400:A:H2'    | 1:A:1401:G:H5'   | 1.98                     | 0.45              |
| 1:A:1458:U:H2'    | 1:A:1459:G:O5'   | 2.17                     | 0.45              |
| 3:C:159:GLY:HA2   | 3:C:193:TYR:CD2  | 2.52                     | 0.45              |
| 13:M:40:ASN:C     | 13:M:40:ASN:ND2  | 2.75                     | 0.45              |
| 13:M:125:ARG:HD2  | 13:M:125:ARG:O   | 2.16                     | 0.45              |
| 17:Q:13:ASP:C     | 17:Q:15:MET:H    | 2.24                     | 0.45              |
| 21:V:2:GLY:C      | 21:V:4:GLY:N     | 2.74                     | 0.45              |
| 1:A:465:G:H2'     | 1:A:467:C:N4     | 2.31                     | 0.45              |
| 1:A:1458:U:H2'    | 1:A:1459:G:C5'   | 2.47                     | 0.45              |
| 5:E:120:THR:HG23  | 5:E:121:LYS:N    | 2.32                     | 0.45              |
| 7:G:146:GLU:HG2   | 7:G:149:ARG:HD3  | 1.99                     | 0.45              |
| 11:K:12:ARG:O     | 11:K:13:GLN:O    | 2.35                     | 0.45              |
| 16:P:6:LEU:HD12   | 16:P:6:LEU:N     | 2.32                     | 0.45              |
| 1:A:52:G:N7       | 1:A:355:A:C2     | 2.85                     | 0.44              |
| 1:A:562:G:H5'     | 1:A:711:A:C1'    | 2.36                     | 0.44              |
| 1:A:852:C:H1'     | 8:H:15:ASN:HD21  | 1.82                     | 0.44              |
| 1:A:960:A:HO2'    | 1:A:1031:U:HO2'  | 1.63                     | 0.44              |
| 1:A:1134:A:OP2    | 10:J:68:HIS:CE1  | 2.70                     | 0.44              |
| 2:B:39:ILE:HG22   | 2:B:40:HIS:H     | 1.82                     | 0.44              |
| 2:B:41:ILE:HD12   | 2:B:41:ILE:H     | 1.81                     | 0.44              |
| 2:B:82:ARG:HG2    | 2:B:82:ARG:HH11  | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:89:GLU:O     | 3:C:93:LYS:HG2   | 2.18                     | 0.44              |
| 3:C:188:LEU:HB3  | 3:C:189:ALA:H    | 1.58                     | 0.44              |
| 5:E:13:ILE:HG13  | 5:E:13:ILE:O     | 2.17                     | 0.44              |
| 9:I:78:LYS:O     | 9:I:78:LYS:HD2   | 2.16                     | 0.44              |
| 20:T:57:ARG:NE   | 20:T:102:GLY:HA2 | 2.32                     | 0.44              |
| 1:A:752:G:H4'    | 1:A:1490:A:H4'   | 1.99                     | 0.44              |
| 1:A:983:A:C8     | 1:A:983:A:H3'    | 2.53                     | 0.44              |
| 1:A:1151:A:H2'   | 1:A:1152:G:H5'   | 1.99                     | 0.44              |
| 7:G:64:GLN:HG2   | 7:G:128:ALA:HB1  | 1.98                     | 0.44              |
| 7:G:154:TYR:O    | 7:G:155:ARG:C    | 2.59                     | 0.44              |
| 9:I:36:TYR:CD2   | 9:I:37:PHE:CE2   | 3.05                     | 0.44              |
| 10:J:71:LEU:O    | 10:J:72:VAL:CB   | 2.65                     | 0.44              |
| 1:A:67:C:O2'     | 1:A:165:A:H1'    | 2.17                     | 0.44              |
| 1:A:634:C:C5'    | 1:A:635:U:OP2    | 2.59                     | 0.44              |
| 1:A:899:G:C6     | 1:A:900:A:C6     | 3.05                     | 0.44              |
| 1:A:1206:A:H5'   | 1:A:1207:C:OP2   | 2.18                     | 0.44              |
| 3:C:26:LYS:H     | 3:C:26:LYS:CD    | 2.17                     | 0.44              |
| 12:L:119:LYS:O   | 12:L:120:TYR:CB  | 2.66                     | 0.44              |
| 1:A:7:G:O2'      | 1:A:8:A:OP1      | 2.32                     | 0.44              |
| 1:A:98:G:H2'     | 1:A:99:C:C6      | 2.52                     | 0.44              |
| 1:A:145:A:H2'    | 1:A:146:A:O4'    | 2.17                     | 0.44              |
| 1:A:949:C:O2'    | 10:J:55:LYS:HA   | 2.17                     | 0.44              |
| 1:A:1262:U:C4'   | 1:A:1263:C:OP2   | 2.64                     | 0.44              |
| 1:A:1305:A:O4'   | 1:A:1343:C:H4'   | 2.18                     | 0.44              |
| 1:A:1417:G:H2'   | 1:A:1418:U:H6    | 1.80                     | 0.44              |
| 3:C:8:ILE:O      | 3:C:9:GLY:C      | 2.60                     | 0.44              |
| 7:G:56:GLN:HB3   | 7:G:60:LYS:HD3   | 1.98                     | 0.44              |
| 8:H:68:ARG:HG2   | 8:H:68:ARG:NH1   | 2.32                     | 0.44              |
| 10:J:26:ALA:CB   | 10:J:85:LEU:HD11 | 2.47                     | 0.44              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:CD   | 2.31                     | 0.44              |
| 13:M:65:LYS:HE3  | 13:M:69:GLU:CG   | 2.37                     | 0.44              |
| 13:M:67:GLU:HB3  | 13:M:68:GLY:H    | 1.58                     | 0.44              |
| 14:N:61:TRP:N    | 14:N:61:TRP:CE3  | 2.85                     | 0.44              |
| 19:S:11:VAL:HA   | 19:S:38:SER:HA   | 1.99                     | 0.44              |
| 20:T:70:SER:HA   | 20:T:73:HIS:CD2  | 2.52                     | 0.44              |
| 23:X:30:G:C4     | 23:X:31:A:N7     | 2.86                     | 0.44              |
| 1:A:577:G:H2'    | 1:A:578:G:H5'    | 2.00                     | 0.44              |
| 1:A:1327:A:HO2'  | 1:A:1328:G:P     | 2.41                     | 0.44              |
| 2:B:119:GLU:O    | 2:B:122:PHE:HB2  | 2.18                     | 0.44              |
| 3:C:6:HIS:CD2    | 3:C:8:ILE:HB     | 2.52                     | 0.44              |
| 6:F:40:VAL:HG22  | 6:F:41:GLU:N     | 2.32                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:O:71:GLN:HB2   | 15:O:78:TYR:CG   | 2.52                     | 0.44              |
| 1:A:50:A:H4'      | 1:A:51:A:OP2     | 2.16                     | 0.44              |
| 1:A:546:A:HO2'    | 1:A:549:G:HO2'   | 1.65                     | 0.44              |
| 1:A:740:U:H2'     | 1:A:741:G:O4'    | 2.17                     | 0.44              |
| 1:A:1110:C:O2'    | 1:A:1111:C:OP1   | 2.34                     | 0.44              |
| 1:A:1111:C:OP2    | 9:I:62:TYR:HE2   | 2.00                     | 0.44              |
| 1:A:1311:U:C2'    | 1:A:1312:G:H5'   | 2.48                     | 0.44              |
| 2:B:14:GLY:N      | 2:B:16:HIS:HE1   | 2.15                     | 0.44              |
| 2:B:44:LEU:O      | 2:B:47:THR:HB    | 2.18                     | 0.44              |
| 3:C:20:SER:HB2    | 3:C:22:TRP:HE1   | 1.83                     | 0.44              |
| 5:E:143:ARG:NH1   | 8:H:77:GLU:CD    | 2.76                     | 0.44              |
| 9:I:18:PHE:O      | 9:I:61:ALA:HA    | 2.17                     | 0.44              |
| 9:I:108:VAL:HG12  | 9:I:109:VAL:N    | 2.33                     | 0.44              |
| 10:J:72:VAL:O     | 10:J:73:ASP:O    | 2.36                     | 0.44              |
| 11:K:40:ILE:HG22  | 11:K:41:THR:HG23 | 1.99                     | 0.44              |
| 1:A:41:G:H2'      | 1:A:42:G:H8      | 1.82                     | 0.44              |
| 1:A:649:G:H5'     | 1:A:709:C:H1'    | 2.00                     | 0.44              |
| 1:A:1110:C:OP1    | 9:I:66:ARG:NH2   | 2.51                     | 0.44              |
| 1:A:1297:G:O2'    | 14:N:18:VAL:HG11 | 2.17                     | 0.44              |
| 1:A:1363:U:H2'    | 1:A:1364:C:H6    | 1.82                     | 0.44              |
| 1:A:1476:A:H1'    | 1:A:1497:G:H5'   | 1.99                     | 0.44              |
| 2:B:25:ASN:HD22   | 2:B:26:PRO:CD    | 2.30                     | 0.44              |
| 2:B:60:ASP:OD1    | 2:B:60:ASP:C     | 2.60                     | 0.44              |
| 5:E:15:ARG:HD2    | 5:E:15:ARG:C     | 2.43                     | 0.44              |
| 9:I:79:LEU:CD1    | 9:I:83:ARG:HD2   | 2.46                     | 0.44              |
| 10:J:32:ALA:HB2   | 10:J:76:ASN:HB2  | 2.00                     | 0.44              |
| 12:L:89:ARG:HA    | 12:L:97:ARG:HA   | 1.99                     | 0.44              |
| 14:N:45:ARG:O     | 14:N:49:HIS:CD2  | 2.71                     | 0.44              |
| 1:A:492:A:H5''    | 4:D:55:ALA:HB2   | 2.00                     | 0.44              |
| 1:A:513:G:O2'     | 1:A:514:U:P      | 2.76                     | 0.44              |
| 1:A:919:G:H2'     | 1:A:920:U:H6     | 1.83                     | 0.44              |
| 1:A:982:A:N6      | 1:A:1019:C:N4    | 2.64                     | 0.44              |
| 1:A:1394:C:H2'    | 1:A:1395:A:C8    | 2.53                     | 0.44              |
| 3:C:11:ARG:NH1    | 3:C:177:THR:O    | 2.51                     | 0.44              |
| 3:C:45:LYS:HB3    | 3:C:45:LYS:HE2   | 1.74                     | 0.44              |
| 4:D:190:ASP:O     | 4:D:191:ARG:C    | 2.60                     | 0.44              |
| 6:F:25:ILE:CD1    | 6:F:82:ARG:HH11  | 2.31                     | 0.44              |
| 12:L:55:VAL:CG1   | 12:L:56:ALA:N    | 2.81                     | 0.44              |
| 13:M:125:ARG:HH12 | 13:M:126:LYS:HG3 | 1.83                     | 0.44              |
| 17:Q:78:GLU:O     | 17:Q:78:GLU:HG3  | 2.16                     | 0.44              |
| 18:R:34:TYR:HB3   | 18:R:69:THR:HG23 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:57:ARG:HH22 | 20:T:100:ILE:CG1 | 2.29                     | 0.44              |
| 20:T:67:ALA:O    | 20:T:73:HIS:CE1  | 2.71                     | 0.44              |
| 1:A:12:U:H4'     | 1:A:509:C:O2'    | 2.18                     | 0.44              |
| 1:A:49:U:O4      | 1:A:359:A:C4     | 2.71                     | 0.44              |
| 1:A:750:A:H2'    | 1:A:751:A:C8     | 2.53                     | 0.44              |
| 1:A:988:G:O2'    | 1:A:989:G:H5'    | 2.18                     | 0.44              |
| 1:A:1039:G:C4    | 1:A:1185:A:C2    | 3.06                     | 0.44              |
| 1:A:1043:G:C6    | 1:A:1044:U:N3    | 2.86                     | 0.44              |
| 1:A:1327:A:O2'   | 1:A:1328:G:P     | 2.76                     | 0.44              |
| 1:A:1478:C:OP2   | 1:A:1481:G:H2'   | 2.17                     | 0.44              |
| 3:C:131:ARG:O    | 3:C:135:LYS:HG3  | 2.17                     | 0.44              |
| 3:C:177:THR:OG1  | 3:C:180:ALA:HB2  | 2.18                     | 0.44              |
| 9:I:13:ALA:HA    | 9:I:67:GLY:O     | 2.18                     | 0.44              |
| 9:I:20:ARG:O     | 9:I:22:GLY:N     | 2.51                     | 0.44              |
| 13:M:108:ARG:NE  | 13:M:108:ARG:HA  | 2.33                     | 0.44              |
| 19:S:80:TYR:O    | 19:S:81:ARG:C    | 2.60                     | 0.44              |
| 1:A:160:G:O2'    | 1:A:161:G:H5'    | 2.18                     | 0.43              |
| 1:A:200:C:H6     | 1:A:200:C:O5'    | 2.01                     | 0.43              |
| 1:A:406:A:N7     | 1:A:408:G:N3     | 2.66                     | 0.43              |
| 1:A:854:C:O2'    | 1:A:855:G:H5'    | 2.18                     | 0.43              |
| 1:A:993:A:H2'    | 1:A:994:A:C8     | 2.53                     | 0.43              |
| 1:A:1258:C:O2'   | 1:A:1260:A:H8    | 2.00                     | 0.43              |
| 1:A:1384:C:H2'   | 1:A:1385:C:O4'   | 2.17                     | 0.43              |
| 2:B:32:ILE:HD13  | 2:B:40:HIS:CE1   | 2.53                     | 0.43              |
| 2:B:112:VAL:O    | 2:B:115:LEU:HB3  | 2.18                     | 0.43              |
| 3:C:138:VAL:HG22 | 3:C:151:VAL:HG23 | 2.00                     | 0.43              |
| 6:F:10:LEU:HB3   | 6:F:84:ASN:O     | 2.18                     | 0.43              |
| 7:G:15:ASP:OD2   | 7:G:17:VAL:HB    | 2.18                     | 0.43              |
| 11:K:33:THR:HG22 | 11:K:39:PRO:HA   | 1.99                     | 0.43              |
| 12:L:41:ARG:CB   | 12:L:41:ARG:CZ   | 2.96                     | 0.43              |
| 20:T:82:SER:O    | 20:T:86:ARG:HG3  | 2.18                     | 0.43              |
| 20:T:86:ARG:HG2  | 20:T:86:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:102:A:C4'    | 1:A:103:C:OP2    | 2.64                     | 0.43              |
| 1:A:919:G:H2'    | 1:A:920:U:C6     | 2.52                     | 0.43              |
| 1:A:980:G:C8     | 1:A:980:G:C3'    | 3.01                     | 0.43              |
| 2:B:228:GLY:O    | 2:B:229:VAL:C    | 2.61                     | 0.43              |
| 3:C:76:VAL:HG11  | 3:C:103:VAL:CG2  | 2.47                     | 0.43              |
| 8:H:126:LYS:C    | 8:H:128:GLY:N    | 2.75                     | 0.43              |
| 9:I:83:ARG:O     | 9:I:86:VAL:N     | 2.50                     | 0.43              |
| 9:I:97:LYS:HB2   | 9:I:102:LEU:HD12 | 1.99                     | 0.43              |
| 13:M:5:ALA:HB2   | 13:M:22:ILE:HD13 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:6:LEU:HB3   | 14:N:23:ARG:HH21 | 1.83                     | 0.43              |
| 1:A:366:G:O2'    | 1:A:367:C:H5'    | 2.18                     | 0.43              |
| 1:A:437:C:H2'    | 1:A:438:C:C6     | 2.51                     | 0.43              |
| 1:A:586:U:H2'    | 1:A:587:G:H8     | 1.83                     | 0.43              |
| 1:A:645:G:O2'    | 1:A:819:G:C5'    | 2.66                     | 0.43              |
| 1:A:1206:A:C4'   | 1:A:1207:C:OP2   | 2.66                     | 0.43              |
| 1:A:1281:G:C2'   | 1:A:1282:U:OP2   | 2.66                     | 0.43              |
| 2:B:16:HIS:O     | 2:B:17:PHE:C     | 2.61                     | 0.43              |
| 3:C:35:GLU:O     | 3:C:36:ASP:C     | 2.62                     | 0.43              |
| 5:E:31:LEU:HD22  | 5:E:43:LEU:CD2   | 2.48                     | 0.43              |
| 7:G:88:PRO:CB    | 7:G:145:ALA:HB1  | 2.48                     | 0.43              |
| 7:G:93:PRO:HA    | 7:G:96:GLN:HE21  | 1.83                     | 0.43              |
| 9:I:3:GLN:HG3    | 9:I:20:ARG:CG    | 2.45                     | 0.43              |
| 18:R:87:ARG:HG2  | 18:R:87:ARG:HH11 | 1.84                     | 0.43              |
| 1:A:52:G:C6      | 1:A:355:A:N3     | 2.87                     | 0.43              |
| 1:A:446:A:H5'    | 16:P:72:ARG:HH21 | 1.79                     | 0.43              |
| 1:A:465:G:C4'    | 1:A:466:A:OP1    | 2.66                     | 0.43              |
| 1:A:468:G:O2'    | 1:A:469:G:H5''   | 2.19                     | 0.43              |
| 1:A:558:G:H4'    | 1:A:559:G:O5'    | 2.18                     | 0.43              |
| 1:A:637:G:C5     | 1:A:638:A:C5     | 3.07                     | 0.43              |
| 1:A:1124:G:H2'   | 1:A:1125:G:H5'   | 2.01                     | 0.43              |
| 1:A:1207:C:N4    | 13:M:104:ARG:HG3 | 2.33                     | 0.43              |
| 2:B:14:GLY:N     | 2:B:16:HIS:CE1   | 2.86                     | 0.43              |
| 2:B:69:LEU:CD1   | 2:B:155:LEU:HD11 | 2.48                     | 0.43              |
| 4:D:145:GLU:OE2  | 4:D:182:LYS:HD2  | 2.18                     | 0.43              |
| 4:D:166:LYS:C    | 4:D:168:ARG:H    | 2.26                     | 0.43              |
| 6:F:92:LYS:HB2   | 6:F:92:LYS:HE3   | 1.74                     | 0.43              |
| 7:G:45:ASP:O     | 7:G:49:ILE:HG13  | 2.18                     | 0.43              |
| 8:H:1:MET:HG2    | 8:H:2:LEU:N      | 2.33                     | 0.43              |
| 12:L:26:ALA:C    | 12:L:27:LEU:O    | 2.62                     | 0.43              |
| 14:N:26:ARG:HE   | 14:N:47:LEU:HD21 | 1.84                     | 0.43              |
| 1:A:48:C:O2'     | 1:A:49:U:P       | 2.71                     | 0.43              |
| 1:A:406:A:C5     | 1:A:408:G:N3     | 2.86                     | 0.43              |
| 1:A:530:A:O2'    | 1:A:531:G:P      | 2.77                     | 0.43              |
| 2:B:20:GLU:HB2   | 2:B:190:THR:HB   | 2.00                     | 0.43              |
| 2:B:178:ARG:NH2  | 8:H:68:ARG:HH22  | 2.16                     | 0.43              |
| 3:C:8:ILE:C      | 3:C:10:PHE:N     | 2.75                     | 0.43              |
| 3:C:26:LYS:HB3   | 10:J:45:ARG:HH21 | 1.83                     | 0.43              |
| 8:H:6:ILE:O      | 8:H:10:LEU:HG    | 2.18                     | 0.43              |
| 8:H:35:ILE:O     | 8:H:39:LEU:HD13  | 2.19                     | 0.43              |
| 8:H:119:LEU:HD13 | 8:H:124:ALA:HA   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:82:ALA:O     | 9:I:86:VAL:HG23  | 2.17                     | 0.43              |
| 10:J:28:ARG:HG3  | 10:J:29:ARG:HG2  | 1.99                     | 0.43              |
| 13:M:87:TYR:O    | 13:M:88:ARG:C    | 2.61                     | 0.43              |
| 1:A:361:C:H4'    | 1:A:362:U:OP1    | 2.18                     | 0.43              |
| 1:A:413:C:H1'    | 1:A:421:G:N2     | 2.33                     | 0.43              |
| 1:A:494:C:O2'    | 1:A:495:U:O5'    | 2.35                     | 0.43              |
| 1:A:1286:G:O2'   | 1:A:1287:A:C8    | 2.72                     | 0.43              |
| 1:A:1291:G:N7    | 19:S:2:PRO:HD3   | 2.34                     | 0.43              |
| 4:D:31:CYS:O     | 4:D:31:CYS:SG    | 2.76                     | 0.43              |
| 6:F:75:LEU:O     | 6:F:79:LEU:HG    | 2.19                     | 0.43              |
| 13:M:10:PRO:CB   | 13:M:18:ALA:HB1  | 2.40                     | 0.43              |
| 1:A:890:A:H4'    | 1:A:891:A:O5'    | 2.18                     | 0.43              |
| 1:A:911:C:H5'    | 1:A:912:A:OP1    | 2.19                     | 0.43              |
| 1:A:1250:A:C2    | 1:A:1294:U:O4'   | 2.72                     | 0.43              |
| 2:B:87:ARG:HB2   | 2:B:219:VAL:HG11 | 2.00                     | 0.43              |
| 2:B:98:LEU:HD12  | 2:B:101:MET:HE3  | 2.00                     | 0.43              |
| 3:C:77:ILE:HA    | 3:C:84:ILE:HB    | 2.01                     | 0.43              |
| 6:F:44:GLY:HA2   | 6:F:59:TYR:CD1   | 2.52                     | 0.43              |
| 8:H:111:ILE:HD12 | 8:H:135:CYS:SG   | 2.59                     | 0.43              |
| 10:J:13:HIS:HB3  | 10:J:68:HIS:CE1  | 2.53                     | 0.43              |
| 13:M:80:ARG:O    | 13:M:84:ILE:HG12 | 2.19                     | 0.43              |
| 13:M:107:ALA:HB3 | 13:M:111:LYS:HD2 | 2.01                     | 0.43              |
| 19:S:20:LEU:HA   | 19:S:23:ASN:HD22 | 1.83                     | 0.43              |
| 1:A:7:G:H21      | 5:E:121:LYS:HG2  | 1.83                     | 0.43              |
| 1:A:250:G:H1'    | 17:Q:16:GLN:NE2  | 2.34                     | 0.43              |
| 1:A:250:G:O6     | 1:A:261:G:O6     | 2.37                     | 0.43              |
| 1:A:814:U:H2'    | 1:A:815:C:C6     | 2.50                     | 0.43              |
| 3:C:83:ARG:O     | 3:C:85:ARG:N     | 2.52                     | 0.43              |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:HD13 | 2.00                     | 0.43              |
| 8:H:10:LEU:CD2   | 8:H:83:ILE:HD11  | 2.49                     | 0.43              |
| 8:H:104:ARG:O    | 8:H:105:ARG:C    | 2.62                     | 0.43              |
| 10:J:6:ILE:HG13  | 10:J:6:ILE:O     | 2.17                     | 0.43              |
| 12:L:102:ARG:HD2 | 12:L:102:ARG:HA  | 1.86                     | 0.43              |
| 14:N:26:ARG:NE   | 14:N:47:LEU:HD21 | 2.33                     | 0.43              |
| 15:O:76:GLU:O    | 15:O:77:ARG:C    | 2.60                     | 0.43              |
| 17:Q:59:ILE:CG2  | 17:Q:71:PHE:HB3  | 2.48                     | 0.43              |
| 19:S:5:LEU:O     | 19:S:6:LYS:HB2   | 2.18                     | 0.43              |
| 21:V:6:ARG:HB3   | 21:V:15:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:208:U:H4'    | 1:A:209:U:OP1    | 2.19                     | 0.43              |
| 1:A:399:U:H2'    | 1:A:400:U:C6     | 2.54                     | 0.43              |
| 1:A:470:U:O5'    | 1:A:470:U:H6     | 2.01                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:494:C:O2'    | 1:A:495:U:H6      | 2.02                     | 0.43              |
| 1:A:798:A:H4'    | 1:A:799:A:OP2     | 2.19                     | 0.43              |
| 1:A:1519:U:H2'   | 1:A:1520:C:O4'    | 2.19                     | 0.43              |
| 2:B:92:TYR:CD2   | 2:B:151:GLY:HA3   | 2.54                     | 0.43              |
| 3:C:6:HIS:CD2    | 3:C:8:ILE:H       | 2.34                     | 0.43              |
| 4:D:3:ARG:O      | 4:D:4:TYR:HB3     | 2.17                     | 0.43              |
| 4:D:70:ILE:HG23  | 4:D:74:GLN:HB2    | 2.00                     | 0.43              |
| 9:I:95:LYS:O     | 9:I:99:LEU:HD23   | 2.19                     | 0.43              |
| 9:I:114:TYR:CE1  | 10:J:59:SER:O     | 2.71                     | 0.43              |
| 1:A:53:A:N1      | 1:A:54:C:C2       | 2.87                     | 0.43              |
| 1:A:872:G:H2'    | 1:A:873:C:C6      | 2.54                     | 0.43              |
| 1:A:1158:G:H8    | 1:A:1158:G:O5'    | 2.02                     | 0.43              |
| 3:C:76:VAL:O     | 3:C:83:ARG:CG     | 2.66                     | 0.43              |
| 4:D:8:VAL:HG21   | 4:D:115:ARG:HH11  | 1.84                     | 0.43              |
| 6:F:45:LEU:H     | 6:F:45:LEU:HD12   | 1.83                     | 0.43              |
| 9:I:9:ARG:CG     | 9:I:14:VAL:HG22   | 2.48                     | 0.43              |
| 16:P:18:ARG:CG   | 16:P:35:LYS:HE3   | 2.47                     | 0.43              |
| 1:A:46:G:O2'     | 1:A:360:U:H1'     | 2.19                     | 0.42              |
| 1:A:143:A:H2'    | 1:A:144:C:C6      | 2.54                     | 0.42              |
| 1:A:278:C:O2'    | 1:A:279:G:H5'     | 2.19                     | 0.42              |
| 1:A:725:G:O2'    | 1:A:726:U:H5'     | 2.19                     | 0.42              |
| 1:A:927:U:H3'    | 13:M:102:ARG:HH21 | 1.84                     | 0.42              |
| 1:A:953:G:OP1    | 14:N:31:ARG:O     | 2.37                     | 0.42              |
| 1:A:1213:U:H5''  | 9:I:124:GLN:O     | 2.20                     | 0.42              |
| 1:A:1374:G:H21   | 1:A:1479:A:H8     | 1.66                     | 0.42              |
| 2:B:204:ASN:HD22 | 2:B:205:ASP:N     | 2.17                     | 0.42              |
| 4:D:76:ARG:O     | 4:D:80:GLU:HG2    | 2.19                     | 0.42              |
| 4:D:182:LYS:NZ   | 4:D:182:LYS:HB2   | 2.34                     | 0.42              |
| 11:K:95:ILE:O    | 11:K:99:GLN:HG3   | 2.19                     | 0.42              |
| 12:L:115:LYS:C   | 12:L:117:ARG:H    | 2.23                     | 0.42              |
| 17:Q:81:ARG:HE   | 17:Q:81:ARG:HB2   | 1.64                     | 0.42              |
| 1:A:8:A:N6       | 4:D:205:GLU:O     | 2.50                     | 0.42              |
| 1:A:545:C:H1'    | 12:L:15:ARG:HD2   | 2.01                     | 0.42              |
| 1:A:1481:G:O2'   | 1:A:1482:G:OP2    | 2.30                     | 0.42              |
| 2:B:78:GLN:HE22  | 2:B:96:ARG:NH1    | 2.10                     | 0.42              |
| 2:B:142:LEU:O    | 2:B:142:LEU:HD23  | 2.20                     | 0.42              |
| 3:C:34:LEU:CD1   | 3:C:38:ARG:HD3    | 2.49                     | 0.42              |
| 9:I:33:PHE:O     | 9:I:35:GLU:N      | 2.52                     | 0.42              |
| 11:K:114:VAL:HA  | 11:K:115:PRO:HD3  | 1.86                     | 0.42              |
| 14:N:33:VAL:HG23 | 14:N:33:VAL:O     | 2.18                     | 0.42              |
| 19:S:11:VAL:HG22 | 19:S:39:THR:O     | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:155:A:H2'    | 1:A:156:A:O5'     | 2.19                     | 0.42              |
| 1:A:319:G:N2     | 1:A:322:A:C8      | 2.87                     | 0.42              |
| 1:A:798:A:HO2'   | 1:A:799:A:P       | 2.41                     | 0.42              |
| 1:A:911:C:C4'    | 1:A:912:A:OP1     | 2.67                     | 0.42              |
| 1:A:915:A:N6     | 1:A:916:G:C6      | 2.87                     | 0.42              |
| 1:A:1062:A:C5'   | 5:E:16:THR:HG21   | 2.49                     | 0.42              |
| 1:A:1168:G:OP1   | 9:I:113:LYS:NZ    | 2.52                     | 0.42              |
| 1:A:1302:C:H2'   | 1:A:1303:C:H5     | 1.84                     | 0.42              |
| 1:A:1432:C:O2'   | 1:A:1433:G:OP2    | 2.36                     | 0.42              |
| 2:B:178:ARG:NH2  | 8:H:68:ARG:NH2    | 2.67                     | 0.42              |
| 10:J:12:ASP:OD2  | 10:J:13:HIS:N     | 2.53                     | 0.42              |
| 10:J:94:VAL:HG12 | 10:J:95:GLU:N     | 2.35                     | 0.42              |
| 13:M:68:GLY:HA2  | 13:M:71:ARG:HD2   | 2.01                     | 0.42              |
| 13:M:96:LEU:O    | 13:M:97:PRO:C     | 2.63                     | 0.42              |
| 20:T:72:LEU:O    | 20:T:73:HIS:O     | 2.36                     | 0.42              |
| 1:A:412:C:H6     | 1:A:412:C:O5'     | 2.01                     | 0.42              |
| 1:A:513:G:O2'    | 23:X:35:U:H4'     | 2.19                     | 0.42              |
| 1:A:952:A:H5'    | 1:A:952:A:C8      | 2.50                     | 0.42              |
| 1:A:972:C:H6     | 1:A:972:C:O5'     | 2.01                     | 0.42              |
| 1:A:1027:C:C2'   | 1:A:1028:A:O5'    | 2.68                     | 0.42              |
| 1:A:1039:G:H5''  | 3:C:154:SER:OG    | 2.20                     | 0.42              |
| 1:A:1074:A:C2    | 1:A:1164:A:C6     | 3.08                     | 0.42              |
| 2:B:209:ARG:HH22 | 2:B:236:TYR:HA    | 1.85                     | 0.42              |
| 3:C:50:ALA:HB2   | 3:C:75:VAL:HG23   | 2.00                     | 0.42              |
| 3:C:174:PRO:HB2  | 3:C:177:THR:HG23  | 2.00                     | 0.42              |
| 17:Q:95:TYR:HA   | 17:Q:98:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:53:A:C2      | 1:A:54:C:H1'      | 2.55                     | 0.42              |
| 1:A:453:G:C3'    | 1:A:454:A:H5''    | 2.49                     | 0.42              |
| 1:A:1106:G:C4'   | 1:A:1107:U:OP1    | 2.55                     | 0.42              |
| 1:A:1210:A:H2'   | 1:A:1211:C:H6     | 1.83                     | 0.42              |
| 2:B:64:ARG:HG2   | 2:B:64:ARG:O      | 2.20                     | 0.42              |
| 9:I:5:TYR:CD1    | 9:I:6:GLY:N       | 2.87                     | 0.42              |
| 11:K:32:ILE:CG2  | 11:K:77:MET:HE2   | 2.49                     | 0.42              |
| 12:L:83:VAL:CG2  | 12:L:100:ILE:HG23 | 2.50                     | 0.42              |
| 13:M:10:PRO:O    | 13:M:45:VAL:HG11  | 2.18                     | 0.42              |
| 19:S:44:MET:O    | 19:S:45:VAL:C     | 2.63                     | 0.42              |
| 1:A:198:U:O3'    | 20:T:57:ARG:HD3   | 2.19                     | 0.42              |
| 1:A:602:U:N3     | 4:D:134:ASP:OD1   | 2.52                     | 0.42              |
| 1:A:612:G:O2'    | 1:A:613:G:H5'     | 2.20                     | 0.42              |
| 1:A:714:G:H5'    | 1:A:749:A:H4'     | 2.02                     | 0.42              |
| 1:A:956:C:H2'    | 1:A:957:C:H5'     | 2.01                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1324:G:H2'  | 1:A:1325:C:C6    | 2.53                     | 0.42              |
| 4:D:62:GLN:HE22 | 4:D:65:ARG:HH12  | 1.67                     | 0.42              |
| 5:E:64:ARG:NH1  | 5:E:64:ARG:CG    | 2.75                     | 0.42              |
| 7:G:36:LYS:O    | 7:G:39:ALA:HB3   | 2.20                     | 0.42              |
| 9:I:112:LYS:HD3 | 9:I:112:LYS:C    | 2.44                     | 0.42              |
| 13:M:23:TYR:HB3 | 13:M:67:GLU:HA   | 2.01                     | 0.42              |
| 16:P:22:THR:HA  | 16:P:33:ILE:HG13 | 2.01                     | 0.42              |
| 20:T:56:MET:HE2 | 20:T:88:VAL:HB   | 2.01                     | 0.42              |
| 1:A:523:G:H2'   | 1:A:524:G:O4'    | 2.19                     | 0.42              |
| 1:A:607:C:H2'   | 1:A:608:G:H8     | 1.85                     | 0.42              |
| 1:A:675:U:H2'   | 1:A:677:A:OP2    | 2.20                     | 0.42              |
| 2:B:226:ARG:HG2 | 2:B:226:ARG:NH1  | 2.31                     | 0.42              |
| 4:D:64:LEU:C    | 4:D:64:LEU:CD2   | 2.92                     | 0.42              |
| 6:F:45:LEU:O    | 6:F:46:ARG:HG2   | 2.20                     | 0.42              |
| 11:K:34:ASP:C   | 11:K:36:ASP:H    | 2.27                     | 0.42              |
| 1:A:135:A:H1'   | 1:A:176:U:O2     | 2.19                     | 0.42              |
| 1:A:162:G:O2'   | 1:A:163:C:H5'    | 2.20                     | 0.42              |
| 1:A:286:C:O2'   | 1:A:287:G:H5'    | 2.20                     | 0.42              |
