



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2018 – 08:37 AM EST

PDB ID : 2VQF
Title : Modified uridines with C5-methylene substituents at the first position of the tRNA anticodon stabilize U-G wobble pairing during decoding
Authors : Kurata, S.; Weixlbaumer, A.; Ohtsuki, T.; Shimazaki, T.; Wada, T.; Kirino, Y.; Takai, K.; Watanabe, K.; Ramakrishnan, V.; Suzuki, T.
Deposited on : 2008-03-14
Resolution : 2.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

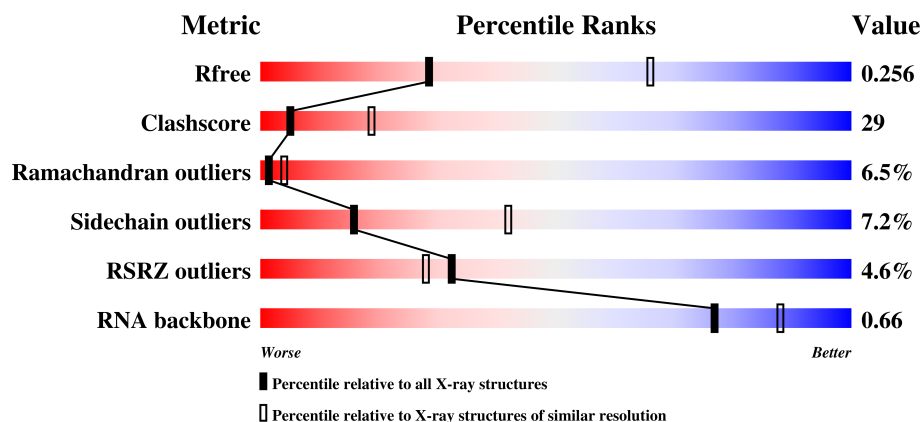
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 111664 | 1716 (2.90-2.90) |
| Clashscore | 122126 | 1924 (2.90-2.90) |
| Ramachandran outliers | 120053 | 1884 (2.90-2.90) |
| Sidechain outliers | 120020 | 1886 (2.90-2.90) |
| RSRZ outliers | 108989 | 1669 (2.90-2.90) |
| RNA backbone | 2636 | 1059 (3.20-2.60) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 1522 | <div> <div>4%</div> <div>39%</div> <div>48%</div> <div>10%</div> <div>..</div> </div> |
| 2 | B | 256 | <div> <div>4%</div> <div>23%</div> <div>56%</div> <div>11%</div> <div>8%</div> </div> |
| 3 | C | 239 | <div> <div>6%</div> <div>30%</div> <div>43%</div> <div>12%</div> <div>13%</div> </div> |
| 4 | D | 209 | <div> <div>6%</div> <div>47%</div> <div>46%</div> <div>5%</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 | 135 | |
| 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 | U | 27 | |
| 22 | X | 6 | |
| 23 | Y | 17 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25 | MG | A | 1607 | - | - | - | X |
| 25 | MG | A | 1610 | - | - | - | X |
| 25 | MG | A | 1612 | - | - | - | X |
| 25 | MG | A | 1615 | - | - | - | X |
| 25 | MG | A | 1618 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25 | MG | A | 1620 | - | - | - | X |
| 25 | MG | A | 1621 | - | - | - | X |
| 25 | MG | A | 1623 | - | - | - | X |
| 25 | MG | A | 1624 | - | - | - | X |
| 25 | MG | A | 1625 | - | - | - | X |
| 25 | MG | A | 1626 | - | - | - | X |
| 25 | MG | A | 1629 | - | - | - | X |
| 25 | MG | A | 1631 | - | - | - | X |
| 25 | MG | A | 1632 | - | - | - | X |
| 25 | MG | A | 1633 | - | - | - | X |
| 25 | MG | A | 1635 | - | - | - | X |
| 25 | MG | A | 1638 | - | - | - | X |
| 25 | MG | A | 1640 | - | - | - | X |
| 25 | MG | A | 1641 | - | - | - | X |
| 25 | MG | A | 1643 | - | - | - | X |
| 25 | MG | A | 1645 | - | - | - | X |
| 25 | MG | A | 1647 | - | - | - | X |
| 25 | MG | A | 1651 | - | - | - | X |
| 25 | MG | A | 1653 | - | - | - | X |
| 25 | MG | A | 1655 | - | - | - | X |
| 25 | MG | A | 1657 | - | - | - | X |
| 25 | MG | A | 1659 | - | - | - | X |
| 25 | MG | A | 1663 | - | - | - | X |
| 25 | MG | A | 1664 | - | - | - | X |
| 25 | MG | A | 1666 | - | - | - | X |
| 25 | MG | A | 1668 | - | - | - | X |
| 25 | MG | A | 1671 | - | - | - | X |
| 25 | MG | A | 1673 | - | - | - | X |
| 25 | MG | A | 1675 | - | - | - | X |
| 25 | MG | A | 1676 | - | - | - | X |
| 25 | MG | A | 1677 | - | - | - | X |
| 25 | MG | A | 1678 | - | - | - | X |
| 25 | MG | A | 1683 | - | - | - | X |
| 25 | MG | A | 1684 | - | - | - | X |
| 25 | MG | A | 1686 | - | - | - | X |
| 25 | MG | A | 1688 | - | - | - | X |
| 25 | MG | A | 1689 | - | - | - | X |
| 25 | MG | A | 1690 | - | - | - | X |
| 25 | MG | A | 1692 | - | - | - | X |
| 25 | MG | A | 1695 | - | - | - | X |
| 25 | MG | A | 1697 | - | - | - | X |
| 25 | MG | A | 1698 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25 | MG | A | 1702 | - | - | - | X |
| 25 | MG | A | 1710 | - | - | - | X |
| 25 | MG | A | 1713 | - | - | - | X |
| 25 | MG | A | 1714 | - | - | - | X |
| 25 | MG | A | 1716 | - | - | - | X |
| 25 | MG | A | 1718 | - | - | - | X |
| 25 | MG | A | 1722 | - | - | - | X |
| 25 | MG | A | 1724 | - | - | - | X |
| 25 | MG | A | 1728 | - | - | - | X |
| 25 | MG | A | 1733 | - | - | - | X |
| 25 | MG | A | 1736 | - | - | - | X |
| 25 | MG | A | 1739 | - | - | - | X |
| 25 | MG | A | 1747 | - | - | - | X |
| 25 | MG | A | 1751 | - | - | - | X |
| 25 | MG | A | 1753 | - | - | - | X |
| 25 | MG | A | 1757 | - | - | - | X |
| 25 | MG | A | 1774 | - | - | - | X |
| 25 | MG | A | 1788 | - | - | - | X |
| 25 | MG | A | 1798 | - | - | - | X |
| 25 | MG | E | 201 | - | - | - | X |
| 25 | MG | N | 102 | - | - | - | X |
| 26 | K | A | 1808 | - | - | - | X |
| 26 | K | A | 1815 | - | - | - | X |
| 26 | K | A | 1817 | - | - | - | X |
| 26 | K | A | 1819 | - | - | - | X |
| 26 | K | A | 1824 | - | - | - | X |
| 26 | K | A | 1825 | - | - | - | X |
| 26 | K | A | 1828 | - | - | - | X |
| 26 | K | A | 1832 | - | - | - | X |
| 26 | K | A | 1833 | - | - | - | X |
| 26 | K | A | 1834 | - | - | - | X |
| 26 | K | A | 1835 | - | - | - | X |
| 26 | K | A | 1839 | - | - | - | X |
| 26 | K | A | 1842 | - | - | - | X |
| 26 | K | A | 1845 | - | - | - | X |
| 26 | K | A | 1847 | - | - | - | X |
| 26 | K | A | 1848 | - | - | - | X |
| 26 | K | A | 1852 | - | - | - | X |
| 26 | K | A | 1853 | - | - | - | X |
| 26 | K | A | 1855 | - | - | - | X |
| 26 | K | A | 1857 | - | - | - | X |
| 26 | K | A | 1858 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 26 | K | A | 1862 | - | - | - | X |
| 26 | K | A | 1863 | - | - | - | X |
| 26 | K | D | 302 | - | - | - | X |
| 26 | K | E | 203 | - | - | - | X |
| 26 | K | I | 203 | - | - | - | X |
| 26 | K | M | 202 | - | - | - | X |
| 26 | K | P | 102 | - | - | - | X |
| 26 | K | R | 102 | - | - | - | X |
| 27 | ZN | D | 301 | - | - | - | X |

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52314 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 | 0 | 0 | 0 |
| | | | 32511 | 14472 | 6016 | 10511 | 1512 | | | |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 235 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1901 | 1213 | 342 | 341 | 5 | | | |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 207 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1613 | 1016 | 315 | 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 | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 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 | S | 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 | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 793 | 498 | 157 | 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 | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 971 | 611 | 196 | 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 | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 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 | 81 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 648 | 414 | 120 | 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 | U | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |

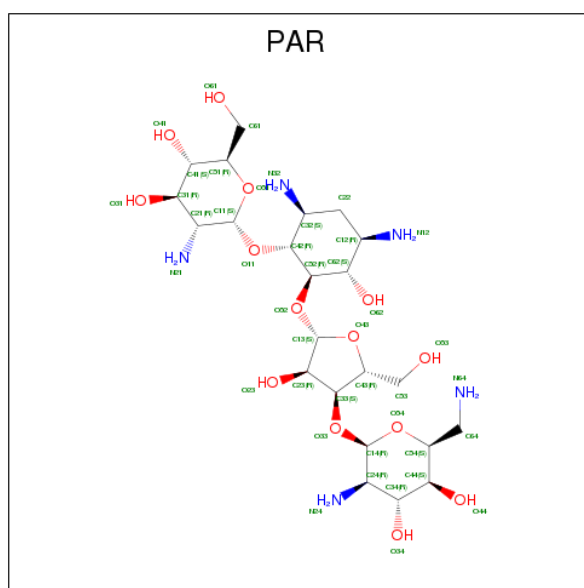
- Molecule 22 is a RNA chain called 5'-R(*UP*UP*GP*AP*AP*AP)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 22 | X | 4 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 82 | 38 | 14 | 27 | 3 | | | |

- Molecule 23 is a RNA chain called 5'-R(*GP*CP*AP*UP*GP*CP*U*TM2P*AP*AP*AP*AP*CP*AP*UP*GP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|-------|
| 23 | Y | 7 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 153 | 70 | 28 | 48 | 6 | 1 | | | |

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 25 | P | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 25 | Q | 2 | Total 2 | Mg 2 | 0 | 0 |
| 25 | K | 1 | Total 1 | Mg 1 | 0 | 0 |
| 25 | E | 1 | Total 1 | Mg 1 | 0 | 0 |
| 25 | B | 1 | Total 1 | Mg 1 | 0 | 0 |
| 25 | I | 2 | Total 2 | Mg 2 | 0 | 0 |
| 25 | A | 203 | Total 203 | Mg 203 | 0 | 0 |
| 25 | N | 1 | Total 1 | Mg 1 | 0 | 0 |
| 25 | R | 1 | Total 1 | Mg 1 | 0 | 0 |
| 25 | M | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 26 | P | 1 | Total 1 | K 1 | 0 | 0 |
| 26 | D | 1 | Total 1 | K 1 | 0 | 0 |
| 26 | K | 1 | Total 1 | K 1 | 0 | 0 |
| 26 | E | 2 | Total 2 | K 2 | 0 | 0 |
| 26 | I | 1 | Total 1 | K 1 | 0 | 0 |
| 26 | A | 63 | Total 63 | K 63 | 0 | 0 |
| 26 | T | 1 | Total 1 | K 1 | 0 | 0 |
| 26 | R | 1 | Total 1 | K 1 | 0 | 0 |
| 26 | S | 1 | Total 1 | K 1 | 0 | 0 |
| 26 | M | 1 | Total 1 | K 1 | 0 | 0 |

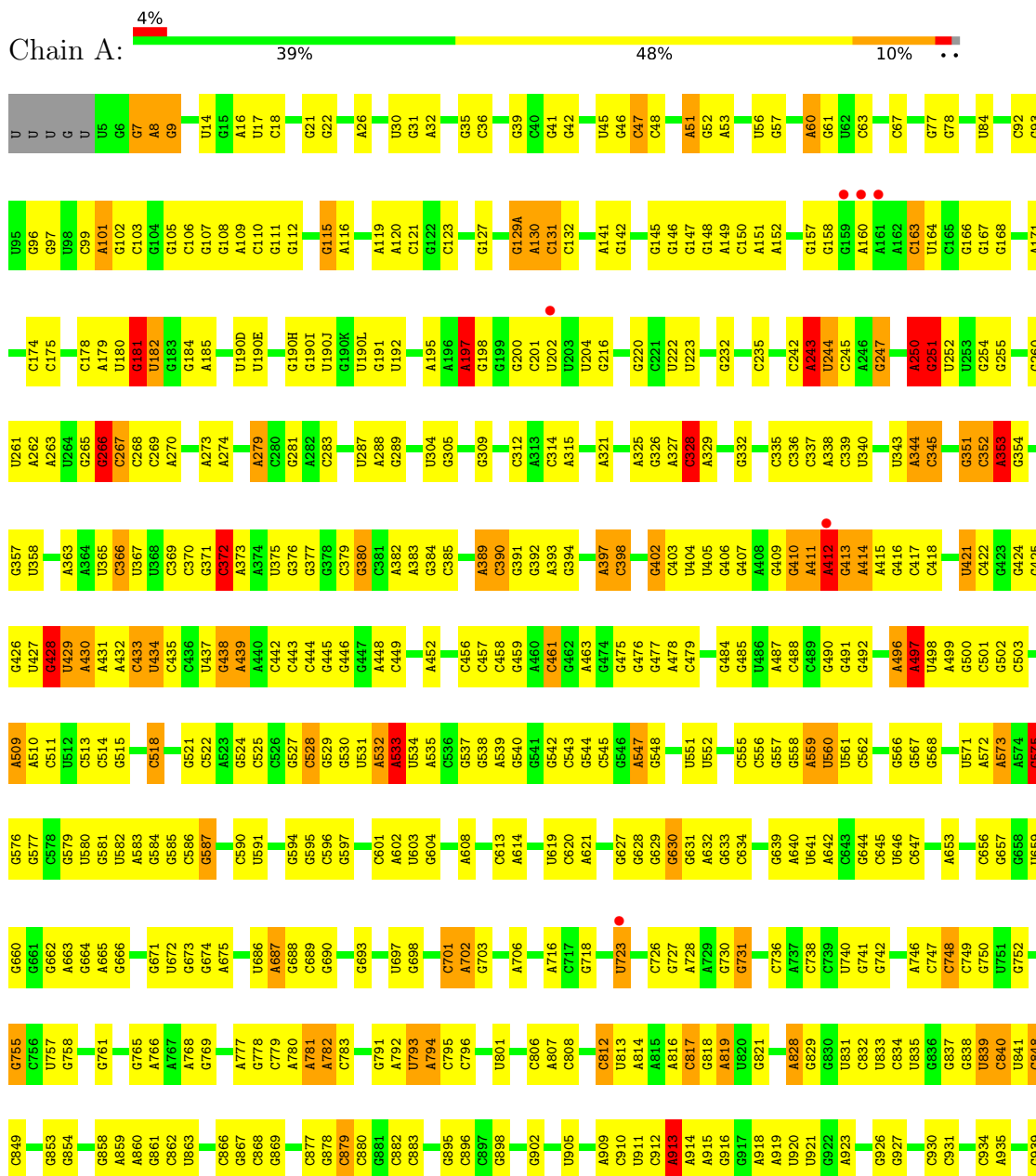
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 27 | D | 1 | Total 1 | Zn 1 | 0 | 0 |
| 27 | N | 1 | Total 1 | Zn 1 | 0 | 0 |