| 1:A:310:A:O2'   | 1:A:311:G:P      | 2.77                     | 0.42              |
| 1:A:639:C:O2'   | 15:O:28:GLN:OE1  | 2.25                     | 0.42              |
| 1:A:1042:C:O2'  | 1:A:1043:G:H5'   | 2.19                     | 0.42              |
| 1:A:1160:A:H2'  | 1:A:1161:A:O4'   | 2.20                     | 0.42              |
| 1:A:1186:U:H2'  | 1:A:1187:G:C8    | 2.55                     | 0.42              |
| 1:A:1367:G:O2'  | 1:A:1368:G:H5'   | 2.20                     | 0.42              |
| 1:A:1384:C:O2   | 1:A:1477:A:N1    | 2.53                     | 0.42              |
| 2:B:50:GLU:HB3  | 2:B:200:ILE:O    | 2.20                     | 0.42              |
| 2:B:181:PHE:HD2 | 8:H:70:GLN:HB3   | 1.85                     | 0.42              |
| 4:D:61:LYS:HE2  | 4:D:206:PHE:CE2  | 2.55                     | 0.42              |
| 5:E:11:ILE:HD12 | 5:E:31:LEU:HD13  | 2.01                     | 0.42              |
| 5:E:28:PHE:O    | 5:E:47:LYS:HA    | 2.20                     | 0.42              |
| 5:E:78:HIS:HD2  | 8:H:107:LEU:HD12 | 1.85                     | 0.42              |
| 7:G:89:MET:HB3  | 7:G:155:ARG:HH12 | 1.84                     | 0.42              |
| 7:G:101:LEU:O   | 7:G:105:VAL:HG23 | 2.18                     | 0.42              |
| 14:N:48:ALA:HB2 | 14:N:53:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:543:U:C4'   | 1:A:544:U:H5''   | 2.44                     | 0.42              |
| 1:A:645:G:O2'   | 1:A:819:G:H5'    | 2.19                     | 0.42              |
| 1:A:839:C:O2'   | 1:A:840:U:H5'    | 2.20                     | 0.42              |
| 1:A:984:C:C5    | 1:A:985:C:C5     | 3.07                     | 0.42              |
| 1:A:1094:C:O2   | 3:C:179:ARG:HB3  | 2.20                     | 0.42              |
| 1:A:1362:U:O2'  | 1:A:1363:U:OP2   | 2.30                     | 0.42              |
| 1:A:1516:C:H5   | 7:G:82:GLY:CA    | 2.22                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:32:LEU:HD12  | 3:C:59:ARG:NH1   | 2.34                     | 0.42              |
| 4:D:24:GLU:C     | 4:D:26:CYS:N     | 2.76                     | 0.42              |
| 7:G:15:ASP:HB3   | 7:G:19:GLY:CA    | 2.50                     | 0.42              |
| 9:I:26:VAL:HG12  | 9:I:28:VAL:HG23  | 2.02                     | 0.42              |
| 11:K:48:ILE:HD11 | 11:K:64:ALA:CA   | 2.43                     | 0.42              |
| 16:P:26:ARG:NH2  | 16:P:31:LYS:HE2  | 2.35                     | 0.42              |
| 19:S:20:LEU:HA   | 19:S:23:ASN:ND2  | 2.34                     | 0.42              |
| 20:T:8:ARG:HB3   | 20:T:9:ASN:H     | 1.71                     | 0.42              |
| 1:A:423:G:OP2    | 4:D:7:PRO:HG3    | 2.20                     | 0.42              |
| 1:A:485:G:P      | 12:L:118:SER:HB3 | 2.59                     | 0.42              |
| 1:A:586:U:H2'    | 1:A:587:G:C8     | 2.55                     | 0.42              |
| 1:A:637:G:C2     | 1:A:638:A:H1'    | 2.55                     | 0.42              |
| 1:A:1006:C:H2'   | 1:A:1007:C:C5'   | 2.48                     | 0.42              |
| 1:A:1183:G:C2    | 14:N:42:ILE:HG21 | 2.55                     | 0.42              |
| 2:B:42:ILE:HD11  | 2:B:190:THR:OG1  | 2.20                     | 0.42              |
| 2:B:187:LEU:HD12 | 2:B:201:ILE:O    | 2.19                     | 0.42              |
| 6:F:33:TYR:CD1   | 6:F:75:LEU:HD23  | 2.54                     | 0.42              |
| 8:H:20:TYR:CE2   | 8:H:75:ARG:HD2   | 2.55                     | 0.42              |
| 9:I:43:ALA:C     | 9:I:45:ALA:H     | 2.26                     | 0.42              |
| 9:I:58:ARG:HG2   | 9:I:58:ARG:NH1   | 2.33                     | 0.42              |
| 9:I:118:LYS:NZ   | 9:I:118:LYS:CB   | 2.83                     | 0.42              |
| 10:J:5:ARG:H     | 10:J:100:THR:HA  | 1.84                     | 0.42              |
| 17:Q:21:VAL:HG21 | 17:Q:59:ILE:HD11 | 2.01                     | 0.42              |
| 20:T:10:LEU:HD13 | 20:T:10:LEU:C    | 2.44                     | 0.42              |
| 1:A:49:U:C4'     | 1:A:50:A:OP2     | 2.60                     | 0.41              |
| 1:A:157:C:H2'    | 1:A:158:U:H6     | 1.83                     | 0.41              |
| 1:A:453:G:H2'    | 1:A:454:A:H5''   | 2.01                     | 0.41              |
| 1:A:545:C:O2'    | 1:A:546:A:OP2    | 2.36                     | 0.41              |
| 1:A:577:G:O2'    | 1:A:578:G:H5'    | 2.20                     | 0.41              |
| 1:A:637:G:C2     | 1:A:638:A:C1'    | 3.03                     | 0.41              |
| 1:A:1123:C:O2'   | 1:A:1124:G:H5'   | 2.19                     | 0.41              |
| 1:A:1124:G:C2'   | 1:A:1125:G:H5'   | 2.49                     | 0.41              |
| 1:A:1237:A:C1'   | 1:A:1239:G:O4'   | 2.66                     | 0.41              |
| 1:A:1281:G:O2'   | 1:A:1282:U:H6    | 2.02                     | 0.41              |
| 2:B:118:LEU:C    | 2:B:120:ALA:N    | 2.78                     | 0.41              |
| 2:B:216:SER:C    | 2:B:218:ALA:N    | 2.77                     | 0.41              |
| 3:C:64:VAL:HG21  | 3:C:99:VAL:HG12  | 2.02                     | 0.41              |
| 3:C:136:GLN:O    | 3:C:139:GLN:HB2  | 2.19                     | 0.41              |
| 3:C:154:SER:OG   | 3:C:196:LEU:HA   | 2.20                     | 0.41              |
| 4:D:8:VAL:CG2    | 4:D:115:ARG:HH11 | 2.32                     | 0.41              |
| 4:D:30:LYS:C     | 4:D:32:ALA:H     | 2.28                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:17:ASP:C    | 10:J:19:SER:N     | 2.76                     | 0.41              |
| 18:R:45:SER:O    | 18:R:47:THR:O     | 2.38                     | 0.41              |
| 19:S:80:TYR:CZ   | 19:S:81:ARG:HD2   | 2.55                     | 0.41              |
| 20:T:41:VAL:O    | 20:T:45:GLN:HB2   | 2.20                     | 0.41              |
| 22:W:2:A:H5'     | 22:W:2:A:C8       | 2.46                     | 0.41              |
| 1:A:16:A:N1      | 1:A:896:A:H2      | 2.17                     | 0.41              |
| 1:A:80:U:H6      | 1:A:80:U:O5'      | 2.03                     | 0.41              |
| 1:A:566:A:H2'    | 1:A:567:G:O4'     | 2.20                     | 0.41              |
| 1:A:584:C:C2     | 1:A:621:G:N2      | 2.88                     | 0.41              |
| 1:A:1218:C:C4'   | 1:A:1315:G:N2     | 2.83                     | 0.41              |
| 1:A:1290:G:C5    | 1:A:1310:A:C2     | 3.08                     | 0.41              |
| 3:C:76:VAL:HG11  | 3:C:103:VAL:HG22  | 2.02                     | 0.41              |
| 8:H:75:ARG:HA    | 8:H:76:PRO:HD3    | 1.83                     | 0.41              |
| 9:I:89:ASN:O     | 9:I:92:TYR:HB2    | 2.20                     | 0.41              |
| 18:R:34:TYR:HA   | 18:R:69:THR:CG2   | 2.50                     | 0.41              |
| 23:X:31:A:C2     | 23:X:32:C:C6      | 3.08                     | 0.41              |
| 1:A:895:A:H2'    | 1:A:896:A:O4'     | 2.19                     | 0.41              |
| 1:A:1259:U:H4'   | 1:A:1260:A:O5'    | 2.20                     | 0.41              |
| 2:B:13:ALA:C     | 2:B:16:HIS:CE1    | 2.97                     | 0.41              |
| 3:C:5:ILE:O      | 3:C:6:HIS:C       | 2.62                     | 0.41              |
| 3:C:113:ALA:HB3  | 3:C:114:PRO:HD3   | 2.02                     | 0.41              |
| 5:E:40:ARG:NH1   | 5:E:68:GLU:OE1    | 2.43                     | 0.41              |
| 7:G:148:ASN:C    | 7:G:150:ALA:H     | 2.28                     | 0.41              |
| 9:I:20:ARG:O     | 9:I:21:PRO:C      | 2.61                     | 0.41              |
| 9:I:79:LEU:HD13  | 9:I:79:LEU:O      | 2.20                     | 0.41              |
| 11:K:99:GLN:HG2  | 11:K:105:VAL:HG21 | 2.01                     | 0.41              |
| 13:M:30:ALA:C    | 13:M:32:GLU:H     | 2.28                     | 0.41              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:HD2   | 1.85                     | 0.41              |
| 15:O:53:HIS:O    | 15:O:57:LEU:HD13  | 2.20                     | 0.41              |
| 19:S:27:GLU:HB3  | 19:S:28:LYS:H     | 1.70                     | 0.41              |
| 1:A:114:C:H4'    | 1:A:115:G:OP1     | 2.20                     | 0.41              |
| 1:A:176:U:H5'    | 1:A:176:U:H6      | 1.86                     | 0.41              |
| 1:A:465:G:HO2'   | 1:A:467:C:N4      | 2.17                     | 0.41              |
| 1:A:497:C:H2'    | 1:A:498:G:C8      | 2.55                     | 0.41              |
| 1:A:522:A:H2'    | 1:A:523:G:C8      | 2.55                     | 0.41              |
| 1:A:525:G:H2'    | 1:A:526:C:C6      | 2.56                     | 0.41              |
| 1:A:725:G:C2'    | 1:A:726:U:H5'     | 2.50                     | 0.41              |
| 1:A:1024:G:C2'   | 1:A:1025:C:H5'    | 2.50                     | 0.41              |
| 1:A:1034:U:H2'   | 1:A:1181:C:H41    | 1.85                     | 0.41              |
| 1:A:1371:C:H2'   | 1:A:1372:U:O4'    | 2.20                     | 0.41              |
| 1:A:1485:G:H2'   | 1:A:1486:C:O4'    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:15:VAL:HB     | 2:B:209:ARG:HB3   | 2.02                     | 0.41              |
| 6:F:67:MET:HB2    | 6:F:68:PRO:CD     | 2.50                     | 0.41              |
| 6:F:69:GLU:O      | 6:F:72:VAL:HG23   | 2.21                     | 0.41              |
| 10:J:49:VAL:O     | 10:J:61:GLU:N     | 2.51                     | 0.41              |
| 17:Q:45:HIS:CD2   | 17:Q:47:PRO:HG3   | 2.55                     | 0.41              |
| 17:Q:63:ARG:O     | 17:Q:65:ILE:CD1   | 2.68                     | 0.41              |
| 1:A:31:G:H1       | 1:A:48:C:H5''     | 1.85                     | 0.41              |
| 1:A:405:G:O6      | 1:A:424:U:O2'     | 2.39                     | 0.41              |
| 1:A:450:C:H2'     | 1:A:451:C:C6      | 2.51                     | 0.41              |
| 1:A:729:A:O2'     | 1:A:730:C:H5'     | 2.21                     | 0.41              |
| 1:A:988:G:H2'     | 1:A:989:G:H8      | 1.84                     | 0.41              |
| 1:A:1286:G:O2'    | 1:A:1287:A:OP2    | 2.34                     | 0.41              |
| 3:C:185:GLY:O     | 3:C:200:ALA:N     | 2.49                     | 0.41              |
| 6:F:6:VAL:HG13    | 6:F:90:VAL:HG22   | 2.01                     | 0.41              |
| 8:H:20:TYR:HE2    | 8:H:75:ARG:HD2    | 1.85                     | 0.41              |
| 9:I:7:THR:HG22    | 9:I:8:GLY:N       | 2.36                     | 0.41              |
| 9:I:40:LEU:C      | 9:I:42:ARG:N      | 2.79                     | 0.41              |
| 10:J:12:ASP:OD2   | 10:J:12:ASP:C     | 2.63                     | 0.41              |
| 12:L:93:LEU:O     | 12:L:94:PRO:C     | 2.62                     | 0.41              |
| 18:R:19:LYS:HD2   | 18:R:19:LYS:N     | 2.25                     | 0.41              |
| 1:A:45:U:H2'      | 1:A:46:G:C8       | 2.56                     | 0.41              |
| 1:A:481:U:H2'     | 1:A:482:A:O5'     | 2.20                     | 0.41              |
| 1:A:954:A:O2'     | 1:A:956:C:OP2     | 2.37                     | 0.41              |
| 2:B:62:ALA:C      | 2:B:64:ARG:H      | 2.27                     | 0.41              |
| 2:B:73:THR:HG23   | 2:B:95:GLN:O      | 2.21                     | 0.41              |
| 3:C:23:TYR:CG     | 3:C:24:ALA:N      | 2.89                     | 0.41              |
| 4:D:135:LEU:HB2   | 4:D:138:TYR:HB2   | 2.01                     | 0.41              |
| 5:E:32:VAL:HG12   | 5:E:58:ALA:HB1    | 2.02                     | 0.41              |
| 5:E:96:PRO:HA     | 5:E:117:ASP:OD2   | 2.20                     | 0.41              |
| 8:H:63:LEU:HD22   | 8:H:63:LEU:H      | 1.85                     | 0.41              |
| 9:I:26:VAL:HA     | 9:I:61:ALA:O      | 2.21                     | 0.41              |
| 12:L:89:ARG:NH2   | 12:L:97:ARG:HH21  | 2.16                     | 0.41              |
| 12:L:104:VAL:O    | 12:L:105:TYR:HB2  | 2.20                     | 0.41              |
| 1:A:246:G:C4'     | 1:A:247:U:O5'     | 2.54                     | 0.41              |
| 1:A:1354:U:H2'    | 1:A:1355:G:O4'    | 2.20                     | 0.41              |
| 1:A:1433:G:H2'    | 1:A:1434:G:O4'    | 2.21                     | 0.41              |
| 25:A:1786:PAR:O52 | 25:A:1786:PAR:C11 | 2.49                     | 0.41              |
| 4:D:157:LEU:HA    | 4:D:160:GLN:HE21  | 1.86                     | 0.41              |
| 5:E:36:ASP:OD2    | 5:E:40:ARG:HB2    | 2.19                     | 0.41              |
| 8:H:72:PRO:O      | 8:H:73:ASP:CB     | 2.69                     | 0.41              |
| 9:I:11:LYS:O      | 9:I:11:LYS:CG     | 2.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:43:ALA:O     | 9:I:44:VAL:C     | 2.64                     | 0.41              |
| 10:J:47:PHE:CZ   | 14:N:37:PHE:HE1  | 2.38                     | 0.41              |
| 17:Q:97:SER:CB   | 17:Q:105:ALA:HB3 | 2.38                     | 0.41              |
| 17:Q:100:LYS:CD  | 17:Q:101:ARG:NE  | 2.84                     | 0.41              |
| 19:S:15:LEU:N    | 19:S:15:LEU:CD2  | 2.82                     | 0.41              |
| 22:W:3:G:H22     | 23:X:34:70U:C2   | 2.32                     | 0.41              |
| 1:A:289:U:OP1    | 1:A:593:G:O2'    | 2.31                     | 0.41              |
| 1:A:565:U:C2     | 1:A:743:G:C6     | 3.08                     | 0.41              |
| 1:A:611:G:H2'    | 1:A:612:G:H8     | 1.85                     | 0.41              |
| 1:A:701:G:H5''   | 1:A:702:C:OP2    | 2.21                     | 0.41              |
| 1:A:1006:C:C6    | 1:A:1006:C:C3'   | 3.04                     | 0.41              |
| 1:A:1043:G:O4'   | 10:J:56:HIS:CE1  | 2.73                     | 0.41              |
| 3:C:10:PHE:CE2   | 3:C:178:LEU:HD13 | 2.56                     | 0.41              |
| 3:C:91:LEU:HD12  | 3:C:101:LEU:HD12 | 2.03                     | 0.41              |
| 3:C:134:ILE:HD11 | 3:C:153:VAL:HG23 | 2.01                     | 0.41              |
| 4:D:173:TRP:CD2  | 4:D:189:PRO:HB3  | 2.56                     | 0.41              |
| 6:F:42:GLU:HG3   | 6:F:61:LEU:CD2   | 2.50                     | 0.41              |
| 7:G:146:GLU:HA   | 7:G:149:ARG:CG   | 2.50                     | 0.41              |
| 7:G:146:GLU:OE1  | 7:G:146:GLU:O    | 2.39                     | 0.41              |
| 17:Q:33:GLY:O    | 17:Q:34:LYS:C    | 2.64                     | 0.41              |
| 17:Q:66:SER:OG   | 17:Q:69:LYS:HB2  | 2.21                     | 0.41              |
| 19:S:24:ALA:C    | 19:S:25:LYS:HG3  | 2.46                     | 0.41              |
| 20:T:57:ARG:HH21 | 20:T:102:GLY:HA2 | 1.86                     | 0.41              |
| 1:A:50:A:C6      | 1:A:356:G:O4'    | 2.74                     | 0.41              |
| 1:A:61:G:H2'     | 1:A:62:U:O4'     | 2.21                     | 0.41              |
| 1:A:123:G:O2'    | 1:A:124:A:OP2    | 2.37                     | 0.41              |
| 1:A:173:A:O2'    | 1:A:174:U:H5'    | 2.21                     | 0.41              |
| 1:A:315:C:H2'    | 1:A:316:A:O4'    | 2.21                     | 0.41              |
| 1:A:400:U:H5''   | 1:A:479:A:C2     | 2.55                     | 0.41              |
| 1:A:422:U:C4     | 1:A:423:G:C6     | 3.08                     | 0.41              |
| 1:A:542:A:H4'    | 1:A:543:U:H5'    | 2.03                     | 0.41              |
| 1:A:545:C:HO2'   | 12:L:15:ARG:HB3  | 1.81                     | 0.41              |
| 1:A:627:G:C5     | 1:A:628:C:C5     | 3.09                     | 0.41              |
| 1:A:835:G:O2'    | 1:A:836:A:H5'    | 2.21                     | 0.41              |
| 1:A:930:G:H2'    | 1:A:931:G:O4'    | 2.21                     | 0.41              |
| 1:A:938:U:C2'    | 1:A:939:C:H5'    | 2.51                     | 0.41              |
| 1:A:1002:G:H8    | 1:A:1002:G:H3'   | 1.86                     | 0.41              |
| 1:A:1067:U:O3'   | 1:A:1068:U:H6    | 2.04                     | 0.41              |
| 1:A:1219:A:C8    | 1:A:1284:C:H1'   | 2.55                     | 0.41              |
| 1:A:1396:U:H2'   | 1:A:1397:G:H8    | 1.86                     | 0.41              |
| 2:B:107:THR:C    | 2:B:109:SER:H    | 2.28                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:131:PRO:HG2  | 2:B:134:GLU:HG3  | 2.02                     | 0.41              |
| 3:C:8:ILE:O      | 3:C:11:ARG:N     | 2.41                     | 0.41              |
| 3:C:60:ALA:HB3   | 3:C:63:ASN:HB2   | 2.03                     | 0.41              |
| 3:C:84:ILE:O     | 3:C:88:ARG:NH1   | 2.53                     | 0.41              |
| 3:C:172:ARG:HB3  | 3:C:174:PRO:HD3  | 2.03                     | 0.41              |
| 3:C:188:LEU:HD22 | 3:C:195:VAL:CG1  | 2.51                     | 0.41              |
| 4:D:3:ARG:O      | 4:D:5:ILE:N      | 2.44                     | 0.41              |
| 9:I:42:ARG:O     | 9:I:43:ALA:C     | 2.63                     | 0.41              |
| 12:L:78:GLN:C    | 12:L:80:HIS:N    | 2.78                     | 0.41              |
| 13:M:29:ARG:HB3  | 13:M:64:TRP:CH2  | 2.56                     | 0.41              |
| 13:M:121:LYS:HE3 | 13:M:121:LYS:HB2 | 1.85                     | 0.41              |
| 14:N:37:PHE:CE2  | 14:N:53:LEU:HD13 | 2.56                     | 0.41              |
| 15:O:17:ARG:NH1  | 15:O:17:ARG:CG   | 2.81                     | 0.41              |
| 15:O:26:GLU:HA   | 15:O:81:LEU:HD11 | 2.02                     | 0.41              |
| 15:O:87:ILE:CG2  | 15:O:88:ARG:N    | 2.83                     | 0.41              |
| 18:R:25:THR:CG2  | 18:R:42:ARG:NH1  | 2.83                     | 0.41              |
| 20:T:86:ARG:O    | 20:T:90:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:105:G:C2'    | 1:A:106:G:H5'    | 2.51                     | 0.41              |
| 1:A:295:A:H8     | 1:A:295:A:O5'    | 2.04                     | 0.41              |
| 1:A:425:A:C2'    | 1:A:426:A:H5'    | 2.51                     | 0.41              |
| 1:A:511:C:H41    | 12:L:49:ASN:ND2  | 2.19                     | 0.41              |
| 1:A:539:C:O2'    | 1:A:540:G:H5'    | 2.21                     | 0.41              |
| 1:A:819:G:C6     | 1:A:828:G:C6     | 3.09                     | 0.41              |
| 1:A:944:C:O5'    | 1:A:944:C:H6     | 2.03                     | 0.41              |
| 1:A:1021:C:H2'   | 1:A:1022:U:C6    | 2.56                     | 0.41              |
| 1:A:1067:U:O3'   | 1:A:1068:U:C6    | 2.74                     | 0.41              |
| 1:A:1093:A:N1    | 3:C:177:THR:CG2  | 2.78                     | 0.41              |
| 1:A:1134:A:O2'   | 1:A:1135:C:H5'   | 2.21                     | 0.41              |
| 1:A:1308:C:O2'   | 1:A:1309:C:H5'   | 2.21                     | 0.41              |
| 1:A:1349:C:H2'   | 1:A:1350:G:O4'   | 2.21                     | 0.41              |
| 2:B:135:GLN:O    | 2:B:139:LYS:HD2  | 2.21                     | 0.41              |
| 4:D:61:LYS:NZ    | 4:D:72:GLU:OE2   | 2.54                     | 0.41              |
| 8:H:104:ARG:NH2  | 8:H:138:TRP:CZ3  | 2.88                     | 0.41              |
| 9:I:82:ALA:CA    | 9:I:96:LEU:HD21  | 2.52                     | 0.41              |
| 9:I:113:LYS:H    | 9:I:119:ALA:HA   | 1.86                     | 0.41              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:N    | 2.19                     | 0.41              |
| 17:Q:95:TYR:HA   | 17:Q:98:LEU:CD1  | 2.51                     | 0.41              |
| 20:T:36:LEU:HA   | 20:T:39:LYS:HB2  | 2.03                     | 0.41              |
| 1:A:421:G:P      | 4:D:36:ARG:HH21  | 2.44                     | 0.40              |
| 1:A:484:C:OP1    | 12:L:117:ARG:NH2 | 2.53                     | 0.40              |
| 1:A:538:C:H2'    | 1:A:539:C:C6     | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:983:A:OP1    | 1:A:983:A:O3'    | 2.38                     | 0.40              |
| 1:A:1363:U:H2'   | 1:A:1364:C:C6    | 2.56                     | 0.40              |
| 2:B:62:ALA:C     | 2:B:64:ARG:N     | 2.79                     | 0.40              |
| 2:B:119:GLU:CG   | 2:B:142:LEU:HD11 | 2.51                     | 0.40              |
| 3:C:117:ALA:HB2  | 3:C:200:ALA:HB2  | 2.04                     | 0.40              |
| 9:I:33:PHE:CZ    | 9:I:43:ALA:HB1   | 2.56                     | 0.40              |
| 10:J:26:ALA:HB2  | 10:J:85:LEU:HD11 | 2.02                     | 0.40              |
| 10:J:64:GLU:HB3  | 14:N:59:ALA:HB2  | 2.03                     | 0.40              |
| 11:K:126:ARG:O   | 11:K:129:SER:N   | 2.54                     | 0.40              |
| 13:M:79:LYS:HD3  | 13:M:83:ASP:OD2  | 2.21                     | 0.40              |
| 15:O:39:LEU:O    | 15:O:43:LEU:HG   | 2.21                     | 0.40              |
| 20:T:57:ARG:HH22 | 20:T:100:ILE:CD1 | 2.33                     | 0.40              |
| 1:A:173:A:H2'    | 1:A:174:U:C6     | 2.56                     | 0.40              |
| 1:A:453:G:C3'    | 1:A:454:A:C5'    | 2.99                     | 0.40              |
| 1:A:549:G:H4'    | 1:A:550:G:OP1    | 2.21                     | 0.40              |
| 1:A:810:U:H5''   | 1:A:811:A:OP2    | 2.20                     | 0.40              |
| 1:A:916:G:H5''   | 7:G:102:ARG:CZ   | 2.51                     | 0.40              |
| 1:A:942:A:HO2'   | 1:A:943:G:P      | 2.45                     | 0.40              |
| 1:A:1162:G:O2'   | 1:A:1163:G:O5'   | 2.37                     | 0.40              |
| 1:A:1167:G:N2    | 1:A:1168:G:H1'   | 2.35                     | 0.40              |
| 1:A:1194:A:H4'   | 1:A:1195:C:OP1   | 2.21                     | 0.40              |
| 7:G:10:ARG:O     | 7:G:10:ARG:HG3   | 2.21                     | 0.40              |
| 7:G:84:ASN:O     | 7:G:85:TYR:CD2   | 2.74                     | 0.40              |
| 9:I:8:GLY:CA     | 9:I:79:LEU:HD12  | 2.39                     | 0.40              |
| 19:S:5:LEU:O     | 19:S:6:LYS:CB    | 2.70                     | 0.40              |
| 1:A:105:G:O2'    | 1:A:106:G:H5'    | 2.21                     | 0.40              |
| 1:A:113:A:O2'    | 1:A:114:C:H5'    | 2.21                     | 0.40              |
| 1:A:257:A:C6     | 1:A:258:A:C6     | 3.09                     | 0.40              |
| 1:A:481:U:O2'    | 1:A:482:A:H5'    | 2.22                     | 0.40              |
| 1:A:837:A:H2'    | 1:A:838:G:O4'    | 2.21                     | 0.40              |
| 1:A:1044:U:H2'   | 1:A:1045:C:C6    | 2.57                     | 0.40              |
| 1:A:1409:U:O2'   | 1:A:1410:A:H5'   | 2.21                     | 0.40              |
| 2:B:134:GLU:C    | 2:B:136:VAL:N    | 2.79                     | 0.40              |
| 3:C:129:ALA:HB3  | 3:C:132:ARG:NH2  | 2.36                     | 0.40              |
| 5:E:76:ILE:O     | 5:E:93:PRO:HB3   | 2.22                     | 0.40              |
| 10:J:27:ALA:HB1  | 10:J:30:SER:OG   | 2.22                     | 0.40              |
| 13:M:96:LEU:O    | 13:M:110:ARG:NH1 | 2.54                     | 0.40              |
| 14:N:10:ALA:C    | 14:N:12:ARG:N    | 2.80                     | 0.40              |
| 1:A:31:G:C2      | 1:A:48:C:H5''    | 2.56                     | 0.40              |
| 1:A:400:U:H5''   | 1:A:479:A:H2     | 1.86                     | 0.40              |
| 1:A:409:A:OP2    | 1:A:423:G:N2     | 2.51                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:975:G:O2'    | 1:A:976:C:H5'     | 2.21                     | 0.40              |
| 1:A:995:G:H2'    | 1:A:996:C:C6      | 2.56                     | 0.40              |
| 1:A:1095:C:H6    | 1:A:1095:C:O5'    | 2.05                     | 0.40              |
| 1:A:1168:G:P     | 9:I:113:LYS:HZ3   | 2.45                     | 0.40              |
| 1:A:1194:A:O2'   | 1:A:1195:C:P      | 2.80                     | 0.40              |
| 2:B:71:VAL:O     | 2:B:71:VAL:HG23   | 2.21                     | 0.40              |
| 2:B:78:GLN:O     | 2:B:94:ASN:ND2    | 2.55                     | 0.40              |
| 2:B:188:ALA:O    | 2:B:202:PRO:HA    | 2.22                     | 0.40              |
| 3:C:106:VAL:O    | 3:C:108:ASN:N     | 2.54                     | 0.40              |
| 3:C:179:ARG:HG3  | 3:C:207:VAL:HA    | 2.03                     | 0.40              |
| 7:G:39:ALA:O     | 7:G:42:ILE:HB     | 2.20                     | 0.40              |
| 9:I:125:TYR:CD2  | 9:I:125:TYR:N     | 2.88                     | 0.40              |
| 13:M:25:ILE:HD11 | 13:M:60:VAL:CG1   | 2.52                     | 0.40              |
| 14:N:33:VAL:HA   | 14:N:39:LEU:O     | 2.22                     | 0.40              |
| 15:O:17:ARG:NH1  | 15:O:77:ARG:NH1   | 2.69                     | 0.40              |
| 1:A:238:A:H4'    | 1:A:239:U:O5'     | 2.21                     | 0.40              |
| 1:A:383:G:HO2'   | 1:A:384:A:P       | 2.44                     | 0.40              |
| 1:A:434:A:C4     | 1:A:480:A:C2      | 3.09                     | 0.40              |
| 1:A:690:C:H2'    | 1:A:691:C:H6      | 1.85                     | 0.40              |
| 1:A:1046:G:N2    | 1:A:1171:G:O2'    | 2.55                     | 0.40              |
| 1:A:1219:A:N7    | 1:A:1284:C:H1'    | 2.36                     | 0.40              |
| 1:A:1283:U:O2'   | 1:A:1284:C:OP1    | 2.34                     | 0.40              |
| 1:A:1345:A:H4'   | 1:A:1346:U:O5'    | 2.21                     | 0.40              |
| 3:C:117:ALA:HB2  | 3:C:200:ALA:CB    | 2.51                     | 0.40              |
| 4:D:61:LYS:C     | 4:D:61:LYS:HD2    | 2.47                     | 0.40              |
| 5:E:69:VAL:HA    | 5:E:70:PRO:HD3    | 1.67                     | 0.40              |
| 7:G:114:ARG:HG2  | 7:G:114:ARG:NH1   | 2.31                     | 0.40              |
| 9:I:80:GLY:C     | 9:I:82:ALA:N      | 2.79                     | 0.40              |
| 13:M:120:LYS:HZ1 | 13:M:123:ALA:HB3  | 1.82                     | 0.40              |
| 14:N:9:LYS:C     | 14:N:9:LYS:CD     | 2.93                     | 0.40              |
| 16:P:6:LEU:N     | 16:P:6:LEU:CD1    | 2.85                     | 0.40              |
| 16:P:63:GLY:O    | 16:P:64:ALA:C     | 2.63                     | 0.40              |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:CD1   | 2.52                     | 0.40              |
| 20:T:57:ARG:NH2  | 20:T:100:ILE:HG12 | 2.35                     | 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 |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 2   | B     | 232/256 (91%)   | 178 (77%)  | 40 (17%)  | 14 (6%)  | 1           | 3   |
| 3   | C     | 204/239 (85%)   | 149 (73%)  | 36 (18%)  | 19 (9%)  | 0           | 1   |
| 4   | D     | 206/209 (99%)   | 171 (83%)  | 27 (13%)  | 8 (4%)   | 2           | 8   |
| 5   | E     | 148/162 (91%)   | 136 (92%)  | 11 (7%)   | 1 (1%)   | 18          | 47  |
| 6   | F     | 99/101 (98%)    | 86 (87%)   | 12 (12%)  | 1 (1%)   | 12          | 38  |
| 7   | G     | 153/156 (98%)   | 130 (85%)  | 18 (12%)  | 5 (3%)   | 3           | 11  |
| 8   | H     | 136/138 (99%)   | 125 (92%)  | 10 (7%)   | 1 (1%)   | 18          | 47  |
| 9   | I     | 125/128 (98%)   | 94 (75%)   | 23 (18%)  | 8 (6%)   | 1           | 3   |
| 10  | J     | 96/105 (91%)    | 69 (72%)   | 20 (21%)  | 7 (7%)   | 1           | 2   |
| 11  | K     | 117/129 (91%)   | 101 (86%)  | 10 (8%)   | 6 (5%)   | 1           | 5   |
| 12  | L     | 122/132 (92%)   | 95 (78%)   | 16 (13%)  | 11 (9%)  | 0           | 1   |
| 13  | M     | 123/126 (98%)   | 90 (73%)   | 25 (20%)  | 8 (6%)   | 1           | 3   |
| 14  | N     | 58/61 (95%)     | 42 (72%)   | 13 (22%)  | 3 (5%)   | 1           | 5   |
| 15  | O     | 86/89 (97%)     | 75 (87%)   | 9 (10%)   | 2 (2%)   | 5           | 18  |
| 16  | P     | 81/88 (92%)     | 68 (84%)   | 13 (16%)  | 0        | 100         | 100 |
| 17  | Q     | 102/105 (97%)   | 90 (88%)   | 7 (7%)    | 5 (5%)   | 1           | 6   |
| 18  | R     | 71/88 (81%)     | 65 (92%)   | 5 (7%)    | 1 (1%)   | 9           | 30  |
| 19  | S     | 78/93 (84%)     | 58 (74%)   | 13 (17%)  | 7 (9%)   | 0           | 1   |
| 20  | T     | 97/106 (92%)    | 80 (82%)   | 8 (8%)    | 9 (9%)   | 0           | 1   |
| 21  | V     | 22/27 (82%)     | 17 (77%)   | 3 (14%)   | 2 (9%)   | 0           | 1   |
| All | All   | 2356/2538 (93%) | 1919 (82%) | 319 (14%) | 118 (5%) | 1           | 5   |

All (118) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 17  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 95  | GLN  |
| 2   | B     | 190 | THR  |
| 3   | C     | 16  | ARG  |
| 3   | C     | 18  | TRP  |
| 3   | C     | 61  | ALA  |
| 3   | C     | 154 | SER  |
| 3   | C     | 189 | ALA  |
| 4   | D     | 20  | TYR  |
| 7   | G     | 155 | ARG  |
| 9   | I     | 41  | VAL  |
| 10  | J     | 55  | LYS  |
| 10  | J     | 73  | ASP  |
| 10  | J     | 90  | LEU  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 115 | LYS  |
| 12  | L     | 116 | SER  |
| 13  | M     | 23  | TYR  |
| 13  | M     | 67  | GLU  |
| 14  | N     | 8   | GLU  |
| 14  | N     | 22  | THR  |
| 17  | Q     | 80  | GLY  |
| 17  | Q     | 81  | ARG  |
| 18  | R     | 87  | ARG  |
| 19  | S     | 30  | LEU  |
| 20  | T     | 73  | HIS  |
| 2   | B     | 11  | LEU  |
| 3   | C     | 65  | ALA  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 205 | GLY  |
| 4   | D     | 22  | LYS  |
| 6   | F     | 100 | ASN  |
| 7   | G     | 17  | VAL  |
| 8   | H     | 83  | ILE  |
| 9   | I     | 44  | VAL  |
| 9   | I     | 101 | PHE  |
| 10  | J     | 54  | PHE  |
| 10  | J     | 60  | ARG  |
| 10  | J     | 72  | VAL  |
| 11  | K     | 13  | GLN  |
| 11  | K     | 35  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 52  | GLY  |
| 11  | K     | 88  | GLY  |
| 12  | L     | 28  | LYS  |
| 12  | L     | 79  | GLU  |
| 12  | L     | 80  | HIS  |
| 13  | M     | 7   | VAL  |
| 13  | M     | 24  | GLY  |
| 13  | M     | 86  | CYS  |
| 17  | Q     | 14  | LYS  |
| 19  | S     | 6   | LYS  |
| 19  | S     | 8   | GLY  |
| 19  | S     | 67  | VAL  |
| 20  | T     | 9   | ASN  |
| 20  | T     | 94  | ALA  |
| 20  | T     | 96  | GLY  |
| 2   | B     | 14  | GLY  |
| 2   | B     | 16  | HIS  |
| 2   | B     | 20  | GLU  |
| 2   | B     | 64  | ARG  |
| 2   | B     | 115 | LEU  |
| 3   | C     | 47  | LEU  |
| 3   | C     | 146 | ALA  |
| 7   | G     | 7   | ALA  |
| 9   | I     | 7   | THR  |
| 9   | I     | 12  | GLU  |
| 9   | I     | 34  | ASN  |
| 9   | I     | 56  | LEU  |
| 13  | M     | 121 | LYS  |
| 15  | O     | 86  | GLY  |
| 17  | Q     | 104 | LYS  |
| 19  | S     | 28  | LYS  |
| 20  | T     | 99  | LEU  |
| 2   | B     | 207 | ALA  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 108 | ASN  |
| 3   | C     | 168 | ALA  |
| 4   | D     | 5   | ILE  |
| 4   | D     | 24  | GLU  |
| 4   | D     | 36  | ARG  |
| 4   | D     | 175 | SER  |
| 9   | I     | 21  | PRO  |
| 12  | L     | 29  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 32  | SER  |
| 19  | S     | 9   | VAL  |
| 20  | T     | 95  | ALA  |
| 20  | T     | 97  | ALA  |
| 20  | T     | 98  | PRO  |
| 20  | T     | 102 | GLY  |
| 21  | V     | 9   | ARG  |
| 2   | B     | 229 | VAL  |
| 3   | C     | 107 | GLN  |
| 5   | E     | 65  | ASN  |
| 7   | G     | 81  | GLY  |
| 11  | K     | 127 | LYS  |
| 12  | L     | 105 | TYR  |
| 17  | Q     | 68  | ARG  |
| 19  | S     | 68  | GLY  |
| 2   | B     | 63  | MET  |
| 4   | D     | 29  | PRO  |
| 10  | J     | 34  | VAL  |
| 12  | L     | 51  | ALA  |
| 12  | L     | 91  | LYS  |
| 2   | B     | 127 | ILE  |
| 2   | B     | 130 | ARG  |
| 3   | C     | 51  | GLY  |
| 3   | C     | 66  | VAL  |
| 13  | M     | 68  | GLY  |
| 21  | V     | 22  | ARG  |
| 3   | C     | 84  | ILE  |
| 3   | C     | 130 | VAL  |
| 4   | D     | 88  | VAL  |
| 7   | G     | 82  | GLY  |
| 11  | K     | 102 | GLY  |
| 13  | M     | 124 | PRO  |
| 15  | O     | 23  | GLY  |