3 Residue-property plots

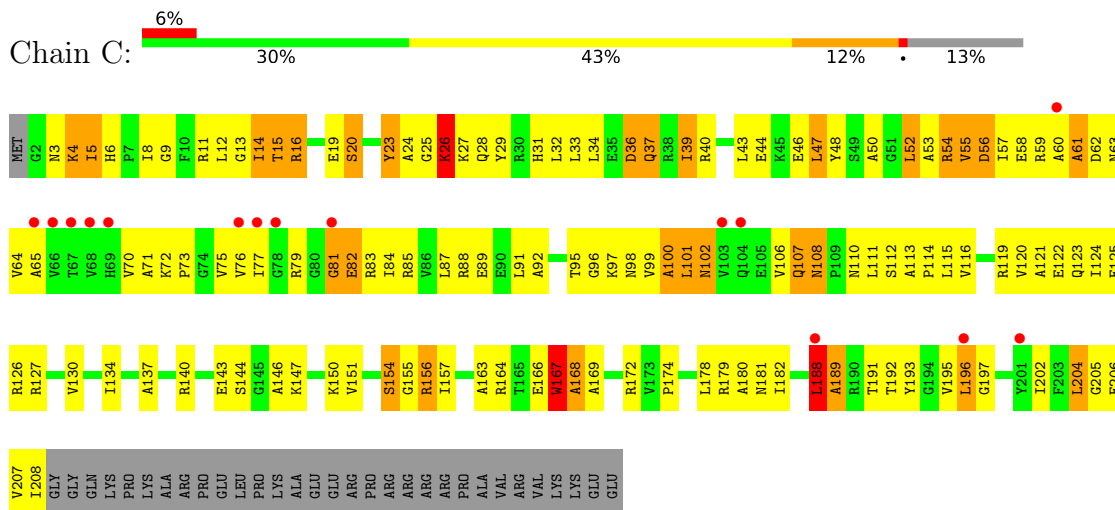
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

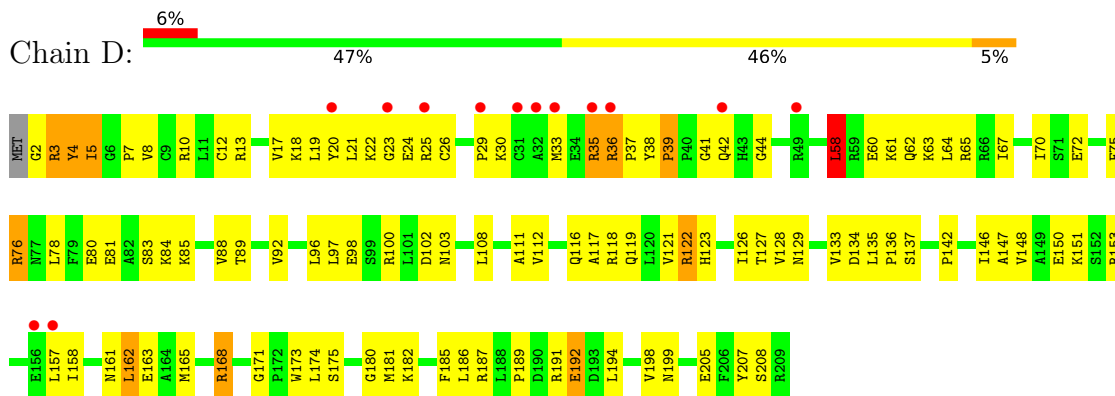




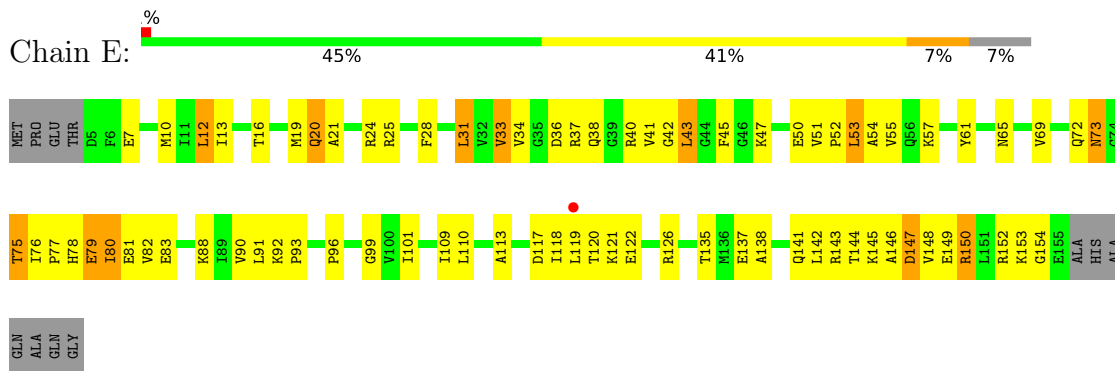
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



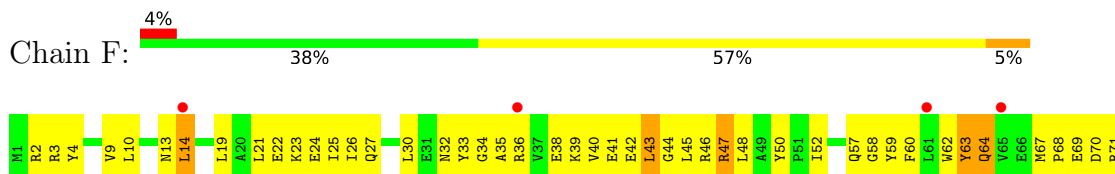
- Molecule 4: 30S RIBOSOMAL PROTEIN S4



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

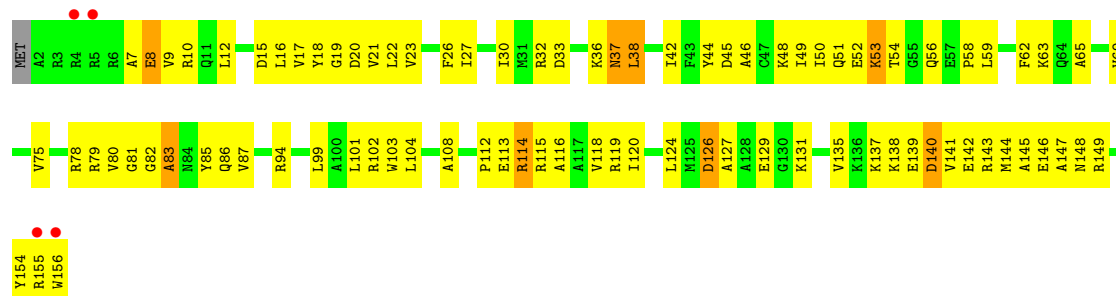
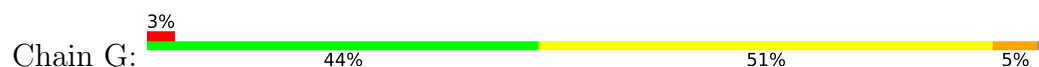


- Molecule 6: 30S RIBOSOMAL PROTEIN S6

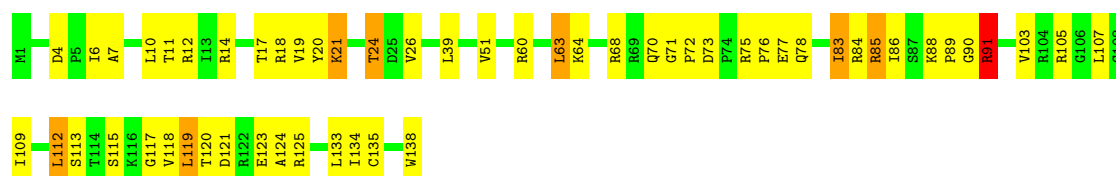




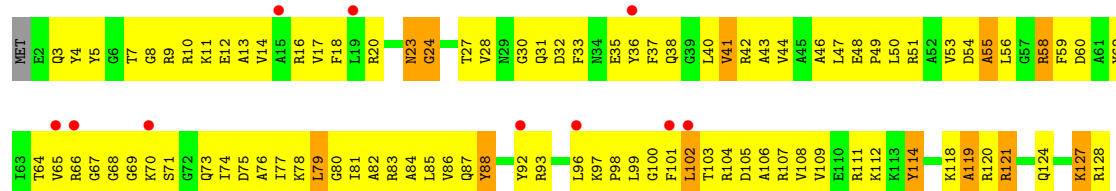
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



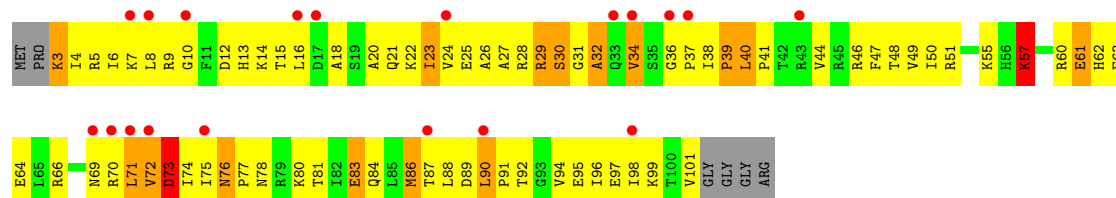
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

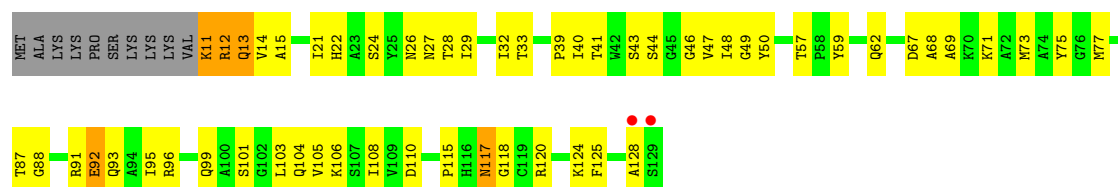


• Molecule 10: 30S RIBOSOMAL PROTEIN S10



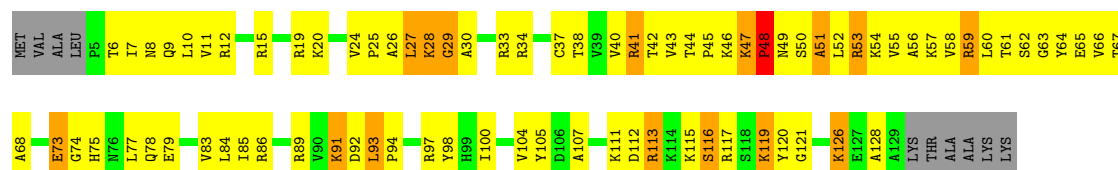
• Molecule 11: 30S RIBOSOMAL PROTEIN S11





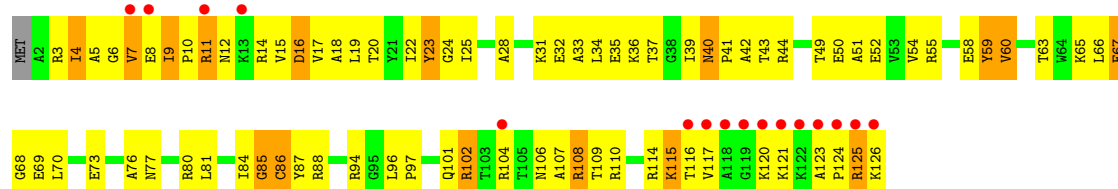
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 32% 49% 11% 7%



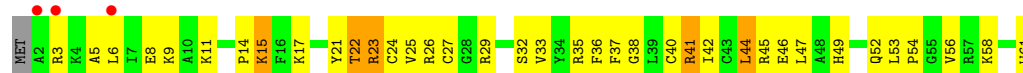
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 13% 34% 52% 13%



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain N: 5% 38% 52% 8%



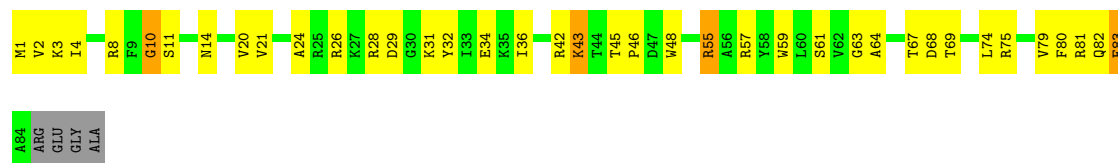
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 4% 56% 38%

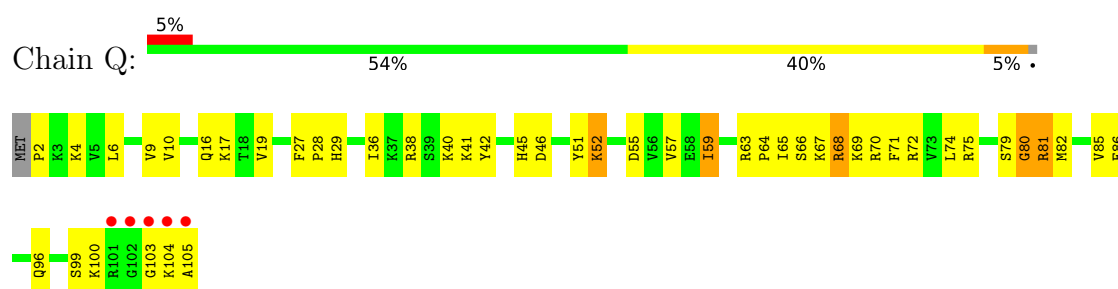


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

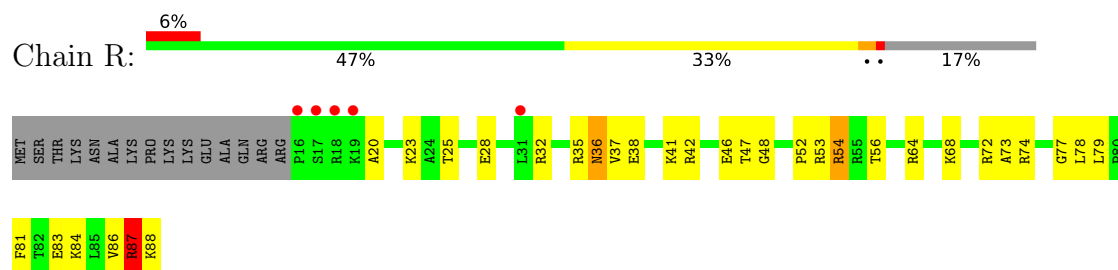
Chain P: 51% 40% 5% 5%



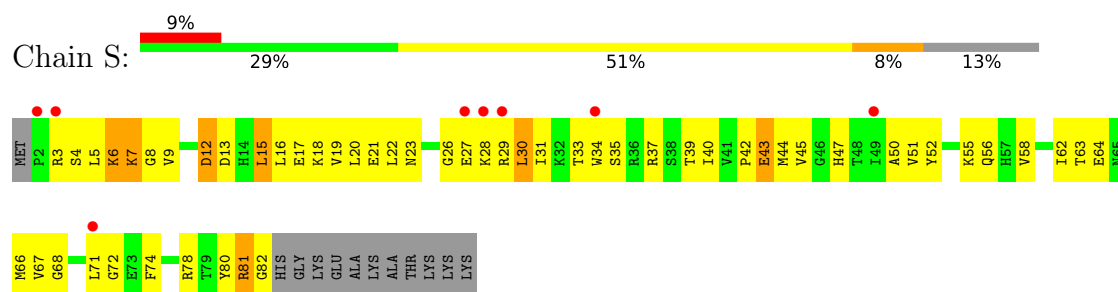
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



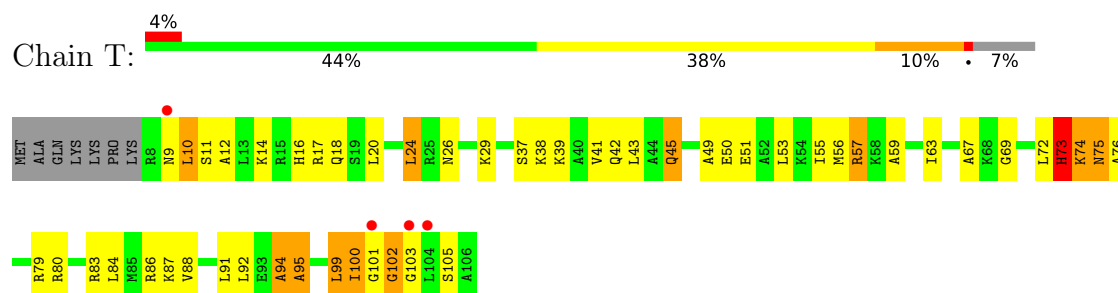
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