### 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 |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | B     | 202/220 (92%)   | 186 (92%)  | 16 (8%)  | 11          | 35 |
| 3   | C     | 160/188 (85%)   | 145 (91%)  | 15 (9%)  | 8           | 27 |
| 4   | D     | 180/181 (99%)   | 170 (94%)  | 10 (6%)  | 19          | 50 |
| 5   | E     | 115/123 (94%)   | 98 (85%)   | 17 (15%) | 3           | 10 |
| 6   | F     | 90/90 (100%)    | 84 (93%)   | 6 (7%)   | 15          | 42 |
| 7   | G     | 126/127 (99%)   | 119 (94%)  | 7 (6%)   | 19          | 50 |
| 8   | H     | 119/119 (100%)  | 110 (92%)  | 9 (8%)   | 12          | 36 |
| 9   | I     | 98/99 (99%)     | 93 (95%)   | 5 (5%)   | 21          | 54 |
| 10  | J     | 87/92 (95%)     | 84 (97%)   | 3 (3%)   | 32          | 68 |
| 11  | K     | 90/99 (91%)     | 86 (96%)   | 4 (4%)   | 25          | 59 |
| 12  | L     | 104/109 (95%)   | 100 (96%)  | 4 (4%)   | 29          | 64 |
| 13  | M     | 100/101 (99%)   | 93 (93%)   | 7 (7%)   | 14          | 40 |
| 14  | N     | 49/50 (98%)     | 44 (90%)   | 5 (10%)  | 7           | 23 |
| 15  | O     | 79/80 (99%)     | 70 (89%)   | 9 (11%)  | 5           | 19 |
| 16  | P     | 72/74 (97%)     | 70 (97%)   | 2 (3%)   | 38          | 73 |
| 17  | Q     | 96/97 (99%)     | 90 (94%)   | 6 (6%)   | 16          | 45 |
| 18  | R     | 64/77 (83%)     | 58 (91%)   | 6 (9%)   | 8           | 27 |
| 19  | S     | 71/80 (89%)     | 67 (94%)   | 4 (6%)   | 19          | 50 |
| 20  | T     | 76/82 (93%)     | 72 (95%)   | 4 (5%)   | 20          | 52 |
| 21  | V     | 19/22 (86%)     | 18 (95%)   | 1 (5%)   | 20          | 52 |
| All | All   | 1997/2110 (95%) | 1857 (93%) | 140 (7%) | 14          | 40 |