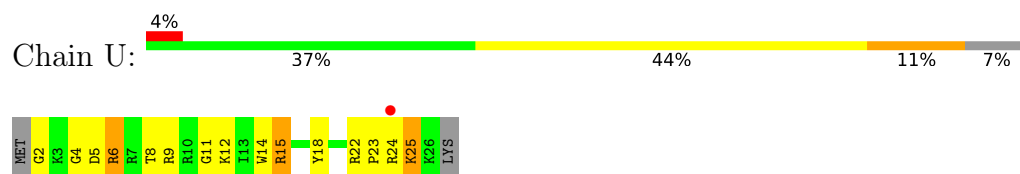
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

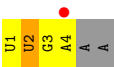


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

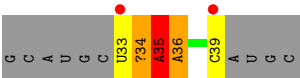
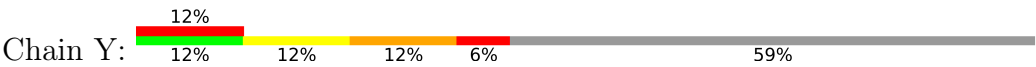


• Molecule 22: 5'-R(*UP*UP*GP*AP*AP*AP)-3'





● Molecule 23: 5'-R(*GP*CP*AP*UP*GP*CP*U*TM2P*AP*AP*AP *AP*CP*AP*UP*GP*C)
-3'



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 402.48Å 402.48Å 175.97Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.92 – 2.90 49.92 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 97.6 (49.92-2.90) 97.4 (49.92-2.80) | Depositor EDS |
| R_{merge} | 0.14 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.52 (at 2.81Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.223 , 0.258 0.225 , 0.256 | Depositor DCC |
| R_{free} test set | 16936 reflections (4.96%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 74.7 | Xtriage |
| Anisotropy | 0.227 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 61.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 52314 | wwPDB-VP |
| Average B, all atoms (Å ²) | 89.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, PAR, ZN, TM2

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 | 1.14 | 14/36390 (0.0%) | 1.01 | 83/56793 (0.1%) |
| 2 | B | 0.35 | 0/1936 | 0.61 | 0/2611 |
| 3 | C | 0.38 | 0/1637 | 0.61 | 0/2207 |
| 4 | D | 0.35 | 0/1733 | 0.57 | 0/2318 |
| 5 | E | 0.46 | 0/1163 | 0.71 | 0/1566 |
| 6 | F | 0.33 | 0/856 | 0.61 | 0/1154 |
| 7 | G | 0.35 | 0/1276 | 0.57 | 0/1709 |
| 8 | H | 0.44 | 0/1136 | 0.73 | 0/1527 |
| 9 | I | 0.35 | 0/1029 | 0.64 | 0/1378 |
| 10 | J | 0.37 | 0/806 | 0.63 | 0/1084 |
| 11 | K | 0.39 | 0/900 | 0.67 | 0/1213 |
| 12 | L | 0.45 | 0/987 | 0.77 | 1/1322 (0.1%) |
| 13 | M | 0.34 | 0/1008 | 0.63 | 0/1347 |
| 14 | N | 0.40 | 0/501 | 0.68 | 0/664 |
| 15 | O | 0.36 | 0/745 | 0.61 | 0/992 |
| 16 | P | 0.48 | 0/717 | 0.73 | 0/965 |
| 17 | Q | 0.43 | 0/870 | 0.74 | 0/1159 |
| 18 | R | 0.37 | 0/603 | 0.61 | 0/799 |
| 19 | S | 0.35 | 0/662 | 0.61 | 0/892 |
| 20 | T | 0.38 | 0/764 | 0.73 | 0/1006 |
| 21 | U | 0.50 | 0/213 | 0.59 | 0/279 |
| 22 | X | 0.38 | 0/91 | 0.67 | 0/140 |
| 23 | Y | 2.01 | 3/140 (2.1%) | 1.36 | 2/216 (0.9%) |
| All | All | 0.95 | 17/56163 (0.0%) | 0.91 | 86/83341 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 4 | 35 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | A | 1179 | A | O3'-P | -77.75 | 0.67 | 1.61 |
| 1 | A | 1331 | G | N3-C4 | 77.20 | 1.89 | 1.35 |
| 1 | A | 1063 | C | O3'-P | -72.79 | 0.73 | 1.61 |
| 1 | A | 1175 | G | O3'-P | -61.89 | 0.86 | 1.61 |
| 1 | A | 1192 | C | O3'-P | -54.97 | 0.95 | 1.61 |
| 1 | A | 1191 | A | O3'-P | -54.09 | 0.96 | 1.61 |
| 1 | A | 1144 | G | O3'-P | -50.43 | 1.00 | 1.61 |
| 1 | A | 1532 | U | O3'-P | -46.97 | 1.04 | 1.61 |
| 1 | A | 1156 | G | O3'-P | -42.86 | 1.09 | 1.61 |
| 1 | A | 1064 | G | O3'-P | 31.21 | 1.98 | 1.61 |
| 1 | A | 1541 | U | O3'-P | -25.77 | 1.30 | 1.61 |
| 1 | A | 1160 | G | O3'-P | -23.93 | 1.32 | 1.61 |
| 23 | Y | 35 | A | O3'-P | -20.26 | 1.36 | 1.61 |
| 23 | Y | 34 | TM2 | O3'-P | -9.96 | 1.49 | 1.61 |
| 1 | A | 1533 | C | O3'-P | 9.56 | 1.72 | 1.61 |
| 23 | Y | 36 | A | O3'-P | -5.41 | 1.54 | 1.61 |
| 1 | A | 243 | A | P-O5' | -5.00 | 1.54 | 1.59 |

All (86) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | A | 1144 | G | P-O3'-C3' | -55.79 | 52.76 | 119.70 |
| 1 | A | 1331 | G | C2-N3-C4 | -52.06 | 85.87 | 111.90 |
| 1 | A | 1127 | G | P-O3'-C3' | -42.98 | 68.12 | 119.70 |
| 1 | A | 1127 | G | OP1-P-O3' | -39.59 | 18.11 | 105.20 |
| 1 | A | 1532 | U | P-O3'-C3' | -38.65 | 73.31 | 119.70 |
| 1 | A | 1064 | G | OP2-P-O3' | -35.66 | 26.76 | 105.20 |
| 1 | A | 1175 | G | O3'-P-O5' | 35.05 | 170.59 | 104.00 |
| 1 | A | 1160 | G | O3'-P-O5' | 34.22 | 169.02 | 104.00 |
| 1 | A | 1179 | A | P-O3'-C3' | -33.26 | 79.79 | 119.70 |
| 1 | A | 1160 | G | P-O3'-C3' | -32.21 | 81.05 | 119.70 |
| 1 | A | 1175 | G | P-O3'-C3' | -31.24 | 82.22 | 119.70 |
| 1 | A | 1532 | U | O3'-P-O5' | 31.08 | 163.05 | 104.00 |
| 1 | A | 1144 | G | O3'-P-O5' | -30.12 | 46.78 | 104.00 |
| 1 | A | 1331 | G | N3-C4-C5 | -30.02 | 113.59 | 128.60 |
| 1 | A | 1063 | C | O3'-P-O5' | -27.82 | 51.13 | 104.00 |
| 1 | A | 1179 | A | OP2-P-O3' | -25.08 | 50.03 | 105.20 |
| 1 | A | 1192 | C | P-O3'-C3' | -22.94 | 92.17 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | A | 1533 | C | P-O3'-C3' | -21.79 | 93.55 | 119.70 |
| 1 | A | 1192 | C | OP2-P-O3' | -21.68 | 57.50 | 105.20 |
| 1 | A | 1532 | U | OP2-P-O3' | -21.02 | 58.96 | 105.20 |
| 1 | A | 1331 | G | N3-C2-N2 | -20.96 | 105.23 | 119.90 |
| 1 | A | 1191 | A | P-O3'-C3' | 20.75 | 144.60 | 119.70 |
| 1 | A | 1160 | G | OP2-P-O3' | -19.55 | 62.19 | 105.20 |
| 1 | A | 1179 | A | O3'-P-O5' | 18.15 | 138.49 | 104.00 |
| 1 | A | 1144 | G | OP1-P-O3' | 17.03 | 142.66 | 105.20 |
| 1 | A | 1063 | C | OP1-P-O3' | 15.96 | 140.30 | 105.20 |
| 1 | A | 1179 | A | OP1-P-O3' | -14.91 | 72.41 | 105.20 |
| 1 | A | 1175 | G | OP2-P-O3' | -13.80 | 74.84 | 105.20 |
| 23 | Y | 34 | TM2 | P-O3'-C3' | 13.75 | 136.20 | 119.70 |
| 1 | A | 1175 | G | OP1-P-O3' | -13.08 | 76.42 | 105.20 |
| 1 | A | 1533 | C | O3'-P-O5' | 12.94 | 128.58 | 104.00 |
| 1 | A | 1160 | G | OP1-P-O3' | -12.46 | 77.78 | 105.20 |
| 1 | A | 1192 | C | OP1-P-O3' | 11.93 | 131.45 | 105.20 |
| 1 | A | 1541 | U | OP2-P-O3' | 11.17 | 129.76 | 105.20 |
| 1 | A | 1156 | G | O3'-P-O5' | 10.71 | 124.35 | 104.00 |
| 1 | A | 1064 | G | O3'-P-O5' | -10.70 | 83.68 | 104.00 |
| 1 | A | 1498 | U | C2'-C3'-O3' | 10.31 | 132.19 | 109.50 |
| 1 | A | 115 | G | C2'-C3'-O3' | 9.92 | 131.33 | 109.50 |
| 1 | A | 1064 | G | OP1-P-O3' | 9.85 | 126.86 | 105.20 |
| 1 | A | 243 | A | C2'-C3'-O3' | 9.49 | 130.39 | 109.50 |
| 1 | A | 1301 | U | C2'-C3'-O3' | 9.17 | 129.68 | 109.50 |
| 1 | A | 1192 | C | O3'-P-O5' | 8.82 | 120.77 | 104.00 |
| 1 | A | 559 | A | C2'-C3'-O3' | 8.81 | 128.89 | 109.50 |
| 1 | A | 812 | C | C2'-C3'-O3' | 8.54 | 128.30 | 109.50 |
| 1 | A | 575 | G | C2'-C3'-O3' | 8.37 | 127.92 | 109.50 |
| 1 | A | 1331 | G | N1-C2-N3 | -8.36 | 118.88 | 123.90 |
| 1 | A | 1541 | U | OP1-P-O3' | -8.22 | 87.12 | 105.20 |
| 1 | A | 412 | A | N9-C1'-C2' | 8.20 | 124.66 | 114.00 |
| 1 | A | 687 | A | C2'-C3'-O3' | 8.10 | 127.31 | 109.50 |
| 1 | A | 60 | A | C2'-C3'-O3' | 8.09 | 127.30 | 109.50 |
| 1 | A | 181 | G | C2'-C3'-O3' | 8.08 | 127.27 | 109.50 |
| 1 | A | 1528 | U | C2'-C3'-O3' | 8.02 | 127.15 | 109.50 |
| 1 | A | 410 | G | C2'-C3'-O3' | 7.95 | 126.99 | 109.50 |
| 1 | A | 1299 | A | N9-C1'-C2' | 7.84 | 124.19 | 114.00 |
| 1 | A | 328 | C | C2'-C3'-O3' | 7.81 | 126.68 | 109.50 |
| 23 | Y | 35 | A | P-O3'-C3' | 7.69 | 128.92 | 119.70 |
| 1 | A | 1503 | A | C2'-C3'-O3' | 7.67 | 126.38 | 109.50 |
| 1 | A | 913 | A | C2'-C3'-O3' | 7.31 | 125.58 | 109.50 |
| 1 | A | 533 | A | C2'-C3'-O3' | 7.11 | 125.14 | 109.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1065 | U | C2'-C3'-O3' | 7.04 | 124.99 | 109.50 |
| 1 | A | 1532 | U | OP1-P-O3' | -6.99 | 89.83 | 105.20 |
| 1 | A | 1191 | A | O3'-P-O5' | 6.91 | 117.12 | 104.00 |
| 1 | A | 1331 | G | N3-C4-N9 | 6.90 | 130.14 | 126.00 |
| 1 | A | 1064 | G | P-O3'-C3' | 6.88 | 127.95 | 119.70 |
| 1 | A | 366 | C | C2'-C3'-O3' | 6.78 | 124.54 | 113.70 |
| 1 | A | 1191 | A | OP2-P-O3' | -6.66 | 90.56 | 105.20 |
| 1 | A | 509 | A | C2'-C3'-O3' | 6.58 | 124.22 | 113.70 |
| 1 | A | 1505 | G | C2'-C3'-O3' | 6.55 | 124.18 | 113.70 |
| 1 | A | 266 | G | C2'-C3'-O3' | 6.50 | 124.10 | 113.70 |
| 1 | A | 372 | C | C2'-C3'-O3' | 6.29 | 123.77 | 113.70 |
| 1 | A | 965 | A | C2'-C3'-O3' | 6.29 | 123.76 | 113.70 |
| 1 | A | 1156 | G | P-O3'-C3' | 5.98 | 126.88 | 119.70 |
| 1 | A | 960 | U | C2'-C3'-O3' | 5.70 | 122.82 | 113.70 |
| 1 | A | 428 | G | C2'-C3'-O3' | 5.63 | 122.71 | 113.70 |
| 12 | L | 119 | LYS | N-CA-C | -5.58 | 95.92 | 111.00 |
| 1 | A | 1502 | A | N9-C1'-C2' | 5.58 | 121.25 | 114.00 |
| 1 | A | 686 | U | N1-C1'-C2' | 5.50 | 121.14 | 114.00 |
| 1 | A | 63 | C | C5'-C4'-C3' | -5.41 | 107.35 | 116.00 |
| 1 | A | 1504 | G | C2'-C3'-O3' | 5.36 | 122.27 | 113.70 |
| 1 | A | 497 | A | C2'-C3'-O3' | 5.24 | 122.09 | 113.70 |
| 1 | A | 389 | A | C5'-C4'-C3' | 5.24 | 124.38 | 116.00 |
| 1 | A | 1533 | C | OP1-P-O3' | -5.22 | 93.72 | 105.20 |
| 1 | A | 748 | C | C2'-C3'-O3' | 5.20 | 122.02 | 113.70 |
| 1 | A | 328 | C | O4'-C1'-N1 | -5.11 | 104.11 | 108.20 |
| 1 | A | 1279 | A | N9-C1'-C2' | 5.11 | 120.64 | 114.00 |
| 1 | A | 353 | A | C5'-C4'-O4' | -5.06 | 103.03 | 109.10 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 115 | G | C3' |
| 1 | A | 243 | A | C3' |
| 1 | A | 410 | G | C3' |
| 1 | A | 412 | A | C1' |

All (35) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1054 | C | Sidechain |
| 1 | A | 1125 | U | Sidechain |
| 1 | A | 1130 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1299 | A | Sidechain |
| 1 | A | 1331 | G | Sidechain |
| 1 | A | 14 | U | Sidechain |
| 1 | A | 1401 | G | Sidechain |
| 1 | A | 1414 | U | Sidechain |
| 1 | A | 1454 | G | Sidechain |
| 1 | A | 1492 | A | Sidechain |
| 1 | A | 1498 | U | Sidechain |
| 1 | A | 1544 | U | Sidechain |
| 1 | A | 197 | A | Sidechain |
| 1 | A | 250 | A | Sidechain |
| 1 | A | 251 | G | Sidechain |
| 1 | A | 265 | G | Sidechain |
| 1 | A | 274 | A | Sidechain |
| 1 | A | 279 | A | Sidechain |
| 1 | A | 380 | G | Sidechain |
| 1 | A | 402 | G | Sidechain |
| 1 | A | 528 | C | Sidechain |
| 1 | A | 529 | G | Sidechain |
| 1 | A | 571 | U | Sidechain |
| 1 | A | 573 | A | Sidechain |
| 1 | A | 575 | G | Sidechain |
| 1 | A | 587 | G | Sidechain |
| 1 | A | 641 | U | Sidechain |
| 1 | A | 656 | C | Sidechain |
| 1 | A | 727 | G | Sidechain |
| 1 | A | 752 | G | Sidechain |
| 1 | A | 84 | U | Sidechain |
| 1 | A | 879 | C | Sidechain |
| 1 | A | 898 | G | Sidechain |
| 1 | A | 905 | U | Sidechain |
| 1 | A | 952 | U | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32511 | 0 | 16403 | 993 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | B | 1901 | 0 | 1951 | 242 | 0 |
| 3 | C | 1613 | 0 | 1677 | 186 | 0 |
| 4 | D | 1703 | 0 | 1767 | 127 | 0 |
| 5 | E | 1147 | 0 | 1206 | 94 | 0 |
| 6 | F | 843 | 0 | 857 | 89 | 0 |
| 7 | G | 1257 | 0 | 1296 | 82 | 0 |
| 8 | H | 1116 | 0 | 1177 | 61 | 0 |
| 9 | I | 1011 | 0 | 1040 | 120 | 0 |
| 10 | J | 793 | 0 | 835 | 142 | 0 |
| 11 | K | 885 | 0 | 904 | 65 | 0 |
| 12 | L | 971 | 0 | 1057 | 110 | 0 |
| 13 | M | 997 | 0 | 1071 | 96 | 0 |
| 14 | N | 492 | 0 | 529 | 50 | 0 |
| 15 | O | 734 | 0 | 771 | 35 | 0 |
| 16 | P | 701 | 0 | 720 | 42 | 0 |
| 17 | Q | 857 | 0 | 930 | 58 | 0 |
| 18 | R | 597 | 0 | 668 | 43 | 0 |
| 19 | S | 648 | 0 | 673 | 71 | 0 |
| 20 | T | 762 | 0 | 859 | 51 | 0 |
| 21 | U | 209 | 0 | 221 | 21 | 0 |
| 22 | X | 82 | 0 | 44 | 18 | 0 |
| 23 | Y | 153 | 0 | 83 | 12 | 0 |
| 24 | A | 42 | 0 | 45 | 1 | 0 |
| 25 | A | 203 | 0 | 0 | 0 | 0 |
| 25 | B | 1 | 0 | 0 | 0 | 0 |
| 25 | E | 1 | 0 | 0 | 0 | 0 |
| 25 | I | 2 | 0 | 0 | 0 | 0 |
| 25 | K | 1 | 0 | 0 | 0 | 0 |
| 25 | M | 1 | 0 | 0 | 0 | 0 |
| 25 | N | 1 | 0 | 0 | 0 | 0 |
| 25 | P | 1 | 0 | 0 | 0 | 0 |
| 25 | Q | 2 | 0 | 0 | 0 | 0 |
| 25 | R | 1 | 0 | 0 | 0 | 0 |
| 26 | A | 63 | 0 | 0 | 0 | 0 |
| 26 | D | 1 | 0 | 0 | 0 | 0 |
| 26 | E | 2 | 0 | 0 | 0 | 0 |
| 26 | I | 1 | 0 | 0 | 0 | 0 |
| 26 | K | 1 | 0 | 0 | 0 | 0 |
| 26 | M | 1 | 0 | 0 | 0 | 0 |
| 26 | P | 1 | 0 | 0 | 0 | 0 |
| 26 | R | 1 | 0 | 0 | 0 | 0 |
| 26 | S | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26 | T | 1 | 0 | 0 | 0 | 0 |
| 27 | D | 1 | 0 | 0 | 0 | 0 |
| 27 | N | 1 | 0 | 0 | 0 | 0 |
| All | All | 52314 | 0 | 36784 | 2557 | 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 29.