All (140) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 16  | HIS  |
| 2   | B     | 21  | ARG  |
| 2   | B     | 25  | ASN  |
| 2   | B     | 40  | HIS  |
| 2   | B     | 80  | ILE  |
| 2   | B     | 83  | MET  |
| 2   | B     | 117 | GLU  |
| 2   | B     | 122 | PHE  |
| 2   | B     | 139 | LYS  |
| 2   | B     | 144 | ARG  |
| 2   | B     | 169 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 170 | GLU  |
| 2   | B     | 178 | ARG  |
| 2   | B     | 215 | LEU  |
| 2   | B     | 221 | LEU  |
| 2   | B     | 231 | GLU  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 5   | ILE  |
| 3   | C     | 12  | LEU  |
| 3   | C     | 14  | ILE  |
| 3   | C     | 26  | LYS  |
| 3   | C     | 38  | ARG  |
| 3   | C     | 42  | LEU  |
| 3   | C     | 52  | LEU  |
| 3   | C     | 105 | GLU  |
| 3   | C     | 127 | ARG  |
| 3   | C     | 139 | GLN  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 192 | THR  |
| 3   | C     | 204 | LEU  |
| 4   | D     | 3   | ARG  |
| 4   | D     | 10  | ARG  |
| 4   | D     | 21  | LEU  |
| 4   | D     | 49  | ARG  |
| 4   | D     | 53  | ASP  |
| 4   | D     | 58  | LEU  |
| 4   | D     | 118 | ARG  |
| 4   | D     | 192 | GLU  |
| 4   | D     | 194 | LEU  |
| 4   | D     | 199 | ASN  |
| 5   | E     | 12  | LEU  |
| 5   | E     | 14  | ARG  |
| 5   | E     | 24  | ARG  |
| 5   | E     | 31  | LEU  |
| 5   | E     | 33  | VAL  |
| 5   | E     | 38  | GLN  |
| 5   | E     | 41  | VAL  |
| 5   | E     | 43  | LEU  |
| 5   | E     | 47  | LYS  |
| 5   | E     | 50  | GLU  |
| 5   | E     | 64  | ARG  |
| 5   | E     | 76  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 80  | ILE  |
| 5   | E     | 89  | ILE  |
| 5   | E     | 116 | THR  |
| 5   | E     | 120 | THR  |
| 5   | E     | 137 | GLU  |
| 6   | F     | 1   | MET  |
| 6   | F     | 10  | LEU  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 27  | GLN  |
| 6   | F     | 55  | ASP  |
| 6   | F     | 82  | ARG  |
| 7   | G     | 5   | ARG  |
| 7   | G     | 12  | LEU  |
| 7   | G     | 16  | LEU  |
| 7   | G     | 45  | ASP  |
| 7   | G     | 73  | MET  |
| 7   | G     | 113 | GLU  |
| 7   | G     | 155 | ARG  |
| 8   | H     | 2   | LEU  |
| 8   | H     | 18  | ARG  |
| 8   | H     | 26  | VAL  |
| 8   | H     | 30  | ARG  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 91  | ARG  |
| 8   | H     | 92  | ARG  |
| 8   | H     | 112 | LEU  |
| 8   | H     | 133 | LEU  |
| 9   | I     | 29  | ASN  |
| 9   | I     | 38  | GLN  |
| 9   | I     | 41  | VAL  |
| 9   | I     | 65  | VAL  |
| 9   | I     | 92  | TYR  |
| 10  | J     | 49  | VAL  |
| 10  | J     | 71  | LEU  |
| 10  | J     | 73  | ASP  |
| 11  | K     | 29  | ILE  |
| 11  | K     | 54  | ARG  |
| 11  | K     | 93  | GLN  |
| 11  | K     | 114 | VAL  |
| 12  | L     | 41  | ARG  |
| 12  | L     | 60  | LEU  |
| 12  | L     | 81  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 118 | SER  |
| 13  | M     | 9   | ILE  |
| 13  | M     | 32  | GLU  |
| 13  | M     | 56  | LEU  |
| 13  | M     | 70  | LEU  |
| 13  | M     | 102 | ARG  |
| 13  | M     | 110 | ARG  |
| 13  | M     | 115 | LYS  |
| 14  | N     | 8   | GLU  |
| 14  | N     | 12  | ARG  |
| 14  | N     | 22  | THR  |
| 14  | N     | 31  | ARG  |
| 14  | N     | 58  | LYS  |
| 15  | O     | 6   | GLU  |
| 15  | O     | 31  | LEU  |
| 15  | O     | 34  | LEU  |
| 15  | O     | 38  | ARG  |
| 15  | O     | 39  | LEU  |
| 15  | O     | 44  | LYS  |
| 15  | O     | 70  | LEU  |
| 15  | O     | 81  | LEU  |
| 15  | O     | 83  | GLU  |
| 16  | P     | 2   | VAL  |
| 16  | P     | 8   | ARG  |
| 17  | Q     | 9   | VAL  |
| 17  | Q     | 14  | LYS  |
| 17  | Q     | 34  | LYS  |
| 17  | Q     | 38  | ARG  |
| 17  | Q     | 74  | LEU  |
| 17  | Q     | 98  | LEU  |
| 18  | R     | 19  | LYS  |
| 18  | R     | 38  | GLU  |
| 18  | R     | 39  | VAL  |
| 18  | R     | 46  | GLU  |
| 18  | R     | 54  | ARG  |
| 18  | R     | 87  | ARG  |
| 19  | S     | 7   | LYS  |
| 19  | S     | 15  | LEU  |
| 19  | S     | 65  | ASN  |
| 19  | S     | 77  | THR  |
| 20  | T     | 39  | LYS  |
| 20  | T     | 73  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 75  | ASN  |
| 20  | T     | 84  | LEU  |
| 21  | V     | 3   | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 25  | ASN  |
| 2   | B     | 78  | GLN  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 212 | GLN  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 6   | HIS  |
| 3   | C     | 69  | HIS  |
| 3   | C     | 139 | GLN  |
| 3   | C     | 170 | GLN  |
| 3   | C     | 176 | HIS  |
| 4   | D     | 42  | GLN  |
| 4   | D     | 45  | GLN  |
| 4   | D     | 62  | GLN  |
| 4   | D     | 123 | HIS  |
| 4   | D     | 129 | ASN  |
| 4   | D     | 160 | GLN  |
| 4   | D     | 199 | ASN  |
| 5   | E     | 56  | GLN  |
| 5   | E     | 73  | ASN  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 27  | GLN  |
| 6   | F     | 100 | ASN  |
| 7   | G     | 11  | GLN  |
| 7   | G     | 13  | GLN  |
| 7   | G     | 56  | GLN  |
| 7   | G     | 68  | ASN  |
| 7   | G     | 96  | GLN  |
| 8   | H     | 15  | ASN  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 31  | GLN  |
| 9   | I     | 73  | GLN  |
| 9   | I     | 124 | GLN  |
| 10  | J     | 13  | HIS  |
| 10  | J     | 56  | HIS  |
| 10  | J     | 62  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 68  | HIS  |
| 10  | J     | 69  | ASN  |
| 10  | J     | 78  | ASN  |
| 10  | J     | 84  | GLN  |
| 11  | K     | 38  | ASN  |
| 11  | K     | 62  | GLN  |
| 11  | K     | 93  | GLN  |
| 11  | K     | 99  | GLN  |
| 11  | K     | 117 | ASN  |
| 12  | L     | 49  | ASN  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 62  | ASN  |
| 14  | N     | 49  | HIS  |
| 15  | O     | 13  | GLN  |
| 15  | O     | 37  | ASN  |
| 16  | P     | 16  | HIS  |
| 16  | P     | 76  | GLN  |
| 17  | Q     | 16  | GLN  |
| 18  | R     | 36  | ASN  |
| 19  | S     | 14  | HIS  |
| 19  | S     | 23  | ASN  |
| 19  | S     | 56  | GLN  |
| 19  | S     | 65  | ASN  |
| 20  | T     | 16  | HIS  |
| 20  | T     | 90  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed         | Backbone Outliers | Pucker Outliers |
|-----|-------|------------------|-------------------|-----------------|
| 1   | A     | 1513/1513 (100%) | 331 (21%)         | 188 (12%)       |
| 22  | W     | 2/3 (66%)        | 1 (50%)           | 0               |
| 23  | X     | 10/11 (90%)      | 4 (40%)           | 2 (20%)         |
| All | All   | 1525/1527 (99%)  | 336 (22%)         | 190 (12%)       |

All (336) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | G    |
| 1   | A     | 8   | A    |
| 1   | A     | 9   | G    |
| 1   | A     | 13  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | U    |
| 1   | A     | 31  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 39  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 49  | U    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 52  | G    |
| 1   | A     | 61  | G    |
| 1   | A     | 65  | U    |
| 1   | A     | 66  | G    |
| 1   | A     | 94  | A    |
| 1   | A     | 102 | A    |
| 1   | A     | 103 | C    |
| 1   | A     | 108 | G    |
| 1   | A     | 109 | A    |
| 1   | A     | 113 | A    |
| 1   | A     | 114 | C    |
| 1   | A     | 115 | G    |
| 1   | A     | 124 | A    |
| 1   | A     | 125 | C    |
| 1   | A     | 138 | G    |
| 1   | A     | 156 | A    |
| 1   | A     | 157 | C    |
| 1   | A     | 167 | U    |
| 1   | A     | 168 | C    |
| 1   | A     | 176 | U    |
| 1   | A     | 189 | U    |
| 1   | A     | 190 | G    |
| 1   | A     | 191 | G    |
| 1   | A     | 201 | A    |
| 1   | A     | 203 | A    |
| 1   | A     | 204 | G    |
| 1   | A     | 207 | C    |
| 1   | A     | 208 | U    |
| 1   | A     | 209 | U    |
| 1   | A     | 210 | U    |
| 1   | A     | 211 | G    |
| 1   | A     | 212 | C    |
| 1   | A     | 239 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 240 | C    |
| 1   | A     | 242 | G    |
| 1   | A     | 246 | G    |
| 1   | A     | 247 | U    |
| 1   | A     | 261 | G    |
| 1   | A     | 262 | C    |
| 1   | A     | 270 | G    |
| 1   | A     | 275 | C    |
| 1   | A     | 276 | G    |
| 1   | A     | 277 | A    |
| 1   | A     | 284 | G    |
| 1   | A     | 301 | G    |
| 1   | A     | 311 | G    |
| 1   | A     | 323 | C    |
| 1   | A     | 324 | A    |
| 1   | A     | 325 | C    |
| 1   | A     | 327 | G    |
| 1   | A     | 340 | C    |
| 1   | A     | 341 | G    |
| 1   | A     | 347 | C    |
| 1   | A     | 348 | A    |
| 1   | A     | 349 | G    |
| 1   | A     | 362 | U    |
| 1   | A     | 363 | U    |
| 1   | A     | 367 | C    |
| 1   | A     | 368 | A    |
| 1   | A     | 384 | A    |
| 1   | A     | 389 | G    |
| 1   | A     | 392 | A    |
| 1   | A     | 393 | C    |
| 1   | A     | 401 | G    |
| 1   | A     | 407 | A    |
| 1   | A     | 408 | G    |
| 1   | A     | 409 | A    |
| 1   | A     | 416 | U    |
| 1   | A     | 417 | C    |
| 1   | A     | 418 | G    |
| 1   | A     | 423 | G    |
| 1   | A     | 424 | U    |
| 1   | A     | 425 | A    |
| 1   | A     | 434 | A    |
| 1   | A     | 442 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 446 | A    |
| 1   | A     | 447 | A    |
| 1   | A     | 454 | A    |
| 1   | A     | 455 | C    |
| 1   | A     | 456 | G    |
| 1   | A     | 465 | G    |
| 1   | A     | 466 | A    |
| 1   | A     | 468 | G    |
| 1   | A     | 469 | G    |
| 1   | A     | 470 | U    |
| 1   | A     | 479 | A    |
| 1   | A     | 480 | A    |
| 1   | A     | 481 | U    |
| 1   | A     | 483 | G    |
| 1   | A     | 491 | C    |
| 1   | A     | 492 | A    |
| 1   | A     | 494 | C    |
| 1   | A     | 495 | U    |
| 1   | A     | 501 | C    |
| 1   | A     | 502 | C    |
| 1   | A     | 505 | C    |
| 1   | A     | 507 | G    |
| 1   | A     | 510 | G    |
| 1   | A     | 513 | G    |
| 1   | A     | 514 | U    |
| 1   | A     | 515 | A    |
| 1   | A     | 516 | A    |
| 1   | A     | 517 | U    |
| 1   | A     | 519 | C    |
| 1   | A     | 531 | G    |
| 1   | A     | 542 | A    |
| 1   | A     | 543 | U    |
| 1   | A     | 544 | U    |
| 1   | A     | 545 | C    |
| 1   | A     | 546 | A    |
| 1   | A     | 549 | G    |
| 1   | A     | 550 | G    |
| 1   | A     | 555 | A    |
| 1   | A     | 556 | A    |
| 1   | A     | 558 | G    |
| 1   | A     | 559 | G    |
| 1   | A     | 560 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 579 | C    |
| 1   | A     | 590 | A    |
| 1   | A     | 624 | U    |
| 1   | A     | 625 | A    |
| 1   | A     | 634 | C    |
| 1   | A     | 635 | U    |
| 1   | A     | 636 | A    |
| 1   | A     | 637 | G    |
| 1   | A     | 648 | A    |
| 1   | A     | 670 | A    |
| 1   | A     | 671 | G    |
| 1   | A     | 678 | A    |
| 1   | A     | 684 | C    |
| 1   | A     | 685 | A    |
| 1   | A     | 686 | G    |
| 1   | A     | 687 | A    |
| 1   | A     | 701 | G    |
| 1   | A     | 704 | G    |
| 1   | A     | 705 | A    |
| 1   | A     | 706 | U    |
| 1   | A     | 707 | G    |
| 1   | A     | 714 | G    |
| 1   | A     | 731 | C    |
| 1   | A     | 732 | C    |
| 1   | A     | 737 | C    |
| 1   | A     | 738 | G    |
| 1   | A     | 760 | A    |
| 1   | A     | 764 | A    |
| 1   | A     | 775 | A    |
| 1   | A     | 776 | U    |
| 1   | A     | 777 | A    |
| 1   | A     | 795 | C    |
| 1   | A     | 796 | U    |
| 1   | A     | 798 | A    |
| 1   | A     | 799 | A    |
| 1   | A     | 800 | C    |
| 1   | A     | 801 | G    |
| 1   | A     | 802 | A    |
| 1   | A     | 803 | U    |
| 1   | A     | 804 | G    |
| 1   | A     | 810 | U    |
| 1   | A     | 811 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 822  | U    |
| 1   | A     | 823  | C    |
| 1   | A     | 824  | U    |
| 1   | A     | 825  | C    |
| 1   | A     | 826  | C    |
| 1   | A     | 835  | G    |
| 1   | A     | 848  | U    |
| 1   | A     | 849  | A    |
| 1   | A     | 850  | A    |
| 1   | A     | 851  | G    |
| 1   | A     | 862  | G    |
| 1   | A     | 866  | A    |
| 1   | A     | 867  | G    |
| 1   | A     | 868  | U    |
| 1   | A     | 891  | A    |
| 1   | A     | 903  | G    |
| 1   | A     | 904  | G    |
| 1   | A     | 911  | C    |
| 1   | A     | 912  | A    |
| 1   | A     | 919  | G    |
| 1   | A     | 922  | G    |
| 1   | A     | 937  | U    |
| 1   | A     | 938  | U    |
| 1   | A     | 943  | G    |
| 1   | A     | 945  | A    |
| 1   | A     | 946  | A    |
| 1   | A     | 948  | G    |
| 1   | A     | 949  | C    |
| 1   | A     | 951  | A    |
| 1   | A     | 952  | A    |
| 1   | A     | 953  | G    |
| 1   | A     | 954  | A    |
| 1   | A     | 959  | U    |
| 1   | A     | 960  | A    |
| 1   | A     | 968  | U    |
| 1   | A     | 970  | G    |
| 1   | A     | 971  | A    |
| 1   | A     | 982  | A    |
| 1   | A     | 983  | A    |
| 1   | A     | 984  | C    |
| 1   | A     | 1003 | U    |
| 1   | A     | 1004 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1005 | C    |
| 1   | A     | 1006 | C    |
| 1   | A     | 1018 | G    |
| 1   | A     | 1024 | G    |
| 1   | A     | 1032 | G    |
| 1   | A     | 1036 | C    |
| 1   | A     | 1046 | G    |
| 1   | A     | 1047 | U    |
| 1   | A     | 1048 | C    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1067 | U    |
| 1   | A     | 1068 | U    |
| 1   | A     | 1076 | G    |
| 1   | A     | 1077 | U    |
| 1   | A     | 1083 | A    |
| 1   | A     | 1084 | A    |
| 1   | A     | 1090 | G    |
| 1   | A     | 1106 | G    |
| 1   | A     | 1107 | U    |
| 1   | A     | 1108 | U    |
| 1   | A     | 1109 | G    |
| 1   | A     | 1111 | C    |
| 1   | A     | 1112 | A    |
| 1   | A     | 1113 | G    |
| 1   | A     | 1119 | C    |
| 1   | A     | 1120 | G    |
| 1   | A     | 1121 | G    |
| 1   | A     | 1122 | C    |
| 1   | A     | 1128 | A    |
| 1   | A     | 1134 | A    |
| 1   | A     | 1139 | A    |
| 1   | A     | 1140 | C    |
| 1   | A     | 1141 | U    |
| 1   | A     | 1142 | G    |
| 1   | A     | 1163 | G    |
| 1   | A     | 1164 | A    |
| 1   | A     | 1165 | G    |
| 1   | A     | 1172 | A    |
| 1   | A     | 1177 | U    |
| 1   | A     | 1178 | G    |
| 1   | A     | 1181 | C    |
| 1   | A     | 1182 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1183 | G    |
| 1   | A     | 1185 | A    |
| 1   | A     | 1193 | U    |
| 1   | A     | 1194 | A    |
| 1   | A     | 1195 | C    |
| 1   | A     | 1196 | G    |
| 1   | A     | 1199 | C    |
| 1   | A     | 1206 | A    |
| 1   | A     | 1207 | C    |
| 1   | A     | 1208 | A    |
| 1   | A     | 1221 | U    |
| 1   | A     | 1222 | G    |
| 1   | A     | 1231 | A    |
| 1   | A     | 1235 | C    |
| 1   | A     | 1236 | G    |
| 1   | A     | 1237 | A    |
| 1   | A     | 1238 | U    |
| 1   | A     | 1239 | G    |
| 1   | A     | 1243 | C    |
| 1   | A     | 1260 | A    |
| 1   | A     | 1261 | A    |
| 1   | A     | 1262 | U    |
| 1   | A     | 1263 | C    |
| 1   | A     | 1266 | A    |
| 1   | A     | 1267 | A    |
| 1   | A     | 1268 | A    |
| 1   | A     | 1270 | A    |
| 1   | A     | 1279 | C    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | G    |
| 1   | A     | 1282 | U    |
| 1   | A     | 1283 | U    |
| 1   | A     | 1284 | C    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1304 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1318 | G    |
| 1   | A     | 1319 | G    |
| 1   | A     | 1327 | A    |
| 1   | A     | 1328 | G    |
| 1   | A     | 1329 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1345 | A    |
| 1   | A     | 1346 | U    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1361 | G    |
| 1   | A     | 1363 | U    |
| 1   | A     | 1376 | A    |
| 1   | A     | 1377 | C    |
| 1   | A     | 1379 | C    |
| 1   | A     | 1380 | A    |
| 1   | A     | 1382 | C    |
| 1   | A     | 1383 | G    |
| 1   | A     | 1424 | G    |
| 1   | A     | 1426 | A    |
| 1   | A     | 1427 | G    |
| 1   | A     | 1432 | C    |
| 1   | A     | 1433 | G    |
| 1   | A     | 1461 | C    |
| 1   | A     | 1469 | A    |
| 1   | A     | 1471 | G    |
| 1   | A     | 1476 | A    |
| 1   | A     | 1479 | A    |
| 1   | A     | 1480 | A    |
| 1   | A     | 1481 | G    |
| 1   | A     | 1482 | G    |
| 1   | A     | 1483 | U    |
| 1   | A     | 1484 | A    |
| 1   | A     | 1494 | G    |
| 1   | A     | 1506 | G    |
| 1   | A     | 1507 | G    |
| 1   | A     | 1510 | C    |
| 1   | A     | 1511 | A    |
| 1   | A     | 1516 | C    |
| 1   | A     | 1519 | U    |
| 22  | W     | 2    | A    |
| 23  | X     | 31   | A    |
| 23  | X     | 32   | C    |
| 23  | X     | 39   | PSU  |
| 23  | X     | 40   | C    |