All (2557) 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:1179:A:N6 | 1:A:1180:A:C2 | 1.81 | 1.49 |
| 1:A:1156:G:O3' | 1:A:1157:A:P | 1.09 | 1.47 |
| 1:A:1331:G:N3 | 1:A:1331:G:C4 | 1.89 | 1.40 |
| 1:A:1191:A:O3' | 1:A:1192:C:P | 0.96 | 1.36 |
| 1:A:1533:C:O2' | 1:A:1534:A:H5' | 1.25 | 1.31 |
| 1:A:1179:A:C6 | 1:A:1180:A:C2 | 2.21 | 1.28 |
| 1:A:1191:A:HO3' | 1:A:1192:C:P | 0.87 | 1.23 |
| 1:A:1156:G:C3' | 1:A:1157:A:P | 2.26 | 1.22 |
| 1:A:1331:G:C2 | 1:A:1331:G:C4 | 2.21 | 1.21 |
| 1:A:1191:A:C3' | 1:A:1192:C:P | 2.31 | 1.17 |
| 22:X:3:G:O2' | 22:X:4:A:H5' | 1.38 | 1.17 |
| 1:A:1156:G:H21 | 1:A:1179:A:N6 | 1.48 | 1.12 |
| 1:A:243:A:H4' | 1:A:244:U:H5' | 1.30 | 1.09 |
| 1:A:1305:G:H22 | 1:A:1331:G:H2' | 1.17 | 1.06 |
| 3:C:64:VAL:HG23 | 3:C:99:VAL:HG11 | 1.39 | 1.05 |
| 3:C:14:ILE:HG22 | 3:C:15:THR:H | 1.16 | 1.05 |
| 1:A:1190:G:H3' | 3:C:3:ASN:ND2 | 1.72 | 1.04 |
| 1:A:266:G:H5'' | 1:A:268:C:H41 | 1.17 | 1.04 |
| 19:S:33:THR:HG22 | 19:S:35:SER:H | 1.23 | 1.04 |
| 1:A:1250:A:H4' | 9:I:68:GLY:H | 1.19 | 1.03 |
| 2:B:60:ASP:HB3 | 2:B:64:ARG:HH12 | 1.22 | 1.03 |
| 1:A:1533:C:O2' | 1:A:1534:A:C5' | 2.07 | 1.03 |
| 1:A:991:U:H5 | 1:A:1212:U:H1' | 1.21 | 1.02 |
| 2:B:208:ILE:HD12 | 2:B:208:ILE:H | 1.22 | 1.02 |
| 1:A:1250:A:H4' | 9:I:68:GLY:N | 1.75 | 1.02 |
| 1:A:1130:A:C4 | 1:A:1146:A:C2 | 2.48 | 1.02 |
| 4:D:7:PRO:HB2 | 4:D:10:ARG:HD2 | 1.43 | 1.01 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 1.42 | 1.01 |
| 1:A:1305:G:N2 | 1:A:1331:G:H2' | 1.77 | 1.00 |
| 1:A:1118:C:O2 | 1:A:1179:A:C5 | 2.15 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 1.42 | 0.99 |
| 4:D:168:ARG:HH11 | 4:D:168:ARG:HB3 | 1.25 | 0.98 |
| 1:A:1179:A:N6 | 1:A:1180:A:H2 | 1.55 | 0.97 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:HG21 | 1.43 | 0.97 |
| 1:A:1116:C:H2' | 1:A:1117:G:H5'' | 1.48 | 0.96 |
| 19:S:28:LYS:HG2 | 19:S:29:ARG:H | 1.27 | 0.96 |
| 3:C:84:ILE:HD11 | 3:C:88:ARG:HH21 | 1.31 | 0.96 |
| 1:A:1118:C:O2 | 1:A:1179:A:C6 | 2.18 | 0.96 |
| 3:C:64:VAL:HB | 3:C:99:VAL:HG21 | 1.43 | 0.96 |
| 11:K:110:ASP:HB2 | 18:R:88:LYS:HD2 | 1.47 | 0.96 |
| 1:A:432:A:H3' | 1:A:433:C:H5'' | 1.48 | 0.95 |
| 1:A:1086:U:H3 | 1:A:1099:G:H22 | 1.06 | 0.95 |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H | 1.31 | 0.95 |
| 1:A:1175:G:N3 | 1:A:1176:A:C8 | 2.35 | 0.95 |
| 22:X:3:G:C2' | 22:X:4:A:H5' | 1.97 | 0.94 |
| 5:E:79:GLU:HG3 | 5:E:93:PRO:HD2 | 1.47 | 0.94 |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA | 1.50 | 0.93 |
| 1:A:1063:C:H3' | 1:A:1064:G:H2' | 1.49 | 0.93 |
| 1:A:1175:G:C4 | 1:A:1176:A:C8 | 2.57 | 0.93 |
| 1:A:1152:A:H5'' | 10:J:13:HIS:HD2 | 1.33 | 0.93 |
| 1:A:1156:G:N2 | 1:A:1179:A:N1 | 2.16 | 0.93 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H | 1.34 | 0.93 |
| 11:K:91:ARG:HD3 | 18:R:88:LYS:HE2 | 1.50 | 0.93 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.09 | 0.93 |
| 1:A:1281:U:H5' | 1:A:1282:C:C5 | 2.03 | 0.92 |
| 1:A:1533:C:HO2' | 1:A:1534:A:H5' | 1.33 | 0.92 |
| 17:Q:67:LYS:HA | 17:Q:70:ARG:HH12 | 1.34 | 0.92 |
| 1:A:1178:G:N2 | 1:A:1180:A:C8 | 2.38 | 0.92 |
| 5:E:80:ILE:CD1 | 5:E:91:LEU:HB2 | 2.00 | 0.91 |
| 12:L:47:LYS:HB3 | 12:L:48:PRO:CD | 1.98 | 0.91 |
| 1:A:972:C:H4' | 10:J:57:LYS:HG2 | 1.51 | 0.91 |
| 3:C:26:LYS:H | 3:C:26:LYS:HD3 | 1.35 | 0.91 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.06 | 0.90 |
| 1:A:1156:G:HO3' | 1:A:1157:A:P | 1.27 | 0.90 |
| 1:A:1179:A:C6 | 1:A:1180:A:N3 | 2.38 | 0.90 |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:H | 1.37 | 0.90 |
| 1:A:1178:G:N2 | 1:A:1180:A:H8 | 1.70 | 0.89 |
| 2:B:18:GLY:HA2 | 2:B:41:ILE:HA | 1.54 | 0.89 |
| 3:C:91:LEU:HD21 | 3:C:99:VAL:H | 1.36 | 0.89 |
| 1:A:1152:A:H5'' | 10:J:13:HIS:CD2 | 2.07 | 0.89 |
| 1:A:991:U:C5 | 1:A:1212:U:H1' | 2.08 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1238:A:H5' | 1:A:1336:C:H41 | 1.38 | 0.89 |
| 7:G:75:VAL:HG21 | 7:G:86:GLN:HB3 | 1.54 | 0.89 |
| 1:A:1367:C:H5' | 10:J:60:ARG:NH1 | 1.88 | 0.89 |
| 1:A:1533:C:H2' | 1:A:1534:A:O5' | 1.73 | 0.89 |
| 12:L:59:ARG:HH11 | 12:L:59:ARG:HB2 | 1.37 | 0.89 |
| 2:B:97:TRP:HZ2 | 2:B:102:LEU:HD13 | 1.38 | 0.89 |
| 13:M:59:TYR:O | 13:M:63:THR:HG22 | 1.72 | 0.88 |
| 2:B:60:ASP:HB3 | 2:B:64:ARG:NH1 | 1.86 | 0.88 |
| 9:I:106:ALA:O | 9:I:108:VAL:HG23 | 1.73 | 0.88 |
| 10:J:49:VAL:HG23 | 14:N:41:ARG:HB2 | 1.56 | 0.88 |
| 5:E:144:THR:HB | 5:E:147:ASP:OD1 | 1.74 | 0.87 |
| 1:A:1116:C:C2' | 1:A:1117:G:H5'' | 2.04 | 0.87 |
| 2:B:91:PRO:HG3 | 2:B:154:LEU:HB2 | 1.55 | 0.87 |
| 1:A:1179:A:N6 | 1:A:1180:A:N1 | 2.22 | 0.87 |
| 6:F:47:ARG:HE | 6:F:47:ARG:H | 1.22 | 0.87 |
| 1:A:1080:A:H5'' | 5:E:16:THR:HG21 | 1.54 | 0.87 |
| 1:A:243:A:C4' | 1:A:244:U:H5' | 2.04 | 0.86 |
| 4:D:150:GLU:CD | 4:D:150:GLU:H | 1.78 | 0.86 |
| 3:C:88:ARG:HG2 | 3:C:101:LEU:HD13 | 1.57 | 0.86 |
| 1:A:718:G:H5' | 11:K:117:ASN:HD22 | 1.40 | 0.86 |
| 2:B:84:GLU:HB3 | 2:B:219:VAL:HG21 | 1.57 | 0.86 |
| 3:C:70:VAL:HG12 | 3:C:72:LYS:H | 1.41 | 0.86 |
| 1:A:1156:G:H21 | 1:A:1179:A:H61 | 1.19 | 0.85 |
| 7:G:69:VAL:HG21 | 7:G:104:LEU:HD21 | 1.58 | 0.85 |
| 19:S:20:LEU:HA | 19:S:23:ASN:HD22 | 1.40 | 0.85 |
| 1:A:129(A):G:O2' | 1:A:190(E):U:H2' | 1.75 | 0.85 |
| 1:A:1137:C:H4' | 1:A:1138:G:C2 | 2.12 | 0.85 |
| 18:R:47:THR:HA | 18:R:83:GLU:HB2 | 1.58 | 0.85 |
| 10:J:30:SER:HB3 | 10:J:84:GLN:HE21 | 1.42 | 0.85 |
| 1:A:975:A:H5' | 1:A:975:A:H8 | 1.40 | 0.84 |
| 3:C:73:PRO:O | 3:C:76:VAL:HG22 | 1.77 | 0.84 |
| 1:A:1035:A:H2' | 1:A:1036:G:H8 | 1.43 | 0.84 |
| 1:A:1156:G:N2 | 1:A:1179:A:H61 | 1.75 | 0.84 |
| 6:F:47:ARG:NE | 6:F:47:ARG:H | 1.74 | 0.84 |
| 19:S:15:LEU:HA | 19:S:18:LYS:HB3 | 1.58 | 0.84 |
| 2:B:25:ASN:C | 2:B:25:ASN:HD22 | 1.81 | 0.84 |
| 1:A:1190:G:OP1 | 3:C:4:LYS:HA | 1.77 | 0.84 |
| 7:G:146:GLU:HG2 | 7:G:149:ARG:HH21 | 1.39 | 0.84 |
| 1:A:1062:U:H2' | 1:A:1063:C:C5 | 2.13 | 0.84 |
| 4:D:23:GLY:HA3 | 4:D:112:VAL:HG22 | 1.60 | 0.84 |
| 14:N:3:ARG:HH21 | 14:N:6:LEU:HD11 | 1.43 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:104:ARG:HD3 | 9:I:105:ASP:H | 1.42 | 0.83 |
| 2:B:8:LYS:HE2 | 2:B:9:GLU:H | 1.42 | 0.83 |
| 7:G:114:ARG:H | 7:G:114:ARG:HD2 | 1.42 | 0.83 |
| 2:B:19:HIS:NE2 | 2:B:206:ASP:HB3 | 1.93 | 0.83 |
| 1:A:1156:G:O3' | 1:A:1157:A:OP2 | 1.93 | 0.82 |
| 9:I:53:VAL:HG21 | 9:I:85:LEU:HD21 | 1.59 | 0.82 |
| 3:C:15:THR:O | 3:C:16:ARG:HB2 | 1.79 | 0.82 |
| 5:E:51:VAL:HB | 5:E:52:PRO:HD3 | 1.61 | 0.82 |
| 1:A:1179:A:O2' | 1:A:1180:A:H5' | 1.78 | 0.82 |
| 22:X:3:G:H1 | 23:Y:34:TM2:H3 | 1.28 | 0.82 |
| 5:E:150:ARG:HH11 | 5:E:150:ARG:HG3 | 1.45 | 0.82 |
| 5:E:50:GLU:HG3 | 5:E:52:PRO:HD2 | 1.61 | 0.82 |
| 1:A:1156:G:N2 | 1:A:1179:A:N6 | 2.27 | 0.82 |
| 1:A:1179:A:H61 | 1:A:1180:A:H2 | 1.24 | 0.81 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.28 | 0.81 |
| 2:B:15:VAL:HG11 | 2:B:209:ARG:HB2 | 1.61 | 0.81 |
| 1:A:351:G:H4' | 1:A:352:C:OP1 | 1.79 | 0.81 |
| 2:B:80:ILE:H | 2:B:80:ILE:HD12 | 1.42 | 0.81 |
| 1:A:1369:C:H2' | 1:A:1370:G:C8 | 2.15 | 0.81 |
| 1:A:432:A:C3' | 1:A:433:C:H5'' | 2.11 | 0.81 |
| 1:A:975:A:H4' | 1:A:976:G:H5'' | 1.62 | 0.80 |
| 11:K:57:THR:HG22 | 11:K:59:TYR:H | 1.44 | 0.80 |
| 2:B:124:SER:HB2 | 2:B:125:PRO:HD2 | 1.61 | 0.80 |
| 5:E:10:MET:SD | 5:E:13:ILE:HD11 | 2.22 | 0.80 |
| 19:S:17:GLU:HA | 19:S:20:LEU:HG | 1.61 | 0.80 |
| 5:E:144:THR:HG22 | 5:E:146:ALA:H | 1.45 | 0.80 |
| 13:M:37:THR:HG23 | 13:M:55:ARG:HD2 | 1.62 | 0.80 |
| 1:A:1054:C:H3' | 1:A:1054:C:O2 | 1.80 | 0.80 |
| 1:A:1305:G:H5' | 21:U:4:GLY:HA3 | 1.62 | 0.80 |
| 17:Q:96:GLN:HB3 | 17:Q:103:GLY:HA3 | 1.64 | 0.80 |
| 19:S:30:LEU:O | 19:S:31:ILE:HD13 | 1.82 | 0.80 |
| 1:A:35:G:H2' | 1:A:36:C:C6 | 2.17 | 0.80 |
| 1:A:438:G:H4' | 1:A:439:A:OP1 | 1.82 | 0.80 |
| 1:A:1190:G:H3' | 3:C:3:ASN:HD21 | 1.46 | 0.80 |
| 10:J:46:ARG:NH1 | 10:J:64:GLU:HB3 | 1.97 | 0.79 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.17 | 0.79 |
| 2:B:132:LYS:HA | 2:B:135:GLN:HB2 | 1.64 | 0.79 |
| 1:A:363:A:H62 | 12:L:28:LYS:HE3 | 1.46 | 0.79 |
| 2:B:193:ASP:HB3 | 2:B:196:LEU:HD13 | 1.62 | 0.79 |
| 2:B:95:GLN:O | 2:B:96:ARG:HD2 | 1.82 | 0.79 |
| 19:S:7:LYS:HD2 | 19:S:7:LYS:O | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 21:U:5:ASP:O | 21:U:11:GLY:HA3 | 1.83 | 0.79 |
| 1:A:1057:G:H5'' | 3:C:154:SER:HB2 | 1.64 | 0.79 |
| 23:Y:33:U:H2' | 23:Y:34:TM2:H3' | 1.63 | 0.79 |
| 2:B:204:ASN:ND2 | 2:B:206:ASP:H | 1.81 | 0.79 |
| 1:A:235:C:H5' | 17:Q:70:ARG:HG2 | 1.62 | 0.79 |
| 1:A:1238:A:H5' | 1:A:1336:C:N4 | 1.98 | 0.79 |
| 7:G:79:ARG:HH12 | 7:G:82:GLY:H | 1.31 | 0.79 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.18 | 0.79 |
| 19:S:13:ASP:HA | 19:S:16:LEU:HB3 | 1.63 | 0.79 |
| 10:J:10:GLY:N | 10:J:16:LEU:HD11 | 1.98 | 0.79 |
| 10:J:84:GLN:O | 10:J:88:LEU:HD12 | 1.83 | 0.78 |
| 1:A:250:A:H4' | 1:A:251:G:O5' | 1.82 | 0.78 |
| 2:B:215:LEU:O | 2:B:219:VAL:HG23 | 1.83 | 0.78 |
| 2:B:42:ILE:H | 2:B:42:ILE:HD12 | 1.48 | 0.78 |
| 2:B:178:ARG:NH2 | 8:H:68:ARG:HH22 | 1.82 | 0.78 |
| 1:A:1527:C:O2' | 1:A:1528:U:H5' | 1.84 | 0.78 |
| 9:I:93:ARG:HB3 | 9:I:93:ARG:NH1 | 1.99 | 0.78 |
| 13:M:54:VAL:O | 13:M:58:GLU:HG2 | 1.84 | 0.78 |
| 1:A:1352:C:H2' | 1:A:1353:G:C8 | 2.18 | 0.78 |
| 1:A:433:C:C5' | 1:A:433:C:H6 | 1.97 | 0.78 |
| 5:E:91:LEU:HD23 | 5:E:120:THR:HG22 | 1.66 | 0.78 |
| 1:A:433:C:H6 | 1:A:433:C:H5' | 1.48 | 0.77 |
| 12:L:47:LYS:HB3 | 12:L:48:PRO:HD3 | 1.64 | 0.77 |
| 1:A:1130:A:C2 | 1:A:1146:A:C4 | 2.71 | 0.77 |
| 7:G:50:ILE:O | 7:G:54:THR:HB | 1.83 | 0.77 |
| 2:B:139:LYS:HD3 | 2:B:139:LYS:O | 1.85 | 0.77 |
| 14:N:22:THR:HB | 14:N:33:VAL:HG21 | 1.65 | 0.77 |
| 15:O:78:TYR:CZ | 15:O:82:ILE:HD11 | 2.19 | 0.77 |
| 9:I:114:TYR:CD2 | 10:J:60:ARG:HB2 | 2.20 | 0.77 |
| 1:A:1003(A):G:H2' | 1:A:1004:A:H4' | 1.67 | 0.77 |
| 2:B:197:VAL:HB | 2:B:200:ILE:HG12 | 1.66 | 0.77 |
| 13:M:36:LYS:HD2 | 13:M:59:TYR:OH | 1.83 | 0.77 |
| 1:A:1281:U:H5' | 1:A:1282:C:H5 | 1.47 | 0.77 |
| 1:A:1497:G:C2' | 1:A:1498:U:H5' | 2.15 | 0.77 |
| 2:B:124:SER:O | 2:B:127:ILE:HG13 | 1.84 | 0.77 |
| 1:A:1065:U:H5'' | 1:A:1190:G:N2 | 2.00 | 0.76 |
| 1:A:1123:A:H4' | 10:J:37:PRO:HD2 | 1.66 | 0.76 |
| 3:C:102:ASN:N | 3:C:102:ASN:HD22 | 1.82 | 0.76 |
| 1:A:1343:G:H1' | 9:I:121:ARG:HH12 | 1.50 | 0.76 |
| 12:L:27:LEU:O | 12:L:29:GLY:N | 2.19 | 0.76 |
| 1:A:1156:G:O3' | 1:A:1157:A:OP1 | 2.02 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:K:33:THR:HG22 | 11:K:39:PRO:HA | 1.67 | 0.76 |
| 13:M:108:ARG:HE | 13:M:108:ARG:HA | 1.49 | 0.76 |
| 1:A:1497:G:O2' | 1:A:1498:U:H5' | 1.86 | 0.76 |
| 12:L:25:PRO:C | 12:L:27:LEU:H | 1.89 | 0.76 |
| 4:D:168:ARG:HB3 | 4:D:168:ARG:NH1 | 2.00 | 0.76 |
| 12:L:28:LYS:C | 12:L:30:ALA:H | 1.87 | 0.76 |
| 1:A:1356:G:H2' | 1:A:1357:A:H8 | 1.48 | 0.76 |
| 14:N:58:LYS:HZ2 | 14:N:58:LYS:HB3 | 1.50 | 0.76 |
| 18:R:47:THR:HG22 | 18:R:48:GLY:H | 1.51 | 0.76 |
| 2:B:48:MET:HA | 2:B:51:LEU:HD12 | 1.68 | 0.75 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.67 | 0.75 |
| 20:T:67:ALA:HA | 20:T:73:HIS:H | 1.49 | 0.75 |
| 7:G:54:THR:HG22 | 7:G:56:GLN:H | 1.50 | 0.75 |
| 12:L:41:ARG:HG2 | 12:L:42:THR:H | 1.50 | 0.75 |
| 6:F:47:ARG:HE | 6:F:47:ARG:N | 1.84 | 0.75 |
| 1:A:1189:C:P | 10:J:51:ARG:HH22 | 2.10 | 0.75 |
| 2:B:218:ALA:O | 2:B:222:ILE:HG13 | 1.85 | 0.75 |
| 5:E:82:VAL:HG21 | 5:E:138:ALA:HA | 1.66 | 0.75 |
| 12:L:57:LYS:HD2 | 12:L:67:THR:HG22 | 1.67 | 0.75 |
| 1:A:948:C:OP1 | 13:M:109:THR:HG22 | 1.87 | 0.75 |
| 1:A:390:C:H2' | 1:A:391:G:H8 | 1.50 | 0.75 |
| 7:G:140:ASP:O | 7:G:144:MET:HB2 | 1.85 | 0.75 |
| 5:E:80:ILE:HD11 | 5:E:91:LEU:HB2 | 1.66 | 0.75 |
| 12:L:46:LYS:HG2 | 12:L:92:ASP:O | 1.87 | 0.75 |
| 22:X:2:U:O2' | 22:X:3:G:H5' | 1.87 | 0.75 |
| 1:A:1529:G:H3' | 1:A:1529:G:OP2 | 1.87 | 0.74 |
| 1:A:718:G:C5' | 11:K:117:ASN:HD22 | 1.99 | 0.74 |
| 2:B:95:GLN:C | 2:B:96:ARG:HD2 | 2.07 | 0.74 |
| 1:A:953:G:H1' | 13:M:125:ARG:HB2 | 1.69 | 0.74 |
| 8:H:90:GLY:O | 8:H:91:ARG:HB2 | 1.85 | 0.74 |
| 1:A:975:A:H5' | 1:A:975:A:C8 | 2.22 | 0.74 |
| 1:A:1161:C:H2' | 1:A:1162:C:C5 | 2.23 | 0.74 |
| 21:U:6:ARG:HD2 | 21:U:15:ARG:HH12 | 1.52 | 0.74 |
| 6:F:2:ARG:HE | 6:F:69:GLU:HG2 | 1.51 | 0.74 |
| 16:P:67:THR:HG22 | 16:P:69:THR:H | 1.53 | 0.74 |
| 1:A:371:G:O2' | 1:A:372:C:H5' | 1.88 | 0.74 |
| 1:A:556:C:O2' | 1:A:557:G:H5' | 1.87 | 0.74 |
| 2:B:172:ILE:H | 2:B:172:ILE:HD12 | 1.51 | 0.74 |
| 4:D:24:GLU:HG2 | 4:D:25:ARG:H | 1.52 | 0.74 |
| 8:H:103:VAL:HG21 | 8:H:109:ILE:O | 1.87 | 0.74 |
| 21:U:15:ARG:HH11 | 21:U:15:ARG:HG2 | 1.53 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1479:C:H2' | 1:A:1480:G:H8 | 1.51 | 0.73 |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:N | 2.02 | 0.73 |
| 6:F:101:ALA:HB2 | 18:R:28:GLU:HB2 | 1.70 | 0.73 |
| 1:A:262:A:H5' | 20:T:74:LYS:HD3 | 1.70 | 0.73 |
| 3:C:44:GLU:HA | 3:C:52:LEU:HD11 | 1.69 | 0.73 |
| 1:A:1533:C:C2' | 1:A:1534:A:O5' | 2.36 | 0.73 |
| 3:C:204:LEU:O | 3:C:204:LEU:HD12 | 1.89 | 0.73 |
| 1:A:1133:G:H2' | 1:A:1134:G:H8 | 1.52 | 0.73 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.24 | 0.73 |
| 9:I:48:GLU:HA | 9:I:51:ARG:HH11 | 1.54 | 0.73 |
| 10:J:6:ILE:HD13 | 10:J:73:ASP:H | 1.54 | 0.73 |
| 15:O:39:LEU:HD12 | 15:O:56:LEU:HD13 | 1.71 | 0.73 |
| 22:X:3:G:HO2' | 22:X:4:A:H5' | 1.53 | 0.73 |
| 12:L:28:LYS:O | 12:L:30:ALA:N | 2.21 | 0.73 |
| 1:A:1095:U:H2' | 1:A:1096:C:C6 | 2.23 | 0.73 |
| 13:M:5:ALA:HB3 | 13:M:8:GLU:HG3 | 1.70 | 0.73 |
| 2:B:51:LEU:HD22 | 2:B:55:PHE:HE1 | 1.53 | 0.73 |
| 12:L:7:ILE:O | 12:L:11:VAL:HG23 | 1.87 | 0.73 |
| 1:A:1175:G:C2 | 1:A:1176:A:C4 | 2.77 | 0.73 |
| 2:B:25:ASN:ND2 | 2:B:27:LYS:H | 1.87 | 0.72 |
| 3:C:107:GLN:H | 3:C:107:GLN:CD | 1.93 | 0.72 |
| 3:C:150:LYS:HG3 | 3:C:169:ALA:HB2 | 1.70 | 0.72 |
| 2:B:204:ASN:HD22 | 2:B:204:ASN:C | 1.93 | 0.72 |
| 14:N:26:ARG:HH12 | 14:N:47:LEU:HD21 | 1.53 | 0.72 |
| 1:A:1247:U:O2' | 1:A:1248:A:H5' | 1.89 | 0.72 |
| 1:A:1373:G:H5'' | 7:G:36:LYS:HB2 | 1.70 | 0.72 |
| 1:A:243:A:H4' | 1:A:244:U:C5' | 2.17 | 0.72 |
| 18:R:46:GLU:CD | 18:R:46:GLU:H | 1.92 | 0.72 |
| 20:T:14:LYS:O | 20:T:18:GLN:HG3 | 1.89 | 0.72 |
| 5:E:144:THR:O | 5:E:148:VAL:HG23 | 1.89 | 0.72 |
| 3:C:34:LEU:HD23 | 3:C:34:LEU:O | 1.87 | 0.72 |
| 9:I:97:LYS:HB3 | 9:I:98:PRO:HD3 | 1.71 | 0.72 |
| 1:A:1152:A:H5' | 10:J:70:ARG:HH22 | 1.55 | 0.72 |
| 13:M:50:GLU:O | 13:M:54:VAL:HG23 | 1.90 | 0.72 |
| 16:P:74:LEU:O | 16:P:79:VAL:HG23 | 1.90 | 0.72 |
| 1:A:1086:U:H3 | 1:A:1099:G:N2 | 1.85 | 0.72 |
| 1:A:1286:A:C8 | 1:A:1287:A:H4' | 2.25 | 0.72 |
| 1:A:382:A:H2' | 1:A:383:A:C8 | 2.25 | 0.71 |
| 6:F:46:ARG:CB | 6:F:47:ARG:HH21 | 2.03 | 0.71 |
| 15:O:16:ALA:HB1 | 15:O:21:ASP:HB3 | 1.73 | 0.71 |
| 13:M:11:ARG:HD3 | 13:M:12:ASN:HB2 | 1.71 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:40:ASN:HB3 | 13:M:43:THR:HG23 | 1.71 | 0.71 |
| 14:N:26:ARG:NH1 | 14:N:47:LEU:HD21 | 2.05 | 0.71 |
| 2:B:88:ALA:HB2 | 2:B:219:VAL:HG13 | 1.73 | 0.71 |
| 9:I:118:LYS:O | 9:I:119:ALA:HB3 | 1.91 | 0.71 |
| 1:A:1250:A:C4' | 9:I:68:GLY:H | 2.01 | 0.71 |
| 1:A:1175:G:C2 | 1:A:1176:A:C5 | 2.78 | 0.71 |
| 13:M:11:ARG:HG3 | 13:M:11:ARG:HH11 | 1.55 | 0.71 |
| 3:C:110:ASN:ND2 | 3:C:140:ARG:HB3 | 2.06 | 0.71 |
| 12:L:38:THR:O | 12:L:79:GLU:HG3 | 1.89 | 0.71 |
| 1:A:1149:C:H2' | 1:A:1150:U:C6 | 2.25 | 0.71 |
| 10:J:18:ALA:O | 10:J:21:GLN:HB2 | 1.91 | 0.71 |
| 1:A:839:U:O2 | 1:A:839:U:H2' | 1.90 | 0.71 |
| 1:A:657:G:H4' | 15:O:28:GLN:HG2 | 1.72 | 0.70 |
| 3:C:6:HIS:HD2 | 3:C:8:ILE:H | 1.38 | 0.70 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N | 2.05 | 0.70 |
| 1:A:254:G:H21 | 17:Q:16:GLN:NE2 | 1.89 | 0.70 |
| 1:A:629:G:H2' | 1:A:630:G:H5'' | 1.72 | 0.70 |
| 1:A:664:G:OP1 | 18:R:64:ARG:HD2 | 1.90 | 0.70 |
| 6:F:46:ARG:HB3 | 6:F:46:ARG:NH1 | 2.06 | 0.70 |
| 1:A:266:G:C8 | 1:A:266:G:H5' | 2.26 | 0.70 |
| 4:D:205:GLU:O | 4:D:208:SER:HB3 | 1.91 | 0.70 |
| 20:T:43:LEU:HD13 | 20:T:51:GLU:HG3 | 1.74 | 0.70 |
| 1:A:1026:G:H3' | 1:A:1027:C:H5'' | 1.72 | 0.70 |
| 1:A:1190:G:C3' | 3:C:3:ASN:HD21 | 2.04 | 0.70 |
| 1:A:1229:A:H2' | 1:A:1230:C:H6 | 1.57 | 0.70 |
| 6:F:44:GLY:HA2 | 6:F:59:TYR:CE1 | 2.27 | 0.70 |
| 6:F:100:ASN:HB2 | 18:R:23:LYS:HE3 | 1.72 | 0.70 |
| 3:C:14:ILE:HG22 | 3:C:15:THR:N | 1.98 | 0.70 |
| 10:J:5:ARG:HA | 10:J:73:ASP:OD1 | 1.91 | 0.70 |
| 1:A:1318:A:H1' | 19:S:37:ARG:HH11 | 1.55 | 0.70 |
| 3:C:23:TYR:CD2 | 3:C:24:ALA:N | 2.60 | 0.70 |
| 10:J:23:ILE:O | 10:J:23:ILE:HG22 | 1.91 | 0.70 |
| 9:I:3:GLN:HE22 | 9:I:20:ARG:HH21 | 1.40 | 0.69 |
| 2:B:80:ILE:HD11 | 2:B:208:ILE:HG23 | 1.73 | 0.69 |
| 19:S:33:THR:HG22 | 19:S:35:SER:N | 2.04 | 0.69 |
| 10:J:32:ALA:HB2 | 10:J:76:ASN:HB2 | 1.73 | 0.69 |
| 17:Q:27:PHE:CE1 | 17:Q:36:ILE:HD11 | 2.28 | 0.69 |
| 1:A:1167:A:H2' | 1:A:1168:A:C8 | 2.28 | 0.69 |
| 10:J:8:LEU:HB2 | 10:J:70:ARG:HB2 | 1.74 | 0.69 |
| 1:A:1175:G:H2' | 1:A:1176:A:H8 | 1.58 | 0.69 |
| 3:C:53:ALA:O | 3:C:54:ARG:HB2 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:143:ARG:NH1 | 8:H:77:GLU:OE2 | 2.26 | 0.69 |
| 9:I:70:LYS:O | 9:I:74:ILE:HG13 | 1.93 | 0.69 |
| 15:O:6:GLU:CD | 15:O:6:GLU:H | 1.96 | 0.69 |
| 1:A:397:A:H5' | 1:A:398:C:OP1 | 1.93 | 0.69 |
| 6:F:62:TRP:C | 6:F:63:TYR:HD2 | 1.97 | 0.69 |
| 8:H:60:ARG:HG3 | 8:H:60:ARG:HH11 | 1.58 | 0.69 |
| 10:J:6:ILE:H | 10:J:6:ILE:HD12 | 1.56 | 0.69 |
| 17:Q:40:LYS:HG3 | 17:Q:41:LYS:N | 2.07 | 0.69 |
| 19:S:4:SER:O | 19:S:5:LEU:HD12 | 1.93 | 0.69 |
| 1:A:1256:A:H2 | 1:A:1277:C:C4 | 2.11 | 0.69 |
| 2:B:196:LEU:H | 2:B:196:LEU:HD12 | 1.57 | 0.69 |
| 1:A:1190:G:C3' | 3:C:3:ASN:ND2 | 2.54 | 0.69 |
| 10:J:30:SER:CB | 10:J:84:GLN:HE21 | 2.05 | 0.69 |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:HG3 | 1.57 | 0.69 |
| 3:C:107:GLN:O | 3:C:108:ASN:HB3 | 1.92 | 0.69 |
| 3:C:26:LYS:CD | 3:C:26:LYS:H | 2.06 | 0.69 |
| 1:A:254:G:OP1 | 17:Q:67:LYS:O | 2.10 | 0.68 |
| 3:C:64:VAL:H | 3:C:99:VAL:HB | 1.58 | 0.68 |
| 9:I:93:ARG:HB3 | 9:I:93:ARG:HH11 | 1.56 | 0.68 |
| 13:M:4:ILE:HG22 | 13:M:5:ALA:N | 2.06 | 0.68 |
| 1:A:701:C:H5'' | 1:A:703:G:O4' | 1.92 | 0.68 |
| 7:G:52:GLU:O | 7:G:53:LYS:HB2 | 1.93 | 0.68 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.29 | 0.68 |
| 7:G:120:ILE:H | 7:G:120:ILE:HD12 | 1.58 | 0.68 |
| 1:A:1016:A:H2' | 1:A:1017:G:O4' | 1.93 | 0.68 |
| 1:A:370:C:O2' | 1:A:371:G:H5' | 1.94 | 0.68 |
| 12:L:126:LYS:HD2 | 12:L:126:LYS:O | 1.94 | 0.68 |
| 1:A:328:C:O2 | 1:A:328:C:H2' | 1.92 | 0.68 |
| 1:A:1057:G:H5'' | 3:C:154:SER:CB | 2.24 | 0.68 |
| 5:E:36:ASP:OD1 | 5:E:38:GLN:N | 2.27 | 0.68 |
| 11:K:124:LYS:HD2 | 11:K:125:PHE:CE1 | 2.27 | 0.68 |
| 1:A:1003(A):G:H2' | 1:A:1004:A:C4' | 2.23 | 0.68 |
| 1:A:1142:G:H2' | 1:A:1143:G:O4' | 1.93 | 0.68 |
| 3:C:121:ALA:O | 3:C:125:GLU:HG3 | 1.94 | 0.68 |
| 10:J:15:THR:HG22 | 10:J:94:VAL:HG23 | 1.76 | 0.68 |
| 10:J:69:ASN:O | 10:J:70:ARG:HD3 | 1.94 | 0.68 |
| 17:Q:65:ILE:N | 17:Q:65:ILE:HD12 | 2.09 | 0.68 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.29 | 0.67 |
| 3:C:50:ALA:HB1 | 3:C:70:VAL:HG11 | 1.76 | 0.67 |
| 4:D:119:GLN:HG2 | 4:D:123:HIS:CD2 | 2.29 | 0.67 |
| 4:D:162:LEU:HD23 | 4:D:162:LEU:O | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1367:C:H5' | 10:J:60:ARG:HH12 | 1.57 | 0.67 |
| 1:A:266:G:H5'' | 1:A:268:C:N4 | 2.01 | 0.67 |
| 7:G:15:ASP:O | 7:G:19:GLY:HA2 | 1.93 | 0.67 |
| 1:A:918:A:H2' | 1:A:919:A:C8 | 2.29 | 0.67 |
| 1:A:1318:A:O2' | 19:S:37:ARG:HD2 | 1.95 | 0.67 |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HG21 | 1.77 | 0.67 |
| 9:I:55:ALA:O | 9:I:56:LEU:HB3 | 1.94 | 0.67 |
| 1:A:1479:C:H2' | 1:A:1480:G:C8 | 2.29 | 0.67 |
| 3:C:123:GLN:O | 3:C:126:ARG:HB3 | 1.94 | 0.67 |
| 19:S:52:TYR:HA | 19:S:56:GLN:O | 1.93 | 0.67 |
| 1:A:1347:G:N2 | 1:A:1373:G:H2' | 2.09 | 0.67 |
| 15:O:4:THR:OG1 | 15:O:7:GLU:HG3 | 1.95 | 0.67 |
| 21:U:6:ARG:HD2 | 21:U:15:ARG:NH1 | 2.09 | 0.67 |
| 2:B:74:LYS:HZ1 | 2:B:206:ASP:HB2 | 1.59 | 0.67 |
| 3:C:188:LEU:O | 3:C:189:ALA:HB2 | 1.95 | 0.67 |
| 6:F:2:ARG:NE | 6:F:69:GLU:HG2 | 2.08 | 0.67 |
| 1:A:1054:C:H2' | 1:A:1055:A:H5'' | 1.77 | 0.67 |
| 1:A:1130:A:N3 | 1:A:1146:A:C2 | 2.62 | 0.67 |
| 2:B:161:ALA:HB1 | 2:B:185:ILE:HD11 | 1.77 | 0.67 |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:CD | 2.07 | 0.67 |
| 10:J:39:PRO:O | 10:J:40:LEU:HB2 | 1.94 | 0.67 |
| 4:D:146:ILE:HD12 | 4:D:146:ILE:N | 2.10 | 0.66 |
| 13:M:19:LEU:O | 13:M:22:ILE:HD13 | 1.95 | 0.66 |
| 17:Q:67:LYS:CA | 17:Q:70:ARG:HH12 | 2.07 | 0.66 |
| 1:A:1156:G:N2 | 1:A:1179:A:C6 | 2.51 | 0.66 |
| 1:A:1193:G:O2' | 1:A:1194:U:H5' | 1.96 | 0.66 |