All (190) RNA pucker outliers are listed below:

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | U    |
| 1   | A     | 7   | G    |
| 1   | A     | 8   | A    |
| 1   | A     | 13  | U    |
| 1   | A     | 30  | U    |
| 1   | A     | 31  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 49  | U    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 60  | A    |
| 1   | A     | 64  | G    |
| 1   | A     | 65  | U    |
| 1   | A     | 102 | A    |
| 1   | A     | 108 | G    |
| 1   | A     | 112 | A    |
| 1   | A     | 114 | C    |
| 1   | A     | 123 | G    |
| 1   | A     | 124 | A    |
| 1   | A     | 155 | A    |
| 1   | A     | 167 | U    |
| 1   | A     | 175 | G    |
| 1   | A     | 188 | U    |
| 1   | A     | 189 | U    |
| 1   | A     | 190 | G    |
| 1   | A     | 203 | A    |
| 1   | A     | 208 | U    |
| 1   | A     | 209 | U    |
| 1   | A     | 238 | A    |
| 1   | A     | 239 | U    |
| 1   | A     | 241 | A    |
| 1   | A     | 245 | A    |
| 1   | A     | 246 | G    |
| 1   | A     | 261 | G    |
| 1   | A     | 269 | A    |
| 1   | A     | 274 | A    |
| 1   | A     | 275 | C    |
| 1   | A     | 276 | G    |
| 1   | A     | 300 | G    |
| 1   | A     | 310 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 322 | A    |
| 1   | A     | 323 | C    |
| 1   | A     | 324 | A    |
| 1   | A     | 339 | A    |
| 1   | A     | 340 | C    |
| 1   | A     | 346 | G    |
| 1   | A     | 348 | A    |
| 1   | A     | 361 | C    |
| 1   | A     | 362 | U    |
| 1   | A     | 367 | C    |
| 1   | A     | 383 | G    |
| 1   | A     | 407 | A    |
| 1   | A     | 408 | G    |
| 1   | A     | 416 | U    |
| 1   | A     | 417 | C    |
| 1   | A     | 423 | G    |
| 1   | A     | 424 | U    |
| 1   | A     | 433 | G    |
| 1   | A     | 445 | A    |
| 1   | A     | 446 | A    |
| 1   | A     | 454 | A    |
| 1   | A     | 455 | C    |
| 1   | A     | 465 | G    |
| 1   | A     | 468 | G    |
| 1   | A     | 469 | G    |
| 1   | A     | 479 | A    |
| 1   | A     | 480 | A    |
| 1   | A     | 482 | A    |
| 1   | A     | 491 | C    |
| 1   | A     | 494 | C    |
| 1   | A     | 500 | G    |
| 1   | A     | 501 | C    |
| 1   | A     | 513 | G    |
| 1   | A     | 514 | U    |
| 1   | A     | 516 | A    |
| 1   | A     | 518 | A    |
| 1   | A     | 530 | A    |
| 1   | A     | 542 | A    |
| 1   | A     | 544 | U    |
| 1   | A     | 545 | C    |
| 1   | A     | 549 | G    |
| 1   | A     | 558 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 559 | G    |
| 1   | A     | 578 | G    |
| 1   | A     | 624 | U    |
| 1   | A     | 636 | A    |
| 1   | A     | 669 | U    |
| 1   | A     | 670 | A    |
| 1   | A     | 684 | C    |
| 1   | A     | 685 | A    |
| 1   | A     | 686 | G    |
| 1   | A     | 700 | C    |
| 1   | A     | 704 | G    |
| 1   | A     | 705 | A    |
| 1   | A     | 731 | C    |
| 1   | A     | 735 | G    |
| 1   | A     | 736 | A    |
| 1   | A     | 775 | A    |
| 1   | A     | 776 | U    |
| 1   | A     | 795 | C    |
| 1   | A     | 798 | A    |
| 1   | A     | 800 | C    |
| 1   | A     | 801 | G    |
| 1   | A     | 802 | A    |
| 1   | A     | 803 | U    |
| 1   | A     | 823 | C    |
| 1   | A     | 847 | U    |
| 1   | A     | 848 | U    |
| 1   | A     | 849 | A    |
| 1   | A     | 850 | A    |
| 1   | A     | 861 | U    |
| 1   | A     | 866 | A    |
| 1   | A     | 867 | G    |
| 1   | A     | 890 | A    |
| 1   | A     | 911 | C    |
| 1   | A     | 937 | U    |
| 1   | A     | 942 | A    |
| 1   | A     | 945 | A    |
| 1   | A     | 948 | G    |
| 1   | A     | 951 | A    |
| 1   | A     | 952 | A    |
| 1   | A     | 953 | G    |
| 1   | A     | 959 | U    |
| 1   | A     | 969 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 970  | G    |
| 1   | A     | 1031 | U    |
| 1   | A     | 1035 | G    |
| 1   | A     | 1046 | G    |
| 1   | A     | 1047 | U    |
| 1   | A     | 1049 | A    |
| 1   | A     | 1067 | U    |
| 1   | A     | 1083 | A    |
| 1   | A     | 1106 | G    |
| 1   | A     | 1110 | C    |
| 1   | A     | 1111 | C    |
| 1   | A     | 1121 | G    |
| 1   | A     | 1127 | C    |
| 1   | A     | 1133 | A    |
| 1   | A     | 1139 | A    |
| 1   | A     | 1141 | U    |
| 1   | A     | 1162 | G    |
| 1   | A     | 1163 | G    |
| 1   | A     | 1164 | A    |
| 1   | A     | 1171 | G    |
| 1   | A     | 1177 | U    |
| 1   | A     | 1182 | A    |
| 1   | A     | 1194 | A    |
| 1   | A     | 1195 | C    |
| 1   | A     | 1205 | G    |
| 1   | A     | 1206 | A    |
| 1   | A     | 1207 | C    |
| 1   | A     | 1220 | A    |
| 1   | A     | 1221 | U    |
| 1   | A     | 1261 | A    |
| 1   | A     | 1262 | U    |
| 1   | A     | 1266 | A    |
| 1   | A     | 1278 | C    |
| 1   | A     | 1279 | C    |
| 1   | A     | 1281 | G    |
| 1   | A     | 1282 | U    |
| 1   | A     | 1283 | U    |
| 1   | A     | 1286 | G    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1316 | C    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1318 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1326 | U    |
| 1   | A     | 1327 | A    |
| 1   | A     | 1328 | G    |
| 1   | A     | 1345 | A    |
| 1   | A     | 1346 | U    |
| 1   | A     | 1362 | U    |
| 1   | A     | 1376 | A    |
| 1   | A     | 1378 | A    |
| 1   | A     | 1379 | C    |
| 1   | A     | 1381 | C    |
| 1   | A     | 1382 | C    |
| 1   | A     | 1426 | A    |
| 1   | A     | 1431 | A    |
| 1   | A     | 1432 | C    |
| 1   | A     | 1475 | U    |
| 1   | A     | 1479 | A    |
| 1   | A     | 1480 | A    |
| 1   | A     | 1481 | G    |
| 1   | A     | 1483 | U    |
| 1   | A     | 1505 | U    |
| 1   | A     | 1506 | G    |
| 23  | X     | 31   | A    |
| 23  | X     | 39   | PSU  |

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

3 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 | $\# Z  > 2$ |
| 23  | 12A  | X     | 37  | 23    | 33,36,37     | 2.96 | 12 (36%)    | 46,52,55    | 2.78 | 19 (41%)    |
| 23  | PSU  | X     | 39  | 23    | 18,21,22     | 1.25 | 2 (11%)     | 21,30,33    | 2.11 | 6 (28%)     |
| 23  | 70U  | X     | 34  | 22,23 | 22,26,27     | 0.56 | 0           | 27,37,40    | 0.73 | 0           |

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

| Mol | Type | Chain | Res | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 23  | 12A  | X     | 37  | 23    | -       | 0/25/43/44 | 0/3/3/3 |
| 23  | PSU  | X     | 39  | 23    | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | 70U  | X     | 34  | 22,23 | -       | 3/13/31/32 | 0/2/2/2 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 23  | X     | 37  | 12A  | C2-S2  | 13.19 | 1.86        | 1.75     |
| 23  | X     | 37  | 12A  | C6-N6  | 4.65  | 1.49        | 1.39     |
| 23  | X     | 37  | 12A  | OG1-CB | 3.95  | 1.53        | 1.43     |
| 23  | X     | 37  | 12A  | C5-C4  | 3.94  | 1.46        | 1.39     |
| 23  | X     | 39  | PSU  | C6-C5  | 3.26  | 1.38        | 1.35     |
| 23  | X     | 37  | 12A  | C5-C6  | -2.98 | 1.34        | 1.41     |
| 23  | X     | 37  | 12A  | C2-N1  | 2.82  | 1.38        | 1.34     |
| 23  | X     | 37  | 12A  | CA-N   | 2.70  | 1.51        | 1.45     |
| 23  | X     | 37  | 12A  | CB-CA  | 2.68  | 1.61        | 1.53     |
| 23  | X     | 37  | 12A  | OXT-C  | 2.41  | 1.38        | 1.30     |
| 23  | X     | 37  | 12A  | C8-N7  | -2.18 | 1.27        | 1.31     |
| 23  | X     | 39  | PSU  | C1'-C5 | 2.13  | 1.55        | 1.50     |
| 23  | X     | 37  | 12A  | C8-N9  | 2.08  | 1.41        | 1.37     |
| 23  | X     | 37  | 12A  | C5-N7  | -2.05 | 1.35        | 1.39     |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | X     | 37  | 12A  | N6-CC-N     | 9.25  | 126.48      | 113.77   |
| 23  | X     | 37  | 12A  | C5-C4-N3    | -6.45 | 120.38      | 127.18   |
| 23  | X     | 37  | 12A  | N3-C4-N9    | 6.40  | 135.11      | 126.99   |
| 23  | X     | 37  | 12A  | OO-CC-N6    | -6.20 | 112.62      | 123.64   |
| 23  | X     | 37  | 12A  | C2M-S2-C2   | -5.18 | 98.36       | 102.25   |
| 23  | X     | 39  | PSU  | N1-C2-N3    | 4.75  | 120.18      | 115.17   |
| 23  | X     | 39  | PSU  | C3'-C2'-C1' | 4.63  | 107.15      | 101.69   |
| 23  | X     | 37  | 12A  | C5-N7-C8    | 4.39  | 110.35      | 103.45   |
| 23  | X     | 39  | PSU  | C4-N3-C2    | -3.79 | 121.15      | 126.37   |
| 23  | X     | 37  | 12A  | OXT-C-O     | -3.18 | 116.87      | 124.08   |
| 23  | X     | 39  | PSU  | O2-C2-N1    | -3.03 | 119.67      | 122.79   |
| 23  | X     | 37  | 12A  | CA-N-CC     | 3.00  | 126.97      | 121.99   |
| 23  | X     | 39  | PSU  | O4'-C4'-C3' | 2.78  | 110.66      | 105.15   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | X     | 37  | 12A  | OXT-C-CA    | 2.77  | 123.77      | 114.15   |
| 23  | X     | 37  | 12A  | C4-C5-N7    | -2.77 | 107.42      | 110.58   |
| 23  | X     | 37  | 12A  | C2-N3-C4    | 2.69  | 119.34      | 112.29   |
| 23  | X     | 37  | 12A  | C6-C5-N7    | 2.52  | 135.18      | 132.43   |
| 23  | X     | 37  | 12A  | O4'-C1'-N9  | 2.49  | 112.88      | 108.09   |
| 23  | X     | 37  | 12A  | N3-C2-N1    | -2.47 | 122.49      | 127.00   |
| 23  | X     | 37  | 12A  | C-CA-N      | 2.39  | 115.43      | 110.17   |
| 23  | X     | 37  | 12A  | N6-C6-N1    | 2.19  | 124.65      | 117.62   |
| 23  | X     | 39  | PSU  | C6-N1-C2    | -2.17 | 120.68      | 122.69   |
| 23  | X     | 37  | 12A  | N9-C8-N7    | -2.13 | 110.91      | 113.94   |
| 23  | X     | 37  | 12A  | O2'-C2'-C1' | 2.03  | 117.10      | 110.10   |
| 23  | X     | 37  | 12A  | C5-C6-N6    | -2.03 | 113.76      | 118.94   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 23  | X     | 34  | 70U  | C4-C5-C5M-C8 |
| 23  | X     | 34  | 70U  | C6-C5-C5M-C8 |
| 23  | X     | 34  | 70U  | C5-C5M-C8-O9 |

There are no ring outliers.

1 monomer is involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | X     | 34  | 70U  | 8       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 188 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 25  | PAR  | A     | 1786 | -    | 44,45,45     | 0.59 | 1 (2%)      | 63,67,67    | 1.38 | 9 (14%)     |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 25  | PAR  | A     | 1786 | -    | -       | 7/18/94/94 | 0/4/4/4 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 25  | A     | 1786 | PAR  | O43-C13 | 2.25 | 1.45        | 1.41     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | A     | 1786 | PAR  | O52-C13-O43 | 3.43  | 114.87      | 111.37   |
| 25  | A     | 1786 | PAR  | O33-C14-C24 | 3.36  | 113.57      | 108.08   |
| 25  | A     | 1786 | PAR  | C32-C22-C12 | -2.97 | 105.93      | 111.02   |
| 25  | A     | 1786 | PAR  | C11-O51-C51 | -2.69 | 108.47      | 113.72   |
| 25  | A     | 1786 | PAR  | C11-O11-C42 | -2.64 | 111.72      | 117.98   |
| 25  | A     | 1786 | PAR  | C13-O52-C52 | -2.48 | 112.10      | 117.98   |
| 25  | A     | 1786 | PAR  | C14-O33-C33 | -2.35 | 112.41      | 117.98   |
| 25  | A     | 1786 | PAR  | O52-C52-C62 | 2.24  | 112.93      | 107.23   |
| 25  | A     | 1786 | PAR  | C44-C34-C24 | -2.18 | 107.37      | 110.99   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | A     | 1786 | PAR  | O54-C14-O33-C33 |
| 25  | A     | 1786 | PAR  | C52-C42-O11-C11 |
| 25  | A     | 1786 | PAR  | C42-C52-O52-C13 |
| 25  | A     | 1786 | PAR  | C62-C52-O52-C13 |
| 25  | A     | 1786 | PAR  | C32-C42-O11-C11 |
| 25  | A     | 1786 | PAR  | C23-C13-O52-C52 |

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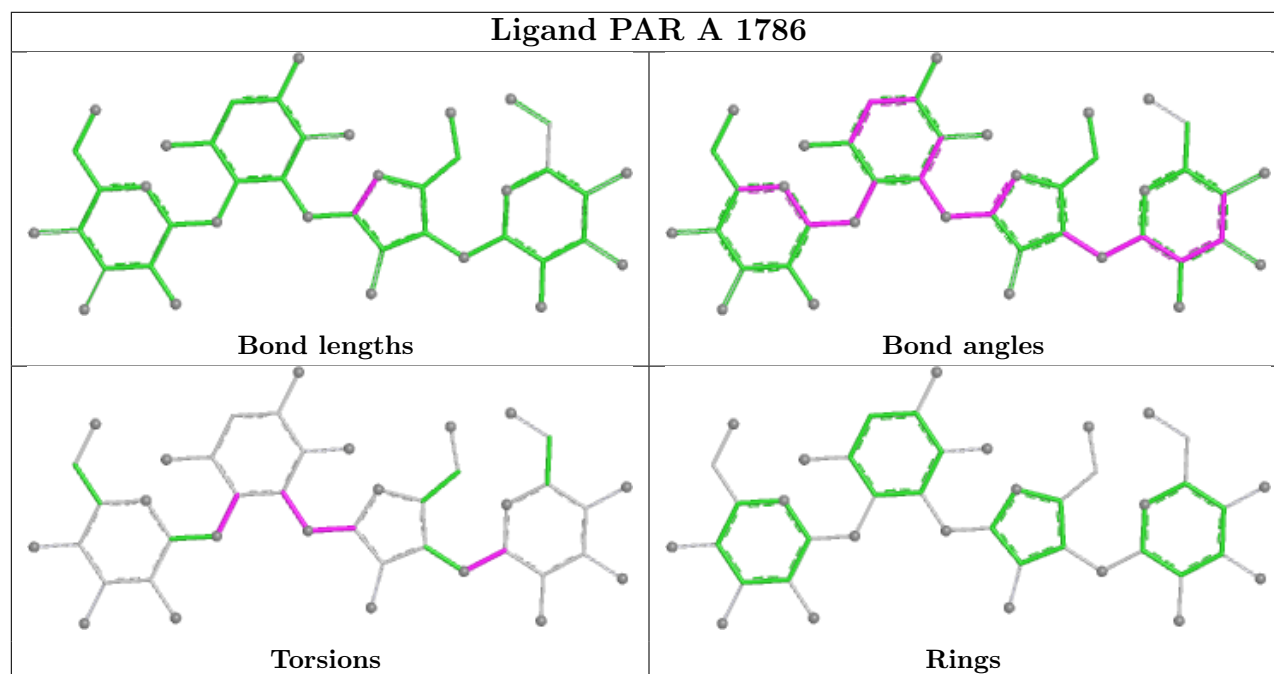
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | A     | 1786 | PAR  | O43-C13-O52-C52 |

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | A     | 1786 | PAR  | 4       | 0            |

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



## 5.7 Other polymers ⓘ

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   | A     | 1512/1513 (99%) | 0.73   | 228 (15%) 5 4 | 28, 54, 117, 169      | 0     |
| 2   | B     | 234/256 (91%)   | 1.99   | 95 (40%) 0 0  | 53, 89, 136, 146      | 0     |
| 3   | C     | 206/239 (86%)   | 1.92   | 85 (41%) 0 0  | 52, 79, 118, 123      | 0     |
| 4   | D     | 208/209 (99%)   | 0.85   | 25 (12%) 9 6  | 46, 64, 86, 96        | 0     |
| 5   | E     | 150/162 (92%)   | 0.39   | 8 (5%) 32 24  | 33, 48, 67, 80        | 0     |
| 6   | F     | 101/101 (100%)  | 1.52   | 24 (23%) 2 1  | 64, 87, 97, 100       | 0     |
| 7   | G     | 155/156 (99%)   | 1.31   | 31 (20%) 3 2  | 51, 76, 105, 118      | 0     |
| 8   | H     | 138/138 (100%)  | 0.22   | 1 (0%) 84 77  | 32, 47, 61, 71        | 0     |
| 9   | I     | 127/128 (99%)   | 1.95   | 51 (40%) 0 0  | 43, 87, 103, 108      | 0     |
| 10  | J     | 98/105 (93%)    | 3.14   | 79 (80%) 0 0  | 52, 113, 141, 145     | 0     |
| 11  | K     | 119/129 (92%)   | 0.92   | 13 (10%) 10 8 | 38, 59, 81, 99        | 0     |
| 12  | L     | 124/132 (93%)   | 0.71   | 16 (12%) 7 6  | 26, 53, 69, 92        | 0     |
| 13  | M     | 125/126 (99%)   | 1.88   | 41 (32%) 1 1  | 57, 73, 126, 145      | 0     |
| 14  | N     | 60/61 (98%)     | 1.88   | 26 (43%) 0 0  | 55, 68, 102, 104      | 0     |
| 15  | O     | 88/89 (98%)     | 0.68   | 6 (6%) 23 17  | 45, 64, 82, 100       | 0     |
| 16  | P     | 83/88 (94%)     | 0.23   | 1 (1%) 76 68  | 39, 49, 60, 84        | 0     |
| 17  | Q     | 104/105 (99%)   | 0.73   | 14 (13%) 7 5  | 35, 50, 100, 129      | 0     |
| 18  | R     | 73/88 (82%)     | 1.15   | 13 (17%) 4 3  | 53, 70, 111, 125      | 0     |
| 19  | S     | 80/93 (86%)     | 2.64   | 50 (62%) 0 0  | 66, 96, 118, 120      | 0     |
| 20  | T     | 99/106 (93%)    | 0.74   | 14 (14%) 6 5  | 32, 52, 74, 79        | 0     |
| 21  | V     | 24/27 (88%)     | 1.58   | 7 (29%) 1 1   | 52, 61, 77, 90        | 0     |
| 22  | W     | 3/3 (100%)      | 0.89   | 0 100 100     | 52, 52, 53, 54        | 0     |
| 23  | X     | 8/11 (72%)      | 2.66   | 5 (62%) 0 0   | 61, 88, 115, 125      | 0     |
| All | All   | 3919/4065 (96%) | 1.09   | 833 (21%) 2 2 | 26, 61, 117, 169      | 0     |