| 2:B:196:LEU:N | 2:B:196:LEU:HD12 | 2.10 | 0.66 |
| 5:E:80:ILE:HD12 | 5:E:91:LEU:HB2 | 1.76 | 0.66 |
| 19:S:22:LEU:HD22 | 19:S:28:LYS:HB2 | 1.78 | 0.66 |
| 1:A:939:G:H2' | 1:A:940:C:C6 | 2.30 | 0.66 |
| 6:F:19:LEU:O | 6:F:23:LYS:HG3 | 1.95 | 0.66 |
| 10:J:15:THR:HG22 | 10:J:94:VAL:CG2 | 2.25 | 0.66 |
| 1:A:1175:G:C2 | 1:A:1176:A:C8 | 2.83 | 0.66 |
| 10:J:32:ALA:H | 10:J:78:ASN:HD21 | 1.42 | 0.66 |
| 19:S:20:LEU:HA | 19:S:23:ASN:ND2 | 2.09 | 0.66 |
| 1:A:818:G:C3' | 1:A:819:A:H5'' | 2.25 | 0.66 |
| 1:A:838:G:H2' | 1:A:839:U:H5'' | 1.76 | 0.66 |
| 6:F:48:LEU:HD13 | 6:F:52:ILE:HD12 | 1.77 | 0.66 |
| 12:L:46:LYS:HE2 | 12:L:47:LYS:HB2 | 1.76 | 0.66 |
| 19:S:5:LEU:O | 19:S:6:LYS:HB2 | 1.95 | 0.66 |
| 1:A:1080:A:C5' | 5:E:16:THR:HG21 | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1502:A:H2 | 1:A:1505:G:N1 | 1.92 | 0.66 |
| 6:F:80:ARG:NH1 | 6:F:88:VAL:HB | 2.10 | 0.66 |
| 19:S:4:SER:C | 19:S:5:LEU:HD12 | 2.15 | 0.66 |
| 4:D:162:LEU:HD13 | 4:D:181:MET:HE2 | 1.78 | 0.66 |
| 9:I:32:ASP:HB3 | 9:I:35:GLU:HB2 | 1.77 | 0.66 |
| 12:L:28:LYS:C | 12:L:30:ALA:N | 2.49 | 0.66 |
| 17:Q:68:ARG:N | 17:Q:70:ARG:NH1 | 2.44 | 0.66 |
| 1:A:141:A:H1' | 1:A:182:U:O2 | 1.95 | 0.66 |
| 2:B:7:VAL:HG11 | 2:B:221:LEU:HD23 | 1.77 | 0.66 |
| 10:J:49:VAL:CG2 | 14:N:41:ARG:HB2 | 2.23 | 0.66 |
| 12:L:43:VAL:HG12 | 12:L:44:THR:N | 2.11 | 0.66 |
| 18:R:87:ARG:HG2 | 18:R:87:ARG:HH11 | 1.59 | 0.66 |
| 20:T:53:LEU:HB2 | 20:T:100:ILE:CG2 | 2.26 | 0.66 |
| 11:K:14:VAL:HG21 | 11:K:40:ILE:HD11 | 1.77 | 0.66 |
| 13:M:15:VAL:HG23 | 13:M:43:THR:O | 1.96 | 0.66 |
| 19:S:20:LEU:HD12 | 19:S:21:GLU:N | 2.10 | 0.66 |
| 23:Y:34:TM2:H2' | 23:Y:35:A:C8 | 2.31 | 0.66 |
| 1:A:1075:C:H5' | 2:B:103:THR:HG21 | 1.79 | 0.65 |
| 1:A:1127:G:H21 | 1:A:1146:A:N6 | 1.94 | 0.65 |
| 1:A:344:A:H4' | 1:A:345:C:OP2 | 1.97 | 0.65 |
| 10:J:9:ARG:HB3 | 10:J:9:ARG:NH1 | 2.11 | 0.65 |
| 1:A:376:G:OP2 | 16:P:67:THR:HG21 | 1.97 | 0.65 |
| 1:A:983:A:H5' | 1:A:984:C:OP2 | 1.96 | 0.65 |
| 2:B:16:HIS:CE1 | 2:B:214:ILE:HG12 | 2.31 | 0.65 |
| 3:C:82:GLU:O | 3:C:85:ARG:HB3 | 1.96 | 0.65 |
| 5:E:137:GLU:O | 5:E:141:GLN:HG3 | 1.97 | 0.65 |
| 6:F:39:LYS:HG3 | 6:F:40:VAL:H | 1.61 | 0.65 |
| 11:K:11:LYS:O | 11:K:11:LYS:HD2 | 1.96 | 0.65 |
| 6:F:100:ASN:HD22 | 18:R:23:LYS:HG2 | 1.61 | 0.65 |
| 1:A:26:A:N6 | 1:A:558:G:H1' | 2.12 | 0.65 |
| 4:D:64:LEU:HD23 | 4:D:64:LEU:C | 2.17 | 0.65 |
| 1:A:1277:C:HO2' | 1:A:1279:A:H8 | 1.41 | 0.65 |
| 1:A:1128:C:O2' | 1:A:1130:A:C8 | 2.50 | 0.65 |
| 1:A:1477:C:H2' | 1:A:1478:C:H6 | 1.62 | 0.65 |
| 12:L:47:LYS:CB | 12:L:48:PRO:HD3 | 2.25 | 0.65 |
| 23:Y:34:TM2:H2' | 23:Y:35:A:H8 | 1.62 | 0.65 |
| 14:N:27:CYS:SG | 14:N:29:ARG:HB2 | 2.36 | 0.65 |
| 19:S:28:LYS:HG2 | 19:S:29:ARG:N | 2.07 | 0.65 |
| 1:A:1066:C:O2' | 1:A:1067:A:H5' | 1.97 | 0.65 |
| 1:A:1175:G:C4 | 1:A:1176:A:N7 | 2.64 | 0.65 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.32 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:39:LYS:HG3 | 6:F:40:VAL:N | 2.11 | 0.65 |
| 17:Q:68:ARG:H | 17:Q:70:ARG:NH1 | 1.95 | 0.65 |
| 9:I:4:TYR:CE1 | 9:I:88:TYR:HA | 2.32 | 0.65 |
| 19:S:62:ILE:HD12 | 19:S:66:MET:HG3 | 1.78 | 0.65 |
| 2:B:80:ILE:N | 2:B:80:ILE:HD12 | 2.11 | 0.64 |
| 3:C:155:GLY:O | 3:C:156:ARG:HB2 | 1.97 | 0.64 |
| 10:J:60:ARG:O | 10:J:61:GLU:HB3 | 1.97 | 0.64 |
| 13:M:23:TYR:O | 13:M:25:ILE:N | 2.30 | 0.64 |
| 1:A:1021:G:O2' | 1:A:1022:G:H5' | 1.96 | 0.64 |
| 1:A:35:G:H2' | 1:A:36:C:H6 | 1.61 | 0.64 |
| 7:G:145:ALA:O | 7:G:146:GLU:HB3 | 1.96 | 0.64 |
| 12:L:24:VAL:HG12 | 12:L:26:ALA:HB2 | 1.79 | 0.64 |
| 9:I:128:ARG:HA | 13:M:126:LYS:HE3 | 1.77 | 0.64 |
| 1:A:109:A:H2' | 1:A:326:G:N2 | 2.11 | 0.64 |
| 2:B:172:ILE:HD12 | 2:B:172:ILE:N | 2.12 | 0.64 |
| 2:B:208:ILE:H | 2:B:208:ILE:CD1 | 1.99 | 0.64 |
| 9:I:50:LEU:HD13 | 9:I:56:LEU:HA | 1.79 | 0.64 |
| 1:A:1156:G:H3' | 1:A:1157:A:P | 2.32 | 0.64 |
| 1:A:1347:G:C8 | 9:I:107:ARG:HB3 | 2.32 | 0.64 |
| 4:D:92:VAL:O | 4:D:96:LEU:HD13 | 1.96 | 0.64 |
| 12:L:34:ARG:O | 12:L:61:THR:HG23 | 1.96 | 0.64 |
| 17:Q:104:LYS:HD3 | 17:Q:105:ALA:H | 1.63 | 0.64 |
| 1:A:1060:C:H2' | 1:A:1061:G:H8 | 1.62 | 0.64 |
| 1:A:415:A:H2' | 1:A:416:G:H8 | 1.61 | 0.64 |
| 1:A:490:G:H2' | 1:A:491:G:H8 | 1.62 | 0.64 |
| 13:M:125:ARG:HD2 | 13:M:125:ARG:O | 1.97 | 0.64 |
| 13:M:3:ARG:HA | 13:M:8:GLU:O | 1.97 | 0.64 |
| 1:A:353:A:H5' | 1:A:353:A:H8 | 1.61 | 0.64 |
| 2:B:231:GLU:CD | 2:B:231:GLU:H | 2.01 | 0.64 |
| 6:F:9:VAL:HB | 6:F:87:ARG:HB2 | 1.79 | 0.64 |
| 1:A:1497:G:H2' | 1:A:1498:U:H5' | 1.80 | 0.64 |
| 2:B:114:ARG:O | 2:B:117:GLU:HB3 | 1.97 | 0.64 |
| 2:B:15:VAL:HG11 | 2:B:209:ARG:CB | 2.28 | 0.64 |
| 5:E:53:LEU:H | 5:E:53:LEU:HD23 | 1.63 | 0.64 |
| 9:I:48:GLU:HA | 9:I:51:ARG:NH1 | 2.12 | 0.64 |
| 10:J:23:ILE:N | 10:J:23:ILE:HD12 | 2.13 | 0.64 |
| 13:M:49:THR:HG22 | 13:M:51:ALA:N | 2.11 | 0.64 |
| 1:A:393:A:O2' | 1:A:394:G:H5' | 1.96 | 0.64 |
| 1:A:524:G:H2' | 1:A:525:C:C6 | 2.33 | 0.64 |
| 3:C:79:ARG:HG3 | 3:C:79:ARG:O | 1.98 | 0.64 |
| 14:N:32:SER:HB3 | 14:N:41:ARG:HB3 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 17:Q:45:HIS:HB3 | 17:Q:72:ARG:HG2 | 1.78 | 0.64 |
| 1:A:1152:A:H2' | 1:A:1153:C:C6 | 2.33 | 0.64 |
| 1:A:1168:A:H2' | 1:A:1169:A:C8 | 2.33 | 0.64 |
| 3:C:52:LEU:H | 3:C:52:LEU:CD2 | 2.10 | 0.64 |
| 10:J:89:ASP:HB2 | 10:J:91:PRO:HD2 | 1.78 | 0.64 |
| 12:L:89:ARG:HA | 12:L:97:ARG:HA | 1.78 | 0.64 |
| 18:R:38:GLU:CD | 18:R:38:GLU:H | 2.01 | 0.64 |
| 14:N:24:CYS:HB2 | 14:N:40:CYS:HB3 | 1.80 | 0.63 |
| 1:A:731:G:OP1 | 1:A:766:A:H1' | 1.98 | 0.63 |
| 4:D:24:GLU:HG2 | 4:D:25:ARG:N | 2.13 | 0.63 |
| 7:G:75:VAL:CG2 | 7:G:86:GLN:HB3 | 2.26 | 0.63 |
| 1:A:1038:C:H2' | 1:A:1039:C:H6 | 1.64 | 0.63 |
| 1:A:1208:C:H2' | 1:A:1209:C:H6 | 1.63 | 0.63 |
| 19:S:64:GLU:O | 19:S:67:VAL:HG23 | 1.98 | 0.63 |
| 1:A:954:G:H21 | 1:A:1227:A:H62 | 1.46 | 0.63 |
| 9:I:127:LYS:O | 9:I:127:LYS:HD2 | 1.98 | 0.63 |
| 10:J:6:ILE:N | 10:J:6:ILE:HD12 | 2.13 | 0.63 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.63 | 0.63 |
| 2:B:80:ILE:CD1 | 2:B:80:ILE:H | 2.10 | 0.63 |
| 3:C:84:ILE:CD1 | 3:C:88:ARG:HH21 | 2.10 | 0.63 |
| 1:A:107:G:C2' | 1:A:108:G:H5' | 2.29 | 0.63 |
| 1:A:1178:G:C2 | 1:A:1180:A:H8 | 2.17 | 0.63 |
| 9:I:17:VAL:HG21 | 9:I:80:GLY:HA3 | 1.80 | 0.63 |
| 20:T:53:LEU:O | 20:T:57:ARG:HD2 | 1.99 | 0.63 |
| 1:A:1366:C:H2' | 1:A:1367:C:C6 | 2.34 | 0.63 |
| 1:A:1477:C:H2' | 1:A:1478:C:C6 | 2.33 | 0.63 |
| 10:J:46:ARG:HG2 | 10:J:46:ARG:HH11 | 1.64 | 0.63 |
| 1:A:1305:G:C5' | 21:U:4:GLY:HA3 | 2.29 | 0.63 |
| 1:A:807:A:H2' | 1:A:808:C:C6 | 2.34 | 0.63 |
| 10:J:22:LYS:HZ2 | 10:J:22:LYS:HB2 | 1.62 | 0.63 |
| 15:O:26:GLU:OE1 | 15:O:77:ARG:HD2 | 1.99 | 0.63 |
| 1:A:421:U:H5' | 1:A:422:C:C5 | 2.33 | 0.63 |
| 3:C:36:ASP:O | 3:C:39:ILE:HB | 1.98 | 0.63 |
| 9:I:69:GLY:O | 9:I:73:GLN:HG3 | 1.98 | 0.63 |
| 1:A:1141:C:H2' | 1:A:1142:G:H8 | 1.64 | 0.62 |
| 1:A:1533:C:C2' | 1:A:1534:A:C5' | 2.76 | 0.62 |
| 8:H:19:VAL:HG23 | 8:H:21:LYS:HD3 | 1.80 | 0.62 |
| 1:A:1192:C:C5 | 1:A:1193:G:C8 | 2.87 | 0.62 |
| 3:C:28:GLN:HA | 3:C:31:HIS:HD2 | 1.63 | 0.62 |
| 4:D:151:LYS:H | 4:D:151:LYS:HD2 | 1.62 | 0.62 |
| 1:A:706:A:O4' | 11:K:29:ILE:HD11 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:47:LYS:CB | 12:L:48:PRO:CD | 2.75 | 0.62 |
| 17:Q:68:ARG:N | 17:Q:70:ARG:HH11 | 1.96 | 0.62 |
| 5:E:12:LEU:HD13 | 5:E:31:LEU:HB2 | 1.81 | 0.62 |
| 5:E:150:ARG:NH1 | 5:E:150:ARG:HG3 | 2.11 | 0.62 |
| 10:J:90:LEU:N | 10:J:91:PRO:CD | 2.62 | 0.62 |
| 14:N:9:LYS:HD3 | 14:N:9:LYS:O | 1.99 | 0.62 |
| 16:P:11:SER:OG | 16:P:14:ASN:HB3 | 1.99 | 0.62 |
| 1:A:1132:C:H2' | 1:A:1133:G:C8 | 2.34 | 0.62 |
| 1:A:1366:C:H2' | 1:A:1367:C:H6 | 1.62 | 0.62 |
| 17:Q:104:LYS:HD3 | 17:Q:105:ALA:N | 2.14 | 0.62 |
| 1:A:1130:A:C5 | 1:A:1146:A:N1 | 2.67 | 0.62 |
| 1:A:1435:G:H2' | 1:A:1436:U:H6 | 1.65 | 0.62 |
| 9:I:7:THR:O | 9:I:83:ARG:HD2 | 2.00 | 0.62 |
| 21:U:12:LYS:HB3 | 21:U:22:ARG:HD2 | 1.81 | 0.62 |
| 1:A:1149:C:H2' | 1:A:1150:U:H6 | 1.62 | 0.62 |
| 1:A:1201:A:H4' | 1:A:1202:G:O5' | 1.99 | 0.62 |
| 1:A:405:U:H3' | 1:A:406:G:H5' | 1.82 | 0.62 |
| 2:B:50:GLU:HB3 | 2:B:200:ILE:O | 2.00 | 0.62 |
| 4:D:64:LEU:HD12 | 4:D:198:VAL:HG11 | 1.82 | 0.62 |
| 6:F:67:MET:HB2 | 6:F:68:PRO:HD2 | 1.82 | 0.62 |
| 7:G:18:TYR:CD2 | 7:G:59:LEU:HB2 | 2.35 | 0.62 |
| 9:I:43:ALA:HA | 9:I:74:ILE:HD13 | 1.82 | 0.62 |
| 19:S:50:ALA:HA | 19:S:58:VAL:O | 1.99 | 0.62 |
| 1:A:107:G:H2' | 1:A:108:G:H5' | 1.82 | 0.62 |
| 1:A:448:A:H2' | 1:A:449:C:C6 | 2.35 | 0.62 |
| 2:B:114:ARG:HD2 | 2:B:117:GLU:HG2 | 1.81 | 0.62 |
| 6:F:3:ARG:HG2 | 6:F:93:SER:OG | 1.99 | 0.62 |
| 13:M:59:TYR:C | 13:M:63:THR:HG22 | 2.19 | 0.62 |
| 21:U:15:ARG:NH1 | 21:U:15:ARG:HG2 | 2.12 | 0.62 |
| 8:H:119:LEU:HB2 | 8:H:123:GLU:HB2 | 1.82 | 0.62 |
| 1:A:1130:A:C6 | 1:A:1146:A:C6 | 2.88 | 0.61 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.34 | 0.61 |
| 10:J:12:ASP:HB3 | 10:J:15:THR:HB | 1.80 | 0.61 |
| 13:M:37:THR:CG2 | 13:M:55:ARG:HD2 | 2.30 | 0.61 |
| 1:A:1062:U:H2' | 1:A:1063:C:C6 | 2.34 | 0.61 |
| 1:A:1326:C:OP1 | 21:U:12:LYS:NZ | 2.32 | 0.61 |
| 1:A:522:C:H41 | 12:L:53:ARG:HH22 | 1.46 | 0.61 |
| 4:D:126:ILE:HG22 | 4:D:127:THR:N | 2.14 | 0.61 |
| 7:G:59:LEU:HD11 | 7:G:63:LYS:HE3 | 1.81 | 0.61 |
| 20:T:45:GLN:C | 20:T:45:GLN:HE21 | 2.04 | 0.61 |
| 1:A:1121:U:H2' | 1:A:1122:U:H6 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:77:ALA:CB | 2:B:211:ILE:HG21 | 2.30 | 0.61 |
| 10:J:98:ILE:HG22 | 10:J:99:LYS:N | 2.15 | 0.61 |
| 1:A:1118:C:O2 | 1:A:1179:A:C4 | 2.52 | 0.61 |
| 1:A:946:A:H2' | 1:A:947:G:H8 | 1.64 | 0.61 |
| 9:I:111:ARG:HG2 | 9:I:112:LYS:N | 2.15 | 0.61 |
| 10:J:6:ILE:HA | 10:J:98:ILE:HG12 | 1.81 | 0.61 |
| 3:C:23:TYR:OH | 10:J:9:ARG:HD3 | 2.00 | 0.61 |
| 2:B:189:ASP:HB2 | 2:B:205:ASP:OD2 | 2.01 | 0.61 |
| 1:A:1251:A:H4' | 9:I:12:GLU:OE2 | 2.00 | 0.61 |
| 10:J:5:ARG:O | 10:J:98:ILE:HG23 | 2.00 | 0.61 |
| 21:U:24:ARG:O | 21:U:25:LYS:HB2 | 2.00 | 0.61 |
| 1:A:1125:U:H3 | 10:J:5:ARG:HH21 | 1.48 | 0.61 |
| 1:A:1128:C:O2' | 1:A:1130:A:H8 | 1.84 | 0.61 |
| 2:B:47:THR:HA | 2:B:202:PRO:HG2 | 1.83 | 0.61 |
| 4:D:150:GLU:HG3 | 4:D:153:ARG:HH12 | 1.63 | 0.61 |
| 3:C:29:TYR:OH | 14:N:54:PRO:HG2 | 2.00 | 0.61 |