All (833) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 238  | LEU  | 9.6  |
| 13  | M     | 119  | GLY  | 9.2  |
| 11  | K     | 128  | ALA  | 8.9  |
| 19  | S     | 3    | ARG  | 8.4  |
| 13  | M     | 118  | ALA  | 8.2  |
| 13  | M     | 125  | ARG  | 8.2  |
| 1   | A     | 1109 | G    | 7.7  |
| 1   | A     | 1111 | C    | 7.6  |
| 7   | G     | 156  | TRP  | 7.6  |
| 1   | A     | 1517 | U    | 7.5  |
| 13  | M     | 124  | PRO  | 7.5  |
| 14  | N     | 13   | THR  | 7.2  |
| 13  | M     | 126  | LYS  | 7.2  |
| 2   | B     | 17   | PHE  | 7.2  |
| 1   | A     | 1112 | A    | 7.1  |
| 19  | S     | 37   | ARG  | 7.0  |
| 19  | S     | 53   | ASN  | 6.9  |
| 17  | Q     | 103  | GLY  | 6.9  |
| 19  | S     | 2    | PRO  | 6.8  |
| 13  | M     | 9    | ILE  | 6.6  |
| 1   | A     | 1519 | U    | 6.6  |
| 17  | Q     | 105  | ALA  | 6.5  |
| 10  | J     | 57   | LYS  | 6.4  |
| 1   | A     | 982  | A    | 6.4  |
| 10  | J     | 27   | ALA  | 6.4  |
| 1   | A     | 983  | A    | 6.3  |
| 2   | B     | 229  | VAL  | 6.3  |
| 18  | R     | 16   | PRO  | 6.3  |
| 1   | A     | 1237 | A    | 6.3  |
| 1   | A     | 1236 | G    | 6.2  |
| 1   | A     | 1516 | C    | 6.1  |
| 9   | I     | 30   | GLY  | 6.1  |
| 2   | B     | 237  | ALA  | 6.1  |
| 4   | D     | 21   | LEU  | 6.1  |
| 4   | D     | 35   | ARG  | 6.1  |
| 9   | I     | 128  | ARG  | 6.1  |
| 10  | J     | 23   | ILE  | 6.0  |
| 2   | B     | 19   | HIS  | 5.9  |
| 1   | A     | 1121 | G    | 5.9  |
| 9   | I     | 27   | THR  | 5.9  |
| 13  | M     | 10   | PRO  | 5.9  |
| 1   | A     | 1108 | U    | 5.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | C            | 2          | GLY         | 5.7         |
| 17         | Q            | 102        | GLY         | 5.7         |
| 1          | A            | 1518       | U           | 5.7         |
| 4          | D            | 3          | ARG         | 5.7         |
| 2          | B            | 131        | PRO         | 5.6         |
| 1          | A            | 515        | A           | 5.5         |
| 1          | A            | 981        | G           | 5.5         |
| 1          | A            | 1239       | G           | 5.5         |
| 1          | A            | 706        | U           | 5.5         |
| 1          | A            | 1036       | C           | 5.5         |
| 2          | B            | 16         | HIS         | 5.5         |
| 2          | B            | 136        | VAL         | 5.4         |
| 3          | C            | 96         | GLY         | 5.4         |
| 1          | A            | 825        | C           | 5.4         |
| 19         | S            | 33         | THR         | 5.3         |
| 19         | S            | 49         | ILE         | 5.3         |
| 4          | D            | 31         | CYS         | 5.3         |
| 2          | B            | 133        | LYS         | 5.3         |
| 10         | J            | 77         | PRO         | 5.2         |
| 10         | J            | 90         | LEU         | 5.2         |
| 1          | A            | 1107       | U           | 5.2         |
| 10         | J            | 37         | PRO         | 5.2         |
| 13         | M            | 117        | VAL         | 5.1         |
| 2          | B            | 122        | PHE         | 5.1         |
| 10         | J            | 75         | ILE         | 5.1         |
| 20         | T            | 74         | LYS         | 5.1         |
| 10         | J            | 85         | LEU         | 5.1         |
| 1          | A            | 1106       | G           | 5.1         |
| 1          | A            | 984        | C           | 5.1         |
| 13         | M            | 4          | ILE         | 5.1         |
| 1          | A            | 1125       | G           | 5.0         |
| 1          | A            | 1126       | G           | 5.0         |
| 3          | C            | 92         | ALA         | 5.0         |
| 19         | S            | 5          | LEU         | 5.0         |
| 23         | X            | 40         | C           | 4.9         |
| 1          | A            | 1113       | G           | 4.9         |
| 2          | B            | 7          | VAL         | 4.9         |
| 10         | J            | 88         | LEU         | 4.9         |
| 13         | M            | 120        | LYS         | 4.9         |
| 1          | A            | 614        | G           | 4.8         |
| 1          | A            | 1009       | G           | 4.8         |
| 5          | E            | 154        | GLY         | 4.8         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | M     | 8    | GLU  | 4.8  |
| 1   | A     | 1005 | C    | 4.8  |
| 2   | B     | 207  | ALA  | 4.8  |
| 10  | J     | 30   | SER  | 4.8  |
| 1   | A     | 1020 | C    | 4.8  |
| 2   | B     | 15   | VAL  | 4.8  |
| 1   | A     | 1002 | G    | 4.8  |
| 1   | A     | 1259 | U    | 4.7  |
| 1   | A     | 1262 | U    | 4.7  |
| 4   | D     | 9    | CYS  | 4.7  |
| 7   | G     | 155  | ARG  | 4.7  |
| 2   | B     | 44   | LEU  | 4.7  |
| 7   | G     | 83   | ALA  | 4.7  |
| 1   | A     | 513  | G    | 4.7  |
| 9   | I     | 102  | LEU  | 4.7  |
| 19  | S     | 20   | LEU  | 4.7  |
| 21  | V     | 6    | ARG  | 4.7  |
| 10  | J     | 15   | THR  | 4.6  |
| 13  | M     | 121  | LYS  | 4.6  |
| 1   | A     | 1010 | C    | 4.6  |
| 4   | D     | 26   | CYS  | 4.6  |
| 19  | S     | 4    | SER  | 4.6  |
| 2   | B     | 230  | VAL  | 4.6  |
| 10  | J     | 81   | THR  | 4.6  |
| 10  | J     | 24   | VAL  | 4.6  |
| 2   | B     | 11   | LEU  | 4.5  |
| 1   | A     | 1117 | U    | 4.5  |
| 10  | J     | 87   | THR  | 4.5  |
| 1   | A     | 1122 | C    | 4.5  |
| 1   | A     | 1127 | C    | 4.5  |
| 11  | K     | 129  | SER  | 4.5  |
| 3   | C     | 167  | TRP  | 4.5  |
| 11  | K     | 36   | ASP  | 4.5  |
| 10  | J     | 28   | ARG  | 4.5  |
| 14  | N     | 30   | ALA  | 4.5  |
| 3   | C     | 87   | LEU  | 4.5  |
| 10  | J     | 71   | LEU  | 4.5  |
| 1   | A     | 413  | C    | 4.4  |
| 2   | B     | 10   | LEU  | 4.4  |
| 1   | A     | 1193 | U    | 4.4  |
| 21  | V     | 25   | LYS  | 4.4  |
| 18  | R     | 17   | SER  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | L     | 26   | ALA  | 4.4  |
| 12  | L     | 128  | ALA  | 4.4  |
| 13  | M     | 116  | THR  | 4.4  |
| 3   | C     | 99   | VAL  | 4.4  |
| 1   | A     | 1163 | G    | 4.4  |
| 9   | I     | 16   | ARG  | 4.4  |
| 2   | B     | 235  | SER  | 4.3  |
| 20  | T     | 100  | ILE  | 4.3  |
| 1   | A     | 211  | G    | 4.3  |
| 10  | J     | 82   | ILE  | 4.3  |
| 1   | A     | 408  | G    | 4.3  |
| 3   | C     | 154  | SER  | 4.3  |
| 3   | C     | 21   | ARG  | 4.3  |
| 13  | M     | 114  | ARG  | 4.3  |
| 10  | J     | 74   | ILE  | 4.2  |
| 1   | A     | 1238 | U    | 4.2  |
| 9   | I     | 56   | LEU  | 4.2  |
| 10  | J     | 32   | ALA  | 4.2  |
| 19  | S     | 16   | LEU  | 4.2  |
| 17  | Q     | 99   | SER  | 4.2  |
| 2   | B     | 234  | PRO  | 4.2  |
| 3   | C     | 61   | ALA  | 4.2  |
| 2   | B     | 203  | GLY  | 4.2  |
| 10  | J     | 93   | GLY  | 4.2  |
| 1   | A     | 1243 | C    | 4.1  |
| 19  | S     | 17   | GLU  | 4.1  |
| 1   | A     | 987  | G    | 4.1  |
| 19  | S     | 26   | GLY  | 4.1  |
| 3   | C     | 77   | ILE  | 4.1  |
| 10  | J     | 86   | MET  | 4.1  |
| 1   | A     | 1241 | C    | 4.1  |
| 13  | M     | 123  | ALA  | 4.1  |
| 10  | J     | 59   | SER  | 4.1  |
| 3   | C     | 97   | LYS  | 4.1  |
| 23  | X     | 33   | U    | 4.1  |
| 10  | J     | 79   | ARG  | 4.1  |
| 13  | M     | 106  | ASN  | 4.1  |
| 2   | B     | 22   | LYS  | 4.1  |
| 3   | C     | 94   | LEU  | 4.0  |
| 2   | B     | 209  | ARG  | 4.0  |
| 9   | I     | 64   | THR  | 4.0  |
| 10  | J     | 34   | VAL  | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1003 | U    | 4.0  |
| 10  | J     | 73   | ASP  | 4.0  |
| 1   | A     | 153  | G    | 4.0  |
| 1   | A     | 1510 | C    | 4.0  |
| 9   | I     | 127  | LYS  | 4.0  |
| 1   | A     | 1240 | C    | 3.9  |
| 9   | I     | 21   | PRO  | 3.9  |
| 10  | J     | 91   | PRO  | 3.9  |
| 10  | J     | 26   | ALA  | 3.9  |
| 14  | N     | 5    | ALA  | 3.9  |
| 1   | A     | 1015 | G    | 3.9  |
| 1   | A     | 1116 | G    | 3.9  |
| 2   | B     | 8    | LYS  | 3.9  |
| 2   | B     | 233  | SER  | 3.9  |
| 2   | B     | 127  | ILE  | 3.9  |
| 21  | V     | 10   | ARG  | 3.9  |
| 1   | A     | 1018 | G    | 3.9  |
| 19  | S     | 6    | LYS  | 3.9  |
| 9   | I     | 119  | ALA  | 3.9  |
| 12  | L     | 19   | ARG  | 3.9  |
| 1   | A     | 1001 | G    | 3.9  |
| 2   | B     | 236  | TYR  | 3.9  |
| 4   | D     | 5    | ILE  | 3.9  |
| 1   | A     | 1235 | C    | 3.9  |
| 10  | J     | 35   | SER  | 3.9  |
| 18  | R     | 46   | GLU  | 3.8  |
| 3   | C     | 207  | VAL  | 3.8  |
| 1   | A     | 637  | G    | 3.8  |
| 1   | A     | 1016 | G    | 3.8  |
| 10  | J     | 80   | LYS  | 3.8  |
| 3   | C     | 74   | GLY  | 3.8  |
| 10  | J     | 16   | LEU  | 3.8  |
| 11  | K     | 90   | GLY  | 3.8  |
| 1   | A     | 1426 | A    | 3.8  |
| 9   | I     | 94   | ALA  | 3.8  |
| 17  | Q     | 98   | LEU  | 3.8  |
| 1   | A     | 1151 | A    | 3.8  |
| 10  | J     | 69   | ASN  | 3.8  |
| 1   | A     | 1129 | C    | 3.8  |
| 7   | G     | 85   | TYR  | 3.8  |
| 9   | I     | 7    | THR  | 3.8  |
| 7   | G     | 5    | ARG  | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | J     | 29   | ARG  | 3.7  |
| 10  | J     | 3    | LYS  | 3.7  |
| 11  | K     | 51   | LYS  | 3.7  |
| 1   | A     | 976  | C    | 3.7  |
| 1   | A     | 1019 | C    | 3.7  |
| 1   | A     | 1114 | C    | 3.7  |
| 1   | A     | 1142 | G    | 3.7  |
| 2   | B     | 232  | PRO  | 3.7  |
| 2   | B     | 240  | GLN  | 3.7  |
| 9   | I     | 38   | GLN  | 3.7  |
| 2   | B     | 148  | TYR  | 3.7  |
| 3   | C     | 23   | TYR  | 3.7  |
| 3   | C     | 98   | ASN  | 3.7  |
| 10  | J     | 100  | THR  | 3.7  |
| 1   | A     | 1403 | G    | 3.7  |
| 19  | S     | 36   | ARG  | 3.7  |
| 13  | M     | 13   | LYS  | 3.7  |
| 2   | B     | 39   | ILE  | 3.7  |
| 19  | S     | 35   | SER  | 3.7  |
| 2   | B     | 89   | GLY  | 3.7  |
| 2   | B     | 132  | LYS  | 3.7  |
| 3   | C     | 70   | VAL  | 3.7  |
| 3   | C     | 155  | GLY  | 3.7  |
| 17  | Q     | 100  | LYS  | 3.7  |
| 6   | F     | 37   | VAL  | 3.7  |
| 2   | B     | 76   | GLN  | 3.6  |
| 1   | A     | 1229 | A    | 3.6  |
| 2   | B     | 123  | ALA  | 3.6  |
| 9   | I     | 15   | ALA  | 3.6  |
| 1   | A     | 1004 | G    | 3.6  |
| 23  | X     | 30   | G    | 3.6  |
| 2   | B     | 224  | GLN  | 3.6  |
| 1   | A     | 1455 | C    | 3.6  |
| 14  | N     | 11   | LYS  | 3.6  |
| 1   | A     | 1115 | G    | 3.6  |
| 3   | C     | 55   | VAL  | 3.6  |
| 3   | C     | 76   | VAL  | 3.6  |
| 10  | J     | 6    | ILE  | 3.6  |
| 10  | J     | 22   | LYS  | 3.6  |
| 18  | R     | 20   | ALA  | 3.6  |
| 10  | J     | 19   | SER  | 3.6  |
| 1   | A     | 1076 | G    | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 144  | ARG  | 3.5  |
| 19  | S     | 8    | GLY  | 3.5  |
| 3   | C     | 86   | VAL  | 3.5  |
| 1   | A     | 52   | G    | 3.5  |
| 14  | N     | 22   | THR  | 3.5  |
| 3   | C     | 100  | ALA  | 3.5  |
| 14  | N     | 10   | ALA  | 3.5  |
| 3   | C     | 57   | ILE  | 3.5  |
| 9   | I     | 18   | PHE  | 3.5  |
| 1   | A     | 731  | C    | 3.5  |
| 2   | B     | 18   | GLY  | 3.5  |
| 7   | G     | 63   | LYS  | 3.5  |
| 10  | J     | 43   | ARG  | 3.5  |
| 10  | J     | 53   | PRO  | 3.5  |
| 14  | N     | 3    | ARG  | 3.5  |
| 2   | B     | 206  | ASP  | 3.5  |
| 10  | J     | 92   | THR  | 3.5  |
| 1   | A     | 980  | G    | 3.4  |
| 1   | A     | 51   | A    | 3.4  |
| 13  | M     | 2    | ALA  | 3.4  |
| 17  | Q     | 96   | GLN  | 3.4  |
| 9   | I     | 85   | LEU  | 3.4  |
| 12  | L     | 18   | VAL  | 3.4  |
| 1   | A     | 979  | G    | 3.4  |
| 1   | A     | 1011 | G    | 3.4  |
| 4   | D     | 25   | ARG  | 3.4  |
| 1   | A     | 209  | U    | 3.4  |
| 1   | A     | 1007 | C    | 3.4  |
| 2   | B     | 227  | GLY  | 3.4  |
| 1   | A     | 1022 | U    | 3.4  |
| 1   | A     | 1192 | U    | 3.4  |
| 10  | J     | 20   | ALA  | 3.4  |
| 7   | G     | 60   | LYS  | 3.4  |
| 13  | M     | 122  | LYS  | 3.4  |
| 2   | B     | 231  | GLU  | 3.4  |
| 3   | C     | 53   | ALA  | 3.4  |
| 19  | S     | 14   | HIS  | 3.4  |
| 10  | J     | 12   | ASP  | 3.4  |
| 19  | S     | 9    | VAL  | 3.3  |
| 3   | C     | 80   | GLY  | 3.3  |
| 17  | Q     | 14   | LYS  | 3.3  |
| 5   | E     | 20   | GLN  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | G     | 76   | ARG  | 3.3  |
| 1   | A     | 1102 | G    | 3.3  |
| 17  | Q     | 104  | LYS  | 3.3  |
| 2   | B     | 140  | HIS  | 3.3  |
| 3   | C     | 50   | ALA  | 3.3  |
| 10  | J     | 33   | GLN  | 3.3  |
| 10  | J     | 5    | ARG  | 3.3  |
| 10  | J     | 45   | ARG  | 3.3  |
| 3   | C     | 25   | GLY  | 3.3  |
| 2   | B     | 9    | GLU  | 3.3  |
| 1   | A     | 1207 | C    | 3.3  |
| 1   | A     | 1402 | C    | 3.3  |
| 2   | B     | 13   | ALA  | 3.3  |
| 10  | J     | 38   | ILE  | 3.3  |
| 10  | J     | 70   | ARG  | 3.3  |
| 10  | J     | 36   | GLY  | 3.3  |
| 4   | D     | 20   | TYR  | 3.3  |
| 14  | N     | 8    | GLU  | 3.3  |
| 1   | A     | 50   | A    | 3.3  |
| 4   | D     | 32   | ALA  | 3.3  |
| 1   | A     | 1457 | G    | 3.3  |
| 2   | B     | 42   | ILE  | 3.2  |
| 1   | A     | 1128 | A    | 3.2  |
| 1   | A     | 1110 | C    | 3.2  |
| 19  | S     | 7    | LYS  | 3.2  |
| 3   | C     | 60   | ALA  | 3.2  |
| 9   | I     | 96   | LEU  | 3.2  |
| 2   | B     | 239  | VAL  | 3.2  |
| 4   | D     | 2    | GLY  | 3.2  |
| 1   | A     | 79   | U    | 3.2  |
| 3   | C     | 91   | LEU  | 3.2  |
| 10  | J     | 18   | ALA  | 3.2  |
| 13  | M     | 11   | ARG  | 3.2  |
| 1   | A     | 991  | G    | 3.2  |
| 9   | I     | 26   | VAL  | 3.2  |
| 3   | C     | 93   | LYS  | 3.2  |
| 10  | J     | 41   | PRO  | 3.2  |
| 9   | I     | 36   | TYR  | 3.2  |
| 19  | S     | 31   | ILE  | 3.2  |
| 1   | A     | 826  | C    | 3.2  |
| 2   | B     | 138  | LEU  | 3.2  |
| 1   | A     | 49   | U    | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 75   | VAL  | 3.2  |
| 10  | J     | 83   | GLU  | 3.2  |
| 16  | P     | 83   | GLU  | 3.2  |
| 9   | I     | 92   | TYR  | 3.1  |
| 4   | D     | 209  | ARG  | 3.1  |
| 6   | F     | 98   | LEU  | 3.1  |
| 7   | G     | 59   | LEU  | 3.1  |
| 9   | I     | 84   | ALA  | 3.1  |
| 1   | A     | 985  | C    | 3.1  |
| 1   | A     | 1509 | U    | 3.1  |
| 14  | N     | 16   | PHE  | 3.1  |
| 20  | T     | 103  | GLY  | 3.1  |
| 1   | A     | 1124 | G    | 3.1  |
| 1   | A     | 1257 | G    | 3.1  |
| 2   | B     | 121  | LEU  | 3.1  |
| 3   | C     | 127  | ARG  | 3.1  |
| 6   | F     | 63   | TYR  | 3.1  |
| 2   | B     | 147  | LYS  | 3.1  |
| 1   | A     | 344  | A    | 3.1  |
| 1   | A     | 972  | C    | 3.1  |
| 1   | A     | 1008 | C    | 3.1  |
| 1   | A     | 1025 | C    | 3.1  |
| 1   | A     | 1263 | C    | 3.1  |
| 9   | I     | 8    | GLY  | 3.1  |
| 10  | J     | 42   | THR  | 3.1  |
| 11  | K     | 127  | LYS  | 3.1  |
| 3   | C     | 69   | HIS  | 3.1  |
| 10  | J     | 17   | ASP  | 3.1  |
| 13  | M     | 7    | VAL  | 3.1  |
| 18  | R     | 22   | VAL  | 3.1  |
| 1   | A     | 407  | A    | 3.1  |
| 1   | A     | 968  | U    | 3.1  |
| 1   | A     | 1104 | U    | 3.1  |
| 7   | G     | 13   | GLN  | 3.1  |
| 3   | C     | 67   | THR  | 3.1  |
| 9   | I     | 19   | LEU  | 3.1  |
| 12  | L     | 60   | LEU  | 3.1  |
| 14  | N     | 14   | PRO  | 3.1  |
| 19  | S     | 77   | THR  | 3.1  |
| 20  | T     | 99   | LEU  | 3.1  |
| 7   | G     | 48   | LYS  | 3.1  |
| 9   | I     | 70   | LYS  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | N     | 9    | LYS  | 3.1  |
| 19  | S     | 32   | LYS  | 3.1  |
| 3   | C     | 22   | TRP  | 3.1  |
| 1   | A     | 990  | U    | 3.1  |
| 4   | D     | 160  | GLN  | 3.0  |
| 6   | F     | 57   | GLN  | 3.0  |
| 9   | I     | 93   | ARG  | 3.0  |
| 2   | B     | 125  | PRO  | 3.0  |
| 19  | S     | 39   | THR  | 3.0  |
| 1   | A     | 970  | G    | 3.0  |
| 1   | A     | 995  | G    | 3.0  |
| 3   | C     | 162  | GLN  | 3.0  |
| 3   | C     | 26   | LYS  | 3.0  |
| 9   | I     | 58   | ARG  | 3.0  |
| 12  | L     | 28   | LYS  | 3.0  |
| 1   | A     | 1123 | C    | 3.0  |
| 12  | L     | 47   | LYS  | 3.0  |
| 2   | B     | 20   | GLU  | 3.0  |
| 3   | C     | 30   | ARG  | 3.0  |
| 10  | J     | 96   | ILE  | 3.0  |
| 3   | C     | 47   | LEU  | 3.0  |
| 7   | G     | 81   | GLY  | 3.0  |
| 1   | A     | 988  | G    | 3.0  |
| 1   | A     | 1171 | G    | 3.0  |
| 1   | A     | 1425 | G    | 3.0  |
| 1   | A     | 1006 | C    | 3.0  |
| 4   | D     | 37   | PRO  | 3.0  |
| 3   | C     | 54   | ARG  | 2.9  |
| 1   | A     | 1194 | A    | 2.9  |
| 7   | G     | 56   | GLN  | 2.9  |
| 1   | A     | 1024 | G    | 2.9  |
| 3   | C     | 68   | VAL  | 2.9  |
| 3   | C     | 95   | THR  | 2.9  |
| 13  | M     | 31   | LYS  | 2.9  |
| 2   | B     | 208  | ILE  | 2.9  |
| 3   | C     | 32   | LEU  | 2.9  |
| 1   | A     | 154  | A    | 2.9  |
| 3   | C     | 56   | ASP  | 2.9  |
| 2   | B     | 120  | ALA  | 2.9  |
| 2   | B     | 139  | LYS  | 2.9  |
| 10  | J     | 4    | ILE  | 2.9  |
| 1   | A     | 210  | U    | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1141 | U    | 2.9  |
| 3   | C     | 101  | LEU  | 2.9  |
| 7   | G     | 12   | LEU  | 2.9  |
| 2   | B     | 38   | GLY  | 2.9  |
| 7   | G     | 52   | GLU  | 2.9  |
| 13  | M     | 35   | GLU  | 2.9  |
| 7   | G     | 2    | ALA  | 2.9  |
| 6   | F     | 36   | ARG  | 2.9  |
| 19  | S     | 81   | ARG  | 2.9  |
| 1   | A     | 208  | U    | 2.9  |
| 19  | S     | 28   | LYS  | 2.9  |
| 19  | S     | 23   | ASN  | 2.9  |
| 7   | G     | 7    | ALA  | 2.9  |
| 2   | B     | 137  | ARG  | 2.9  |
| 3   | C     | 112  | SER  | 2.9  |
| 1   | A     | 973  | A    | 2.9  |
| 1   | A     | 1266 | A    | 2.9  |
| 3   | C     | 119  | ARG  | 2.9  |
| 6   | F     | 79   | LEU  | 2.9  |
| 2   | B     | 228  | GLY  | 2.8  |
| 9   | I     | 87   | GLN  | 2.8  |
| 10  | J     | 95   | GLU  | 2.8  |
| 20  | T     | 68   | LYS  | 2.8  |
| 12  | L     | 89   | ARG  | 2.8  |
| 2   | B     | 83   | MET  | 2.8  |
| 9   | I     | 2    | GLU  | 2.8  |
| 10  | J     | 94   | VAL  | 2.8  |
| 20  | T     | 12   | ALA  | 2.8  |
| 10  | J     | 11   | PHE  | 2.8  |
| 6   | F     | 84   | ASN  | 2.8  |
| 10  | J     | 58   | ASP  | 2.8  |
| 14  | N     | 7    | ILE  | 2.8  |
| 1   | A     | 1401 | G    | 2.8  |
| 1   | A     | 1017 | A    | 2.8  |
| 7   | G     | 73   | MET  | 2.8  |
| 10  | J     | 7    | LYS  | 2.8  |
| 10  | J     | 84   | GLN  | 2.8  |
| 4   | D     | 24   | GLU  | 2.8  |
| 2   | B     | 92   | TYR  | 2.8  |
| 13  | M     | 21   | TYR  | 2.8  |
| 17  | Q     | 101  | ARG  | 2.8  |
| 14  | N     | 2    | ALA  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | G     | 16   | LEU  | 2.8  |
| 1   | A     | 1143 | C    | 2.8  |
| 3   | C     | 62   | ASP  | 2.8  |
| 19  | S     | 38   | SER  | 2.8  |
| 18  | R     | 19   | LYS  | 2.8  |
| 1   | A     | 1012 | A    | 2.8  |
| 2   | B     | 141  | GLU  | 2.8  |
| 10  | J     | 89   | ASP  | 2.8  |
| 10  | J     | 99   | LYS  | 2.8  |
| 19  | S     | 18   | LYS  | 2.8  |
| 23  | X     | 32   | C    | 2.8  |
| 4   | D     | 7    | PRO  | 2.8  |
| 11  | K     | 54   | ARG  | 2.7  |
| 10  | J     | 44   | VAL  | 2.7  |
| 1   | A     | 1479 | A    | 2.7  |
| 3   | C     | 24   | ALA  | 2.7  |
| 19  | S     | 34   | TRP  | 2.7  |
| 1   | A     | 343  | G    | 2.7  |
| 1   | A     | 1156 | G    | 2.7  |
| 6   | F     | 19   | LEU  | 2.7  |
| 3   | C     | 181  | ASN  | 2.7  |
| 13  | M     | 109  | THR  | 2.7  |
| 7   | G     | 55   | GLY  | 2.7  |
| 7   | G     | 79   | ARG  | 2.7  |
| 9   | I     | 3    | GLN  | 2.7  |
| 14  | N     | 57   | ARG  | 2.7  |
| 1   | A     | 417  | C    | 2.7  |
| 1   | A     | 1021 | C    | 2.7  |
| 19  | S     | 67   | VAL  | 2.7  |
| 17  | Q     | 95   | TYR  | 2.7  |
| 1   | A     | 1242 | A    | 2.7  |
| 1   | A     | 465  | G    | 2.7  |
| 1   | A     | 707  | G    | 2.7  |
| 1   | A     | 989  | G    | 2.7  |
| 2   | B     | 124  | SER  | 2.7  |
| 6   | F     | 47   | ARG  | 2.7  |
| 2   | B     | 49   | GLU  | 2.7  |
| 3   | C     | 90   | GLU  | 2.7  |
| 12  | L     | 79   | GLU  | 2.7  |
| 3   | C     | 128  | PHE  | 2.7  |
| 9   | I     | 79   | LEU  | 2.7  |
| 10  | J     | 40   | LEU  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | S     | 25   | LYS  | 2.7  |
| 1   | A     | 1261 | A    | 2.7  |
| 1   | A     | 824  | U    | 2.7  |
| 1   | A     | 1118 | U    | 2.7  |
| 3   | C     | 83   | ARG  | 2.7  |
| 1   | A     | 1032 | G    | 2.7  |
| 1   | A     | 1120 | G    | 2.7  |
| 2   | B     | 45   | GLN  | 2.7  |
| 2   | B     | 78   | GLN  | 2.7  |
| 2   | B     | 95   | GLN  | 2.7  |
| 2   | B     | 32   | ILE  | 2.7  |
| 2   | B     | 223  | ILE  | 2.7  |
| 3   | C     | 65   | ALA  | 2.7  |
| 20  | T     | 94   | ALA  | 2.7  |
| 14  | N     | 31   | ARG  | 2.7  |
| 21  | V     | 9    | ARG  | 2.7  |
| 19  | S     | 54   | GLY  | 2.7  |
| 1   | A     | 516  | A    | 2.7  |
| 1   | A     | 1023 | A    | 2.7  |
| 17  | Q     | 12   | SER  | 2.7  |
| 19  | S     | 24   | ALA  | 2.6  |
| 1   | A     | 1459 | G    | 2.6  |
| 20  | T     | 73   | HIS  | 2.6  |
| 3   | C     | 88   | ARG  | 2.6  |
| 2   | B     | 94   | ASN  | 2.6  |
| 2   | B     | 145  | LEU  | 2.6  |
| 4   | D     | 22   | LYS  | 2.6  |
| 9   | I     | 65   | VAL  | 2.6  |
| 1   | A     | 1267 | A    | 2.6  |
| 1   | A     | 246  | G    | 2.6  |
| 1   | A     | 975  | G    | 2.6  |
| 1   | A     | 1014 | G    | 2.6  |
| 3   | C     | 201  | TYR  | 2.6  |
| 10  | J     | 31   | GLY  | 2.6  |
| 12  | L     | 17   | LYS  | 2.6  |
| 2   | B     | 221  | LEU  | 2.6  |
| 3   | C     | 82   | GLU  | 2.6  |
| 1   | A     | 974  | U    | 2.6  |
| 6   | F     | 1    | MET  | 2.6  |
| 6   | F     | 60   | PHE  | 2.6  |
| 8   | H     | 1    | MET  | 2.6  |
| 19  | S     | 66   | MET  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 454  | A    | 2.6  |
| 1   | A     | 1185 | A    | 2.6  |
| 17  | Q     | 97   | SER  | 2.6  |
| 23  | X     | 31   | A    | 2.6  |
| 10  | J     | 10   | GLY  | 2.6  |
| 1   | A     | 1264 | G    | 2.6  |
| 7   | G     | 61   | VAL  | 2.6  |
| 18  | R     | 25   | THR  | 2.6  |
| 2   | B     | 116  | GLU  | 2.6  |
| 10  | J     | 78   | ASN  | 2.6  |
| 1   | A     | 340  | C    | 2.6  |
| 3   | C     | 20   | SER  | 2.6  |
| 7   | G     | 149  | ARG  | 2.6  |
| 14  | N     | 12   | ARG  | 2.6  |
| 3   | C     | 81   | GLY  | 2.6  |
| 2   | B     | 29   | ALA  | 2.6  |
| 3   | C     | 110  | ASN  | 2.6  |
| 9   | I     | 55   | ALA  | 2.6  |
| 11  | K     | 117  | ASN  | 2.6  |
| 1   | A     | 613  | G    | 2.5  |
| 1   | A     | 1000 | G    | 2.5  |
| 1   | A     | 1013 | G    | 2.5  |
| 1   | A     | 1152 | G    | 2.5  |
| 1   | A     | 1158 | G    | 2.5  |
| 1   | A     | 1244 | C    | 2.5  |
| 1   | A     | 1456 | C    | 2.5  |
| 14  | N     | 15   | LYS  | 2.5  |
| 3   | C     | 73   | PRO  | 2.5  |
| 2   | B     | 52   | GLU  | 2.5  |
| 3   | C     | 28   | GLN  | 2.5  |
| 6   | F     | 70   | ASP  | 2.5  |
| 1   | A     | 1035 | G    | 2.5  |
| 1   | A     | 455  | C    | 2.5  |
| 19  | S     | 22   | LEU  | 2.5  |
| 21  | V     | 23   | PRO  | 2.5  |
| 10  | J     | 72   | VAL  | 2.5  |
| 1   | A     | 971  | A    | 2.5  |
| 18  | R     | 28   | GLU  | 2.5  |
| 3   | C     | 118  | GLN  | 2.5  |
| 3   | C     | 71   | ALA  | 2.5  |
| 21  | V     | 24   | ARG  | 2.5  |
| 1   | A     | 969  | U    | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | N     | 60   | SER  | 2.5  |
| 2   | B     | 118  | LEU  | 2.5  |
| 3   | C     | 188  | LEU  | 2.5  |
| 13  | M     | 85   | GLY  | 2.5  |
| 2   | B     | 97   | TRP  | 2.5  |
| 6   | F     | 6    | VAL  | 2.5  |
| 9   | I     | 17   | VAL  | 2.5  |
| 19  | S     | 19   | VAL  | 2.5  |
| 1   | A     | 1258 | C    | 2.5  |
| 5   | E     | 133  | TYR  | 2.5  |
| 13  | M     | 59   | TYR  | 2.5  |
| 3   | C     | 89   | GLU  | 2.5  |
| 10  | J     | 47   | PHE  | 2.5  |
| 13  | M     | 105  | THR  | 2.5  |
| 1   | A     | 1256 | A    | 2.5  |
| 3   | C     | 72   | LYS  | 2.5  |
| 2   | B     | 108  | ILE  | 2.5  |
| 12  | L     | 62   | SER  | 2.5  |
| 21  | V     | 4    | GLY  | 2.5  |
| 4   | D     | 187  | ARG  | 2.5  |
| 1   | A     | 1247 | G    | 2.5  |
| 1   | A     | 1297 | G    | 2.5  |
| 1   | A     | 83   | A    | 2.5  |
| 1   | A     | 1249 | A    | 2.5  |
| 15  | O     | 87   | ILE  | 2.4  |
| 13  | M     | 6    | GLY  | 2.4  |
| 3   | C     | 40   | ARG  | 2.4  |
| 13  | M     | 93   | ARG  | 2.4  |
| 1   | A     | 994  | A    | 2.4  |
| 4   | D     | 36   | ARG  | 2.4  |
| 9   | I     | 11   | LYS  | 2.4  |
| 10  | J     | 21   | GLN  | 2.4  |
| 3   | C     | 103  | VAL  | 2.4  |
| 1   | A     | 245  | A    | 2.4  |
| 1   | A     | 1268 | A    | 2.4  |
| 1   | A     | 1508 | A    | 2.4  |
| 13  | M     | 3    | ARG  | 2.4  |
| 13  | M     | 115  | LYS  | 2.4  |
| 1   | A     | 1255 | G    | 2.4  |
| 1   | A     | 1286 | G    | 2.4  |
| 6   | F     | 66   | GLU  | 2.4  |
| 1   | A     | 1283 | U    | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | K     | 25   | TYR  | 2.4  |
| 10  | J     | 8    | LEU  | 2.4  |
| 9   | I     | 14   | VAL  | 2.4  |
| 3   | C     | 36   | ASP  | 2.4  |
| 9   | I     | 66   | ARG  | 2.4  |
| 14  | N     | 4    | LYS  | 2.4  |
| 15  | O     | 64   | ARG  | 2.4  |
| 7   | G     | 90   | GLU  | 2.4  |
| 13  | M     | 58   | GLU  | 2.4  |
| 11  | K     | 79   | SER  | 2.4  |
| 1   | A     | 423  | G    | 2.4  |
| 1   | A     | 953  | G    | 2.4  |
| 1   | A     | 1202 | G    | 2.4  |
| 10  | J     | 13   | HIS  | 2.4  |
| 19  | S     | 62   | ILE  | 2.4  |
| 6   | F     | 91   | VAL  | 2.3  |
| 18  | R     | 21   | LYS  | 2.3  |
| 6   | F     | 97   | PHE  | 2.3  |
| 1   | A     | 1080 | C    | 2.3  |
| 1   | A     | 1140 | C    | 2.3  |
| 1   | A     | 1181 | C    | 2.3  |
| 1   | A     | 1195 | C    | 2.3  |
| 1   | A     | 978  | A    | 2.3  |
| 1   | A     | 1105 | A    | 2.3  |
| 19  | S     | 71   | LEU  | 2.3  |
| 1   | A     | 1177 | U    | 2.3  |
| 4   | D     | 40   | PRO  | 2.3  |
| 19  | S     | 55   | LYS  | 2.3  |
| 1   | A     | 405  | G    | 2.3  |
| 1   | A     | 1281 | G    | 2.3  |
| 2   | B     | 130  | ARG  | 2.3  |
| 13  | M     | 88   | ARG  | 2.3  |
| 6   | F     | 58   | GLY  | 2.3  |
| 10  | J     | 76   | ASN  | 2.3  |
| 11  | K     | 52   | GLY  | 2.3  |
| 13  | M     | 12   | ASN  | 2.3  |
| 2   | B     | 109  | SER  | 2.3  |
| 9   | I     | 126  | SER  | 2.3  |
| 1   | A     | 48   | C    | 2.3  |
| 1   | A     | 157  | C    | 2.3  |
| 1   | A     | 212  | C    | 2.3  |
| 1   | A     | 1027 | C    | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1198 | C    | 2.3  |
| 1   | A     | 1265 | C    | 2.3  |
| 2   | B     | 33   | TYR  | 2.3  |
| 3   | C     | 14   | ILE  | 2.3  |
| 3   | C     | 84   | ILE  | 2.3  |
| 15  | O     | 22   | THR  | 2.3  |
| 5   | E     | 9    | LYS  | 2.3  |
| 2   | B     | 23   | ARG  | 2.3  |
| 19  | S     | 42   | PRO  | 2.3  |
| 9   | I     | 57   | GLY  | 2.3  |
| 20  | T     | 95   | ALA  | 2.3  |
| 12  | L     | 33   | ARG  | 2.3  |
| 20  | T     | 83   | ARG  | 2.3  |
| 1   | A     | 823  | C    | 2.3  |
| 1   | A     | 1295 | C    | 2.3  |
| 19  | S     | 11   | VAL  | 2.3  |
| 1   | A     | 5    | U    | 2.3  |
| 12  | L     | 63   | GLY  | 2.3  |
| 2   | B     | 37   | ASN  | 2.3  |
| 9   | I     | 12   | GLU  | 2.3  |
| 19  | S     | 13   | ASP  | 2.3  |
| 12  | L     | 115  | LYS  | 2.3  |
| 19  | S     | 70   | LYS  | 2.3  |
| 10  | J     | 98   | ILE  | 2.3  |
| 7   | G     | 4    | ARG  | 2.3  |
| 13  | M     | 20   | THR  | 2.3  |
| 1   | A     | 996  | C    | 2.2  |
| 1   | A     | 1461 | C    | 2.2  |
| 3   | C     | 105  | GLU  | 2.2  |
| 6   | F     | 35   | ALA  | 2.2  |
| 6   | F     | 61   | LEU  | 2.2  |
| 2   | B     | 110  | GLN  | 2.2  |
| 17  | Q     | 17   | LYS  | 2.2  |
| 9   | I     | 90   | PRO  | 2.2  |
| 1   | A     | 1405 | G    | 2.2  |
| 1   | A     | 1424 | G    | 2.2  |
| 9   | I     | 22   | GLY  | 2.2  |
| 15  | O     | 6    | GLU  | 2.2  |
| 1   | A     | 1199 | C    | 2.2  |
| 1   | A     | 1260 | A    | 2.2  |
| 1   | A     | 1480 | A    | 2.2  |
| 9   | I     | 111  | ARG  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | M     | 102  | ARG  | 2.2  |
| 6   | F     | 65   | VAL  | 2.2  |
| 9   | I     | 114  | TYR  | 2.2  |
| 19  | S     | 52   | TYR  | 2.2  |
| 3   | C     | 205  | GLY  | 2.2  |
| 11  | K     | 77   | MET  | 2.2  |
| 1   | A     | 433  | G    | 2.2  |
| 1   | A     | 1138 | G    | 2.2  |
| 1   | A     | 1246 | G    | 2.2  |
| 1   | A     | 1031 | U    | 2.2  |
| 3   | C     | 63   | ASN  | 2.2  |
| 1   | A     | 1119 | C    | 2.2  |
| 1   | A     | 1145 | C    | 2.2  |
| 1   | A     | 1348 | C    | 2.2  |
| 9   | I     | 68   | GLY  | 2.2  |
| 18  | R     | 88   | LYS  | 2.2  |
| 2   | B     | 61   | LEU  | 2.2  |
| 14  | N     | 6    | LEU  | 2.2  |
| 9   | I     | 52   | ALA  | 2.2  |
| 14  | N     | 20   | ALA  | 2.2  |
| 7   | G     | 10   | ARG  | 2.2  |
| 7   | G     | 143  | ARG  | 2.2  |
| 14  | N     | 29   | ARG  | 2.2  |
| 1   | A     | 1507 | G    | 2.2  |
| 9   | I     | 105  | ASP  | 2.2  |
| 10  | J     | 39   | PRO  | 2.2  |
| 1   | A     | 1135 | C    | 2.2  |
| 4   | D     | 4    | TYR  | 2.2  |
| 19  | S     | 10   | PHE  | 2.2  |
| 2   | B     | 98   | LEU  | 2.2  |
| 3   | C     | 52   | LEU  | 2.2  |
| 6   | F     | 21   | LEU  | 2.2  |
| 19  | S     | 30   | LEU  | 2.2  |
| 19  | S     | 27   | GLU  | 2.2  |
| 4   | D     | 73   | ARG  | 2.1  |
| 12  | L     | 59   | ARG  | 2.1  |
| 18  | R     | 72   | ARG  | 2.1  |
| 2   | B     | 113  | HIS  | 2.1  |
| 9   | I     | 29   | ASN  | 2.1  |
| 2   | B     | 165  | VAL  | 2.1  |
| 3   | C     | 106  | VAL  | 2.1  |
| 9   | I     | 28   | VAL  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 152  | G    | 2.1  |
| 10  | J     | 14   | LYS  | 2.1  |
| 1   | A     | 1134 | A    | 2.1  |
| 5   | E     | 22   | GLY  | 2.1  |
| 14  | N     | 28   | GLY  | 2.1  |
| 19  | S     | 79   | THR  | 2.1  |
| 9   | I     | 101  | PHE  | 2.1  |
| 18  | R     | 29   | PHE  | 2.1  |
| 2   | B     | 85   | ALA  | 2.1  |
| 3   | C     | 146  | ALA  | 2.1  |
| 4   | D     | 34   | GLU  | 2.1  |
| 7   | G     | 57   | GLU  | 2.1  |
| 18  | R     | 42   | ARG  | 2.1  |
| 2   | B     | 135  | GLN  | 2.1  |
| 1   | A     | 998  | U    | 2.1  |
| 1   | A     | 1034 | U    | 2.1  |
| 1   | A     | 1458 | U    | 2.1  |
| 3   | C     | 17   | ASP  | 2.1  |
| 5   | E     | 5    | ASP  | 2.1  |
| 2   | B     | 28   | PHE  | 2.1  |
| 1   | A     | 1133 | A    | 2.1  |
| 2   | B     | 111  | ARG  | 2.1  |
| 13  | M     | 5    | ALA  | 2.1  |
| 1   | A     | 1159 | G    | 2.1  |
| 1   | A     | 1162 | G    | 2.1  |
| 1   | A     | 1451 | G    | 2.1  |
| 5   | E     | 80   | ILE  | 2.1  |
| 15  | O     | 13   | GLN  | 2.1  |
| 2   | B     | 93   | VAL  | 2.1  |
| 4   | D     | 33   | MET  | 2.1  |
| 7   | G     | 53   | LYS  | 2.1  |
| 13  | M     | 27   | LYS  | 2.1  |
| 12  | L     | 92   | ASP  | 2.1  |
| 20  | T     | 10   | LEU  | 2.1  |
| 5   | E     | 150  | ARG  | 2.1  |
| 7   | G     | 154  | TYR  | 2.1  |
| 10  | J     | 97   | GLU  | 2.1  |
| 1   | A     | 1269 | A    | 2.1  |
| 1   | A     | 966  | C    | 2.1  |
| 1   | A     | 1155 | G    | 2.1  |
| 1   | A     | 1178 | G    | 2.1  |
| 1   | A     | 1303 | C    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 31   | HIS  | 2.1  |
| 1   | A     | 1452 | G    | 2.1  |
| 3   | C     | 66   | VAL  | 2.1  |
| 9   | I     | 86   | VAL  | 2.1  |
| 11  | K     | 11   | LYS  | 2.1  |
| 14  | N     | 17   | LYS  | 2.1  |
| 2   | B     | 43   | ASP  | 2.1  |
| 14  | N     | 35   | ARG  | 2.1  |
| 3   | C     | 44   | GLU  | 2.1  |
| 14  | N     | 32   | SER  | 2.0  |
| 20  | T     | 11   | SER  | 2.0  |
| 19  | S     | 57   | HIS  | 2.0  |
| 1   | A     | 993  | A    | 2.0  |
| 19  | S     | 41   | VAL  | 2.0  |
| 6   | F     | 12   | PRO  | 2.0  |
| 20  | T     | 98   | PRO  | 2.0  |
| 1   | A     | 1230 | C    | 2.0  |
| 3   | C     | 78   | GLY  | 2.0  |
| 3   | C     | 79   | ARG  | 2.0  |
| 15  | O     | 86   | GLY  | 2.0  |
| 1   | A     | 1130 | U    | 2.0  |
| 2   | B     | 54   | THR  | 2.0  |
| 3   | C     | 27   | LYS  | 2.0  |
| 6   | F     | 43   | LEU  | 2.0  |
| 4   | D     | 50   | ARG  | 2.0  |
| 7   | G     | 6    | ARG  | 2.0  |
| 9   | I     | 9    | ARG  | 2.0  |
| 10  | J     | 9    | ARG  | 2.0  |
| 2   | B     | 211  | ILE  | 2.0  |
| 6   | F     | 25   | ILE  | 2.0  |
| 20  | T     | 106  | ALA  | 2.0  |
| 2   | B     | 35   | GLU  | 2.0  |
| 2   | B     | 143  | GLU  | 2.0  |
| 13  | M     | 65   | LYS  | 2.0  |
| 13  | M     | 64   | TRP  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23  | PSU  | X     | 39  | 20/21 | 0.76 | 0.21 | 88,88,91,91                 | 0     |
| 23  | 70U  | X     | 34  | 25/26 | 0.81 | 0.18 | 61,70,80,82                 | 0     |
| 23  | 12A  | X     | 37  | 34/35 | 0.83 | 0.21 | 69,72,72,72                 | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 24  | MG   | A     | 1725 | 1/1   | -0.26 | 0.89 | 38,38,38,38                 | 1     |
| 24  | MG   | A     | 1757 | 1/1   | -0.25 | 0.87 | 0,0,0,0                     | 1     |
| 24  | MG   | A     | 1644 | 1/1   | -0.06 | 1.25 | 60,60,60,60                 | 1     |
| 24  | MG   | A     | 1695 | 1/1   | 0.09  | 0.78 | 33,33,33,33                 | 1     |
| 24  | MG   | A     | 1694 | 1/1   | 0.10  | 1.69 | 69,69,69,69                 | 1     |
| 24  | MG   | A     | 1696 | 1/1   | 0.10  | 0.80 | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1638 | 1/1   | 0.15  | 1.13 | 50,50,50,50                 | 1     |
| 24  | MG   | A     | 1701 | 1/1   | 0.15  | 2.27 | 27,27,27,27                 | 1     |
| 24  | MG   | A     | 1777 | 1/1   | 0.17  | 1.60 | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1752 | 1/1   | 0.18  | 0.74 | 27,27,27,27                 | 1     |
| 24  | MG   | A     | 1702 | 1/1   | 0.22  | 1.07 | 57,57,57,57                 | 1     |
| 24  | MG   | A     | 1712 | 1/1   | 0.22  | 0.74 | 21,21,21,21                 | 1     |
| 24  | MG   | A     | 1639 | 1/1   | 0.23  | 2.94 | 64,64,64,64                 | 1     |
| 24  | MG   | A     | 1736 | 1/1   | 0.24  | 1.45 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1724 | 1/1   | 0.26  | 0.88 | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1697 | 1/1   | 0.29  | 1.83 | 55,55,55,55                 | 1     |
| 24  | MG   | A     | 1707 | 1/1   | 0.31  | 1.40 | 33,33,33,33                 | 1     |
| 24  | MG   | A     | 1776 | 1/1   | 0.32  | 0.91 | 64,64,64,64                 | 1     |
| 24  | MG   | A     | 1607 | 1/1   | 0.33  | 0.86 | 107,107,107,107             | 1     |
| 24  | MG   | A     | 1602 | 1/1   | 0.34  | 0.28 | 86,86,86,86                 | 0     |
| 24  | MG   | A     | 1734 | 1/1   | 0.35  | 0.75 | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1666 | 1/1   | 0.35  | 1.14 | 55,55,55,55                 | 1     |
| 24  | MG   | A     | 1624 | 1/1   | 0.36  | 0.57 | 82,82,82,82                 | 1     |
| 24  | MG   | A     | 1706 | 1/1   | 0.38  | 1.60 | 6,6,6,6                     | 1     |
| 24  | MG   | A     | 1616 | 1/1   | 0.46  | 1.90 | 74,74,74,74                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1708 | 1/1   | 0.47 | 1.52 | 51,51,51,51                 | 1     |
| 24  | MG   | A     | 1622 | 1/1   | 0.50 | 0.42 | 54,54,54,54                 | 1     |
| 24  | MG   | A     | 1689 | 1/1   | 0.52 | 0.87 | 27,27,27,27                 | 1     |
| 24  | MG   | A     | 1645 | 1/1   | 0.53 | 0.44 | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1610 | 1/1   | 0.54 | 0.45 | 66,66,66,66                 | 0     |
| 24  | MG   | A     | 1604 | 1/1   | 0.55 | 0.82 | 111,111,111,111             | 0     |
| 24  | MG   | A     | 1759 | 1/1   | 0.55 | 0.56 | 15,15,15,15                 | 1     |
| 24  | MG   | A     | 1758 | 1/1   | 0.56 | 1.14 | 40,40,40,40                 | 1     |
| 24  | MG   | A     | 1658 | 1/1   | 0.58 | 0.58 | 43,43,43,43                 | 1     |
| 24  | MG   | A     | 1699 | 1/1   | 0.58 | 0.79 | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1623 | 1/1   | 0.58 | 0.69 | 67,67,67,67                 | 1     |
| 24  | MG   | A     | 1750 | 1/1   | 0.59 | 0.66 | 43,43,43,43                 | 1     |
| 24  | MG   | A     | 1760 | 1/1   | 0.59 | 0.71 | 6,6,6,6                     | 1     |
| 24  | MG   | A     | 1629 | 1/1   | 0.61 | 1.05 | 39,39,39,39                 | 1     |
| 24  | MG   | A     | 1739 | 1/1   | 0.61 | 0.50 | 33,33,33,33                 | 1     |
| 24  | MG   | A     | 1621 | 1/1   | 0.62 | 0.55 | 18,18,18,18                 | 1     |
| 24  | MG   | A     | 1780 | 1/1   | 0.63 | 0.90 | 0,0,0,0                     | 1     |
| 24  | MG   | A     | 1731 | 1/1   | 0.65 | 0.54 | 18,18,18,18                 | 1     |
| 24  | MG   | A     | 1617 | 1/1   | 0.65 | 1.24 | 50,50,50,50                 | 1     |
| 24  | MG   | A     | 1767 | 1/1   | 0.65 | 0.50 | 17,17,17,17                 | 1     |
| 24  | MG   | A     | 1749 | 1/1   | 0.66 | 0.37 | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1636 | 1/1   | 0.67 | 0.52 | 42,42,42,42                 | 1     |
| 24  | MG   | A     | 1614 | 1/1   | 0.67 | 0.64 | 49,49,49,49                 | 1     |
| 24  | MG   | A     | 1635 | 1/1   | 0.68 | 0.65 | 18,18,18,18                 | 1     |
| 24  | MG   | A     | 1603 | 1/1   | 0.68 | 0.56 | 63,63,63,63                 | 0     |
| 24  | MG   | A     | 1704 | 1/1   | 0.68 | 1.18 | 10,10,10,10                 | 1     |
| 24  | MG   | A     | 1669 | 1/1   | 0.68 | 1.27 | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1730 | 1/1   | 0.69 | 0.44 | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1751 | 1/1   | 0.70 | 1.77 | 29,29,29,29                 | 1     |
| 24  | MG   | A     | 1633 | 1/1   | 0.70 | 0.91 | 57,57,57,57                 | 1     |
| 24  | MG   | A     | 1773 | 1/1   | 0.71 | 0.51 | 35,35,35,35                 | 1     |
| 24  | MG   | A     | 1605 | 1/1   | 0.71 | 0.44 | 33,33,33,33                 | 1     |
| 24  | MG   | A     | 1630 | 1/1   | 0.72 | 0.47 | 59,59,59,59                 | 1     |
| 24  | MG   | A     | 1608 | 1/1   | 0.72 | 0.72 | 62,62,62,62                 | 1     |
| 24  | MG   | A     | 1613 | 1/1   | 0.73 | 0.34 | 25,25,25,25                 | 1     |
| 24  | MG   | A     | 1601 | 1/1   | 0.73 | 0.17 | 51,51,51,51                 | 0     |
| 24  | MG   | A     | 1753 | 1/1   | 0.73 | 0.97 | 31,31,31,31                 | 1     |
| 24  | MG   | A     | 1661 | 1/1   | 0.73 | 0.43 | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1727 | 1/1   | 0.74 | 0.45 | 6,6,6,6                     | 1     |
| 24  | MG   | A     | 1625 | 1/1   | 0.74 | 0.45 | 0,0,0,0                     | 1     |
| 24  | MG   | A     | 1671 | 1/1   | 0.75 | 0.57 | 41,41,41,41                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1683 | 1/1   | 0.75 | 0.39 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1700 | 1/1   | 0.75 | 1.18 | 32,32,32,32                 | 1     |
| 24  | MG   | A     | 1619 | 1/1   | 0.75 | 0.60 | 57,57,57,57                 | 1     |
| 24  | MG   | A     | 1733 | 1/1   | 0.76 | 0.50 | 35,35,35,35                 | 1     |
| 24  | MG   | A     | 1715 | 1/1   | 0.76 | 0.63 | 44,44,44,44                 | 1     |
| 24  | MG   | A     | 1741 | 1/1   | 0.77 | 0.97 | 33,33,33,33                 | 1     |
| 24  | MG   | A     | 1717 | 1/1   | 0.77 | 0.53 | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1754 | 1/1   | 0.77 | 0.51 | 31,31,31,31                 | 1     |
| 24  | MG   | A     | 1785 | 1/1   | 0.77 | 0.61 | 17,17,17,17                 | 1     |
| 24  | MG   | A     | 1632 | 1/1   | 0.78 | 0.81 | 31,31,31,31                 | 1     |
| 24  | MG   | A     | 1768 | 1/1   | 0.78 | 0.91 | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1660 | 1/1   | 0.78 | 0.42 | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1667 | 1/1   | 0.78 | 0.73 | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1726 | 1/1   | 0.78 | 0.32 | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1735 | 1/1   | 0.78 | 0.34 | 3,3,3,3                     | 1     |
| 24  | MG   | A     | 1716 | 1/1   | 0.78 | 0.44 | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1745 | 1/1   | 0.79 | 1.59 | 13,13,13,13                 | 1     |
| 24  | MG   | A     | 1631 | 1/1   | 0.79 | 0.29 | 54,54,54,54                 | 1     |
| 24  | MG   | A     | 1775 | 1/1   | 0.79 | 0.37 | 16,16,16,16                 | 1     |
| 24  | MG   | A     | 1719 | 1/1   | 0.79 | 2.10 | 35,35,35,35                 | 1     |
| 24  | MG   | A     | 1722 | 1/1   | 0.79 | 0.75 | 22,22,22,22                 | 1     |
| 24  | MG   | A     | 1684 | 1/1   | 0.79 | 1.29 | 16,16,16,16                 | 1     |
| 24  | MG   | A     | 1662 | 1/1   | 0.79 | 0.55 | 32,32,32,32                 | 1     |
| 24  | MG   | A     | 1781 | 1/1   | 0.80 | 0.37 | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1650 | 1/1   | 0.80 | 0.40 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1641 | 1/1   | 0.81 | 0.37 | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1656 | 1/1   | 0.81 | 0.46 | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1765 | 1/1   | 0.81 | 0.27 | 0,0,0,0                     | 1     |
| 24  | MG   | A     | 1672 | 1/1   | 0.81 | 0.86 | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1738 | 1/1   | 0.81 | 0.39 | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1783 | 1/1   | 0.81 | 0.93 | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1676 | 1/1   | 0.81 | 0.45 | 44,44,44,44                 | 1     |
| 24  | MG   | A     | 1657 | 1/1   | 0.82 | 0.73 | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1652 | 1/1   | 0.82 | 0.65 | 30,30,30,30                 | 1     |
| 24  | MG   | A     | 1711 | 1/1   | 0.82 | 0.64 | 62,62,62,62                 | 1     |
| 24  | MG   | A     | 1705 | 1/1   | 0.82 | 1.74 | 39,39,39,39                 | 1     |
| 24  | MG   | A     | 1713 | 1/1   | 0.82 | 0.33 | 31,31,31,31                 | 1     |
| 24  | MG   | A     | 1743 | 1/1   | 0.82 | 0.90 | 17,17,17,17                 | 1     |
| 24  | MG   | A     | 1612 | 1/1   | 0.82 | 0.38 | 25,25,25,25                 | 1     |
| 24  | MG   | B     | 301  | 1/1   | 0.82 | 0.19 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1693 | 1/1   | 0.83 | 0.28 | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1755 | 1/1   | 0.83 | 0.80 | 44,44,44,44                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1664 | 1/1   | 0.84 | 0.37 | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1769 | 1/1   | 0.84 | 0.48 | 2,2,2,2                     | 1     |
| 24  | MG   | A     | 1772 | 1/1   | 0.84 | 0.59 | 32,32,32,32                 | 1     |
| 24  | MG   | A     | 1675 | 1/1   | 0.84 | 0.37 | 29,29,29,29                 | 1     |
| 26  | ZN   | D     | 301  | 1/1   | 0.84 | 0.47 | 100,100,100,100             | 0     |
| 24  | MG   | A     | 1740 | 1/1   | 0.85 | 0.85 | 29,29,29,29                 | 1     |
| 24  | MG   | A     | 1674 | 1/1   | 0.85 | 0.43 | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1721 | 1/1   | 0.85 | 0.47 | 21,21,21,21                 | 1     |
| 24  | MG   | A     | 1710 | 1/1   | 0.85 | 0.32 | 25,25,25,25                 | 1     |
| 24  | MG   | A     | 1690 | 1/1   | 0.85 | 0.24 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1680 | 1/1   | 0.85 | 1.26 | 45,45,45,45                 | 1     |
| 24  | MG   | A     | 1729 | 1/1   | 0.86 | 0.25 | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1742 | 1/1   | 0.86 | 0.23 | 2,2,2,2                     | 1     |
| 24  | MG   | A     | 1659 | 1/1   | 0.86 | 0.31 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1709 | 1/1   | 0.86 | 0.17 | 8,8,8,8                     | 1     |
| 24  | MG   | A     | 1703 | 1/1   | 0.86 | 0.54 | 40,40,40,40                 | 1     |
| 24  | MG   | A     | 1654 | 1/1   | 0.86 | 0.50 | 45,45,45,45                 | 1     |
| 24  | MG   | A     | 1682 | 1/1   | 0.87 | 0.51 | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1746 | 1/1   | 0.87 | 1.03 | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1678 | 1/1   | 0.87 | 1.12 | 40,40,40,40                 | 1     |
| 24  | MG   | A     | 1627 | 1/1   | 0.87 | 0.17 | 6,6,6,6                     | 1     |
| 24  | MG   | A     | 1770 | 1/1   | 0.88 | 1.37 | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1762 | 1/1   | 0.88 | 0.26 | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1732 | 1/1   | 0.88 | 0.62 | 13,13,13,13                 | 1     |
| 24  | MG   | A     | 1686 | 1/1   | 0.88 | 0.25 | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1723 | 1/1   | 0.88 | 0.58 | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1615 | 1/1   | 0.88 | 0.27 | 39,39,39,39                 | 0     |
| 24  | MG   | A     | 1764 | 1/1   | 0.89 | 0.45 | 29,29,29,29                 | 1     |
| 24  | MG   | A     | 1663 | 1/1   | 0.89 | 0.38 | 47,47,47,47                 | 1     |
| 24  | MG   | A     | 1756 | 1/1   | 0.89 | 0.37 | 16,16,16,16                 | 1     |
| 24  | MG   | A     | 1655 | 1/1   | 0.89 | 0.44 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1606 | 1/1   | 0.89 | 0.47 | 47,47,47,47                 | 1     |
| 24  | MG   | A     | 1628 | 1/1   | 0.89 | 0.68 | 47,47,47,47                 | 1     |
| 24  | MG   | A     | 1784 | 1/1   | 0.89 | 0.93 | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1771 | 1/1   | 0.89 | 1.04 | 46,46,46,46                 | 1     |
| 24  | MG   | A     | 1646 | 1/1   | 0.89 | 0.81 | 42,42,42,42                 | 1     |
| 24  | MG   | A     | 1670 | 1/1   | 0.89 | 0.44 | 13,13,13,13                 | 1     |
| 24  | MG   | A     | 1647 | 1/1   | 0.90 | 0.70 | 55,55,55,55                 | 1     |
| 24  | MG   | A     | 1779 | 1/1   | 0.90 | 0.81 | 15,15,15,15                 | 1     |
| 24  | MG   | A     | 1698 | 1/1   | 0.90 | 0.32 | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1718 | 1/1   | 0.90 | 0.65 | 31,31,31,31                 | 1     |
| 24  | MG   | A     | 1782 | 1/1   | 0.90 | 0.41 | 13,13,13,13                 | 1     |

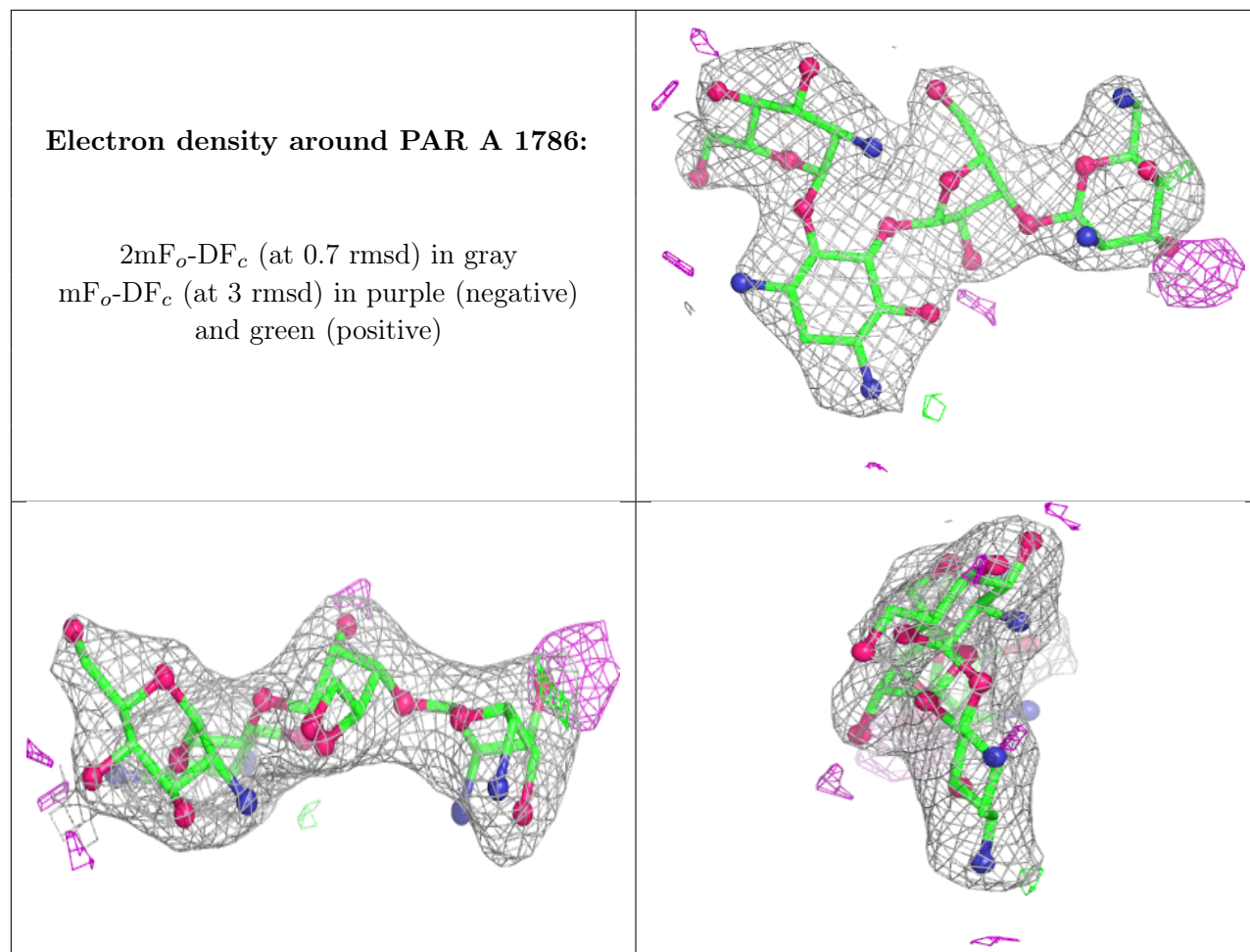
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1668 | 1/1   | 0.91 | 0.21 | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1620 | 1/1   | 0.91 | 0.28 | 52,52,52,52                 | 1     |
| 24  | MG   | A     | 1688 | 1/1   | 0.91 | 0.31 | 22,22,22,22                 | 1     |
| 24  | MG   | A     | 1677 | 1/1   | 0.91 | 1.03 | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1653 | 1/1   | 0.91 | 0.40 | 21,21,21,21                 | 1     |
| 24  | MG   | A     | 1637 | 1/1   | 0.91 | 0.31 | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1642 | 1/1   | 0.91 | 0.60 | 44,44,44,44                 | 1     |
| 24  | MG   | A     | 1618 | 1/1   | 0.91 | 0.27 | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1665 | 1/1   | 0.92 | 0.10 | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1649 | 1/1   | 0.92 | 0.26 | 21,21,21,21                 | 1     |
| 24  | MG   | A     | 1681 | 1/1   | 0.92 | 0.47 | 41,41,41,41                 | 1     |
| 24  | MG   | A     | 1737 | 1/1   | 0.92 | 0.46 | 0,0,0,0                     | 1     |
| 24  | MG   | A     | 1778 | 1/1   | 0.92 | 0.33 | 7,7,7,7                     | 1     |
| 24  | MG   | A     | 1748 | 1/1   | 0.92 | 0.69 | 39,39,39,39                 | 1     |
| 24  | MG   | A     | 1766 | 1/1   | 0.92 | 0.72 | 43,43,43,43                 | 1     |
| 24  | MG   | A     | 1609 | 1/1   | 0.93 | 0.40 | 39,39,39,39                 | 1     |
| 24  | MG   | A     | 1626 | 1/1   | 0.93 | 0.14 | 15,15,15,15                 | 1     |
| 24  | MG   | A     | 1685 | 1/1   | 0.93 | 0.88 | 37,37,37,37                 | 1     |
| 24  | MG   | A     | 1691 | 1/1   | 0.93 | 0.12 | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1747 | 1/1   | 0.93 | 0.27 | 19,19,19,19                 | 1     |
| 25  | PAR  | A     | 1786 | 42/42 | 0.93 | 0.12 | 34,40,52,55                 | 0     |
| 24  | MG   | A     | 1679 | 1/1   | 0.93 | 0.35 | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1714 | 1/1   | 0.94 | 0.22 | 13,13,13,13                 | 1     |
| 24  | MG   | A     | 1640 | 1/1   | 0.94 | 0.28 | 101,101,101,101             | 1     |
| 24  | MG   | A     | 1720 | 1/1   | 0.94 | 0.91 | 13,13,13,13                 | 1     |
| 24  | MG   | A     | 1774 | 1/1   | 0.95 | 0.61 | 21,21,21,21                 | 1     |
| 24  | MG   | A     | 1673 | 1/1   | 0.95 | 0.16 | 0,0,0,0                     | 1     |
| 24  | MG   | A     | 1648 | 1/1   | 0.95 | 0.37 | 37,37,37,37                 | 0     |
| 24  | MG   | A     | 1687 | 1/1   | 0.95 | 0.64 | 22,22,22,22                 | 1     |
| 24  | MG   | A     | 1634 | 1/1   | 0.95 | 0.32 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1761 | 1/1   | 0.96 | 0.61 | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1728 | 1/1   | 0.96 | 0.27 | 5,5,5,5                     | 1     |
| 24  | MG   | A     | 1763 | 1/1   | 0.96 | 0.17 | 0,0,0,0                     | 1     |
| 24  | MG   | A     | 1692 | 1/1   | 0.96 | 0.57 | 31,31,31,31                 | 1     |
| 24  | MG   | A     | 1744 | 1/1   | 0.97 | 0.43 | 33,33,33,33                 | 1     |
| 24  | MG   | A     | 1611 | 1/1   | 0.97 | 0.39 | 37,37,37,37                 | 0     |
| 24  | MG   | A     | 1651 | 1/1   | 0.97 | 0.92 | 29,29,29,29                 | 1     |
| 24  | MG   | A     | 1643 | 1/1   | 0.98 | 0.40 | 31,31,31,31                 | 1     |
| 26  | ZN   | N     | 101  | 1/1   | 0.99 | 0.05 | 60,60,60,60                 | 0     |

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

orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.