| 2:B:231:GLU:HB3 | 2:B:232:PRO:HD2 | 1.83 | 0.61 |
| 6:F:4:TYR:HD1 | 6:F:92:LYS:HA | 1.66 | 0.61 |
| 7:G:108:ALA:O | 7:G:119:ARG:HD2 | 2.01 | 0.61 |
| 9:I:53:VAL:O | 9:I:54:ASP:HB2 | 2.01 | 0.61 |
| 19:S:17:GLU:O | 19:S:21:GLU:HG3 | 2.00 | 0.61 |
| 1:A:984:C:H2' | 1:A:985:C:H6 | 1.66 | 0.61 |
| 4:D:189:PRO:HB2 | 4:D:194:LEU:HD21 | 1.83 | 0.61 |
| 2:B:178:ARG:O | 8:H:71:GLY:HA2 | 2.01 | 0.61 |
| 1:A:1370:G:O2' | 1:A:1371:G:H5' | 2.01 | 0.61 |
| 1:A:579:G:H5' | 1:A:728:A:C1' | 2.27 | 0.61 |
| 2:B:204:ASN:HD22 | 2:B:205:ASP:N | 1.99 | 0.61 |
| 3:C:36:ASP:HA | 3:C:39:ILE:HD12 | 1.82 | 0.61 |
| 6:F:69:GLU:CD | 6:F:69:GLU:H | 2.03 | 0.61 |
| 1:A:1307:U:H5' | 13:M:109:THR:HG21 | 1.82 | 0.61 |
| 1:A:1286:A:H2' | 1:A:1287:A:H4' | 1.83 | 0.61 |
| 1:A:575:G:OP1 | 1:A:575:G:H4' | 2.01 | 0.61 |
| 2:B:114:ARG:HA | 2:B:117:GLU:HB3 | 1.81 | 0.61 |
| 3:C:70:VAL:HG12 | 3:C:71:ALA:N | 2.16 | 0.61 |
| 4:D:30:LYS:HA | 4:D:35:ARG:HH12 | 1.66 | 0.61 |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:N | 1.99 | 0.61 |
| 1:A:1260:C:O5' | 1:A:1284:C:H4' | 2.01 | 0.60 |
| 1:A:818:G:O2' | 1:A:819:A:H5'' | 2.01 | 0.60 |
| 2:B:141:GLU:O | 2:B:144:ARG:HG2 | 2.01 | 0.60 |
| 1:A:542:G:OP1 | 4:D:10:ARG:NH2 | 2.33 | 0.60 |
| 5:E:144:THR:HG22 | 5:E:146:ALA:N | 2.14 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:53:LEU:N | 5:E:53:LEU:HD23 | 2.15 | 0.60 |
| 9:I:9:ARG:HA | 9:I:13:ALA:O | 2.01 | 0.60 |
| 1:A:1229:A:H2' | 1:A:1230:C:C6 | 2.34 | 0.60 |
| 2:B:114:ARG:NH1 | 2:B:118:LEU:HD21 | 2.17 | 0.60 |
| 3:C:60:ALA:O | 3:C:61:ALA:HB2 | 2.01 | 0.60 |
| 4:D:162:LEU:HD13 | 4:D:181:MET:CE | 2.31 | 0.60 |
| 5:E:80:ILE:H | 5:E:80:ILE:HD12 | 1.66 | 0.60 |
| 6:F:46:ARG:HB3 | 6:F:47:ARG:HH21 | 1.67 | 0.60 |
| 6:F:93:SER:O | 6:F:94:GLN:HG3 | 2.01 | 0.60 |
| 10:J:32:ALA:H | 10:J:78:ASN:ND2 | 1.98 | 0.60 |
| 1:A:1068:G:H8 | 1:A:1068:G:OP2 | 1.84 | 0.60 |
| 1:A:1286:A:H8 | 1:A:1287:A:H4' | 1.66 | 0.60 |
| 2:B:97:TRP:HH2 | 2:B:176:GLU:CD | 2.04 | 0.60 |
| 4:D:10:ARG:HG3 | 4:D:10:ARG:HH11 | 1.66 | 0.60 |
| 1:A:1127:G:N2 | 1:A:1146:A:N6 | 2.49 | 0.60 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.36 | 0.60 |
| 1:A:818:G:C2' | 1:A:819:A:H5'' | 2.31 | 0.60 |
| 2:B:60:ASP:O | 2:B:64:ARG:HG3 | 2.00 | 0.60 |
| 1:A:1026:G:H3' | 1:A:1027:C:C5' | 2.31 | 0.60 |
| 1:A:1234:C:O2' | 1:A:1235:U:H5' | 2.01 | 0.60 |
| 1:A:1438:G:H2' | 1:A:1439:C:C6 | 2.37 | 0.60 |
| 2:B:10:LEU:HG | 2:B:48:MET:CE | 2.32 | 0.60 |
| 6:F:2:ARG:HE | 6:F:69:GLU:CG | 2.13 | 0.60 |
| 1:A:1024:G:H3' | 1:A:1025:U:H5'' | 1.82 | 0.60 |
| 1:A:1132:C:H2' | 1:A:1133:G:H8 | 1.66 | 0.60 |
| 2:B:80:ILE:HG21 | 2:B:212:GLN:HA | 1.84 | 0.60 |
| 4:D:150:GLU:N | 4:D:150:GLU:CD | 2.54 | 0.60 |
| 6:F:47:ARG:O | 6:F:47:ARG:HG2 | 2.00 | 0.60 |
| 7:G:140:ASP:HA | 7:G:143:ARG:HH21 | 1.67 | 0.60 |
| 8:H:119:LEU:HD12 | 8:H:124:ALA:HA | 1.82 | 0.60 |
| 14:N:58:LYS:HB3 | 14:N:58:LYS:NZ | 2.17 | 0.60 |
| 1:A:190(L):U:O2 | 20:T:105:SER:HB2 | 2.02 | 0.60 |
| 20:T:43:LEU:HD11 | 20:T:55:ILE:HD12 | 1.83 | 0.60 |
| 1:A:1022:G:H2' | 1:A:1023:G:H8 | 1.67 | 0.60 |
| 1:A:1316:G:N2 | 1:A:1318:A:H3' | 2.17 | 0.60 |
| 1:A:1412:C:H2' | 1:A:1413:A:C8 | 2.36 | 0.60 |
| 1:A:45:U:H2' | 1:A:46:G:C8 | 2.37 | 0.60 |
| 9:I:93:ARG:CB | 9:I:93:ARG:HH11 | 2.14 | 0.60 |
| 18:R:47:THR:HG22 | 18:R:48:GLY:N | 2.17 | 0.60 |
| 18:R:86:VAL:O | 18:R:87:ARG:HG2 | 2.02 | 0.60 |
| 2:B:143:GLU:O | 2:B:147:LYS:HG3 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:75:LYS:HE2 | 2:B:96:ARG:HH22 | 1.67 | 0.60 |
| 5:E:69:VAL:HG21 | 5:E:113:ALA:HB1 | 1.84 | 0.60 |
| 1:A:1249:C:O2' | 9:I:73:GLN:NE2 | 2.35 | 0.60 |
| 10:J:14:LYS:O | 10:J:18:ALA:HB3 | 2.01 | 0.60 |
| 19:S:13:ASP:HA | 19:S:16:LEU:CB | 2.31 | 0.60 |
| 9:I:30:GLY:O | 9:I:31:GLN:HG3 | 2.02 | 0.60 |
| 17:Q:67:LYS:O | 17:Q:68:ARG:CB | 2.49 | 0.60 |
| 18:R:42:ARG:NH1 | 18:R:42:ARG:HB3 | 2.16 | 0.60 |
| 1:A:1256:A:C2 | 1:A:1277:C:C4 | 2.89 | 0.60 |
| 1:A:383:A:H2' | 1:A:384:G:H5' | 1.84 | 0.60 |
| 1:A:457:C:H2' | 1:A:458:C:H6 | 1.67 | 0.60 |
| 2:B:12:GLU:C | 2:B:14:GLY:H | 2.05 | 0.60 |
| 5:E:82:VAL:HG21 | 5:E:138:ALA:CA | 2.32 | 0.60 |
| 10:J:44:VAL:HG22 | 10:J:66:ARG:HB3 | 1.83 | 0.60 |
| 1:A:1054:C:C3' | 1:A:1054:C:O2 | 2.49 | 0.59 |
| 1:A:1347:G:O2' | 1:A:1348:U:P | 2.60 | 0.59 |
| 1:A:853:G:O2' | 1:A:854:G:H5' | 2.01 | 0.59 |
| 3:C:116:VAL:HG21 | 3:C:202:ILE:HD11 | 1.83 | 0.59 |
| 4:D:24:GLU:O | 4:D:25:ARG:HB3 | 2.01 | 0.59 |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:CA | 2.30 | 0.59 |
| 16:P:28:ARG:HG3 | 16:P:29:ASP:OD2 | 2.03 | 0.59 |
| 1:A:112:G:H5' | 1:A:389:A:H4' | 1.83 | 0.59 |
| 2:B:213:LEU:O | 2:B:217:ARG:HG2 | 2.02 | 0.59 |
| 2:B:84:GLU:OE1 | 2:B:216:SER:HA | 2.02 | 0.59 |
| 10:J:24:VAL:O | 10:J:28:ARG:HG3 | 2.02 | 0.59 |
| 10:J:27:ALA:HA | 10:J:81:THR:HG23 | 1.83 | 0.59 |
| 1:A:232:G:H1' | 1:A:262:A:N1 | 2.17 | 0.59 |
| 1:A:746:A:O2' | 1:A:747:C:H5' | 2.02 | 0.59 |
| 2:B:23:ARG:NH1 | 2:B:24:TRP:HA | 2.18 | 0.59 |
| 3:C:79:ARG:HG2 | 3:C:82:GLU:HG2 | 1.83 | 0.59 |
| 9:I:44:VAL:HG12 | 9:I:51:ARG:NH2 | 2.17 | 0.59 |
| 10:J:76:ASN:O | 10:J:78:ASN:N | 2.35 | 0.59 |
| 22:X:3:G:C2' | 22:X:4:A:C5' | 2.77 | 0.59 |
| 2:B:102:LEU:HD12 | 2:B:102:LEU:N | 2.17 | 0.59 |
| 9:I:17:VAL:CG2 | 9:I:80:GLY:HA3 | 2.33 | 0.59 |
| 1:A:1392:G:O2' | 1:A:1502:A:H5'' | 2.01 | 0.59 |
| 2:B:168:THR:OG1 | 2:B:192:SER:HB3 | 2.02 | 0.59 |
| 6:F:82:ARG:HB2 | 6:F:85:VAL:HG23 | 1.85 | 0.59 |
| 7:G:85:TYR:O | 7:G:87:VAL:HG23 | 2.03 | 0.59 |
| 9:I:118:LYS:O | 9:I:119:ALA:CB | 2.51 | 0.59 |
| 9:I:16:ARG:HB2 | 9:I:64:THR:HB | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1130:A:N3 | 1:A:1146:A:N3 | 2.50 | 0.59 |
| 3:C:54:ARG:CG | 3:C:55:VAL:H | 2.15 | 0.59 |
| 10:J:8:LEU:CD1 | 10:J:20:ALA:HB2 | 2.33 | 0.59 |
| 1:A:1175:G:N2 | 1:A:1176:A:C4 | 2.71 | 0.59 |
| 1:A:942:G:H2' | 1:A:943:U:H6 | 1.66 | 0.59 |
| 5:E:90:VAL:O | 5:E:120:THR:HA | 2.03 | 0.59 |
| 9:I:103:THR:HG22 | 9:I:104:ARG:O | 2.02 | 0.59 |
| 12:L:54:LYS:N | 12:L:54:LYS:HD2 | 2.18 | 0.59 |
| 19:S:15:LEU:O | 19:S:19:VAL:HG12 | 2.03 | 0.59 |
| 1:A:1176:A:H2' | 1:A:1177:G:C8 | 2.38 | 0.59 |
| 1:A:1330:U:C4 | 1:A:1331:G:N3 | 2.71 | 0.59 |
| 2:B:223:ILE:C | 2:B:225:ALA:H | 2.06 | 0.59 |
| 2:B:42:ILE:HG21 | 2:B:202:PRO:O | 2.01 | 0.59 |
| 12:L:75:HIS:HD2 | 12:L:77:LEU:H | 1.49 | 0.59 |
| 12:L:83:VAL:HG22 | 12:L:84:LEU:N | 2.18 | 0.59 |
| 13:M:17:VAL:O | 13:M:20:THR:HB | 2.02 | 0.59 |
| 20:T:75:ASN:N | 20:T:75:ASN:OD1 | 2.36 | 0.59 |
| 1:A:1130:A:C4 | 1:A:1146:A:N1 | 2.70 | 0.59 |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:CG1 | 2.33 | 0.59 |
| 1:A:522:C:H41 | 12:L:53:ARG:NH2 | 2.00 | 0.59 |
| 11:K:110:ASP:CB | 18:R:88:LYS:HD2 | 2.27 | 0.59 |
| 19:S:17:GLU:HA | 19:S:20:LEU:CG | 2.31 | 0.59 |
| 2:B:42:ILE:H | 2:B:42:ILE:CD1 | 2.15 | 0.59 |
| 3:C:154:SER:OG | 3:C:155:GLY:N | 2.33 | 0.59 |
| 8:H:4:ASP:OD2 | 8:H:7:ALA:HB2 | 2.03 | 0.59 |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:HB3 | 1.85 | 0.59 |
| 18:R:52:PRO:HB3 | 18:R:54:ARG:NH1 | 2.17 | 0.59 |
| 1:A:390:C:O3' | 16:P:28:ARG:NH2 | 2.35 | 0.58 |
| 2:B:42:ILE:N | 2:B:42:ILE:HD12 | 2.17 | 0.58 |
| 3:C:37:GLN:HE22 | 14:N:52:GLN:HE22 | 1.51 | 0.58 |
| 10:J:8:LEU:HD12 | 10:J:20:ALA:HB2 | 1.86 | 0.58 |
| 1:A:1056:U:H5' | 3:C:163:ALA:HB2 | 1.84 | 0.58 |
| 1:A:1085:U:H3' | 1:A:1086:U:H5 | 1.67 | 0.58 |
| 2:B:122:PHE:HE2 | 2:B:139:LYS:HG2 | 1.68 | 0.58 |
| 7:G:120:ILE:N | 7:G:120:ILE:HD12 | 2.17 | 0.58 |
| 8:H:120:THR:OG1 | 8:H:123:GLU:HG3 | 2.03 | 0.58 |
| 8:H:119:LEU:HD12 | 8:H:124:ALA:N | 2.18 | 0.58 |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:HG13 | 1.83 | 0.58 |
| 1:A:1006:C:H2' | 1:A:1007:C:H6 | 1.65 | 0.58 |
| 1:A:314:C:O2' | 1:A:315:A:H5' | 2.02 | 0.58 |
| 1:A:940:C:H2' | 1:A:941:G:H8 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:47:LEU:N | 3:C:47:LEU:HD12 | 2.18 | 0.58 |
| 4:D:3:ARG:HD2 | 4:D:118:ARG:HE | 1.68 | 0.58 |
| 7:G:46:ALA:O | 7:G:50:ILE:HG12 | 2.02 | 0.58 |
| 1:A:1366:C:C2 | 1:A:1367:C:C5 | 2.91 | 0.58 |
| 1:A:1428:A:H2' | 1:A:1429:C:C6 | 2.39 | 0.58 |
| 1:A:426:G:O2' | 1:A:427:U:H5' | 2.04 | 0.58 |
| 1:A:792:A:H4' | 1:A:793:U:O5' | 2.03 | 0.58 |
| 4:D:191:ARG:O | 4:D:191:ARG:HD2 | 2.03 | 0.58 |
| 1:A:1101:A:H4' | 1:A:1102:A:O5' | 2.04 | 0.58 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.38 | 0.58 |
| 1:A:833:U:H2' | 1:A:834:C:C6 | 2.38 | 0.58 |
| 2:B:97:TRP:CZ2 | 2:B:102:LEU:HD13 | 2.29 | 0.58 |
| 2:B:232:PRO:O | 2:B:233:SER:HB2 | 2.03 | 0.58 |
| 6:F:23:LYS:O | 6:F:27:GLN:HG2 | 2.02 | 0.58 |
| 16:P:67:THR:HG22 | 16:P:68:ASP:N | 2.19 | 0.58 |
| 22:X:3:G:H2' | 22:X:4:A:H5' | 1.82 | 0.58 |
| 1:A:1339:A:H2' | 1:A:1340:A:O4' | 2.04 | 0.58 |
| 1:A:427:U:OP1 | 4:D:13:ARG:NH2 | 2.36 | 0.58 |
| 5:E:75:THR:HG23 | 5:E:76:ILE:N | 2.18 | 0.58 |
| 6:F:47:ARG:HA | 6:F:57:GLN:HG2 | 1.84 | 0.58 |
| 9:I:82:ALA:O | 9:I:86:VAL:HG23 | 2.04 | 0.58 |
| 10:J:3:LYS:N | 10:J:3:LYS:HD3 | 2.19 | 0.58 |
| 10:J:32:ALA:HB2 | 10:J:76:ASN:CB | 2.33 | 0.58 |
| 12:L:41:ARG:CG | 12:L:42:THR:H | 2.15 | 0.58 |
| 20:T:37:SER:O | 20:T:41:VAL:HG23 | 2.04 | 0.58 |
| 20:T:83:ARG:HB3 | 20:T:87:LYS:NZ | 2.18 | 0.58 |
| 1:A:1342:C:O2' | 1:A:1343:G:H5' | 2.04 | 0.58 |
| 1:A:179:A:H2' | 1:A:180:U:C6 | 2.38 | 0.58 |
| 1:A:496:A:H4' | 1:A:497:A:O5' | 2.02 | 0.58 |
| 3:C:77:ILE:C | 3:C:83:ARG:HB3 | 2.24 | 0.58 |
| 9:I:5:TYR:O | 9:I:84:ALA:HA | 2.04 | 0.58 |
| 20:T:45:GLN:HB2 | 20:T:91:LEU:HD13 | 1.84 | 0.58 |
| 1:A:353:A:H5' | 1:A:353:A:C8 | 2.39 | 0.58 |
| 10:J:47:PHE:CE2 | 14:N:37:PHE:HE1 | 2.21 | 0.58 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 2.04 | 0.58 |
| 1:A:273:A:H1' | 17:Q:16:GLN:NE2 | 2.19 | 0.58 |
| 1:A:433:C:C6 | 1:A:433:C:H5' | 2.36 | 0.58 |
| 2:B:166:ASP:OD2 | 2:B:169:LYS:HB2 | 2.04 | 0.58 |
| 1:A:939:G:H5'' | 7:G:102:ARG:NH2 | 2.18 | 0.58 |
| 1:A:1250:A:H4' | 9:I:68:GLY:CA | 2.33 | 0.58 |
| 19:S:80:TYR:O | 19:S:82:GLY:N | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1137:C:H4' | 1:A:1138:G:N1 | 2.19 | 0.57 |
| 1:A:1175:G:N1 | 1:A:1176:A:C5 | 2.72 | 0.57 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.38 | 0.57 |
| 1:A:47:C:H5'' | 1:A:365:U:C6 | 2.39 | 0.57 |
| 1:A:706:A:C4' | 11:K:29:ILE:HD11 | 2.33 | 0.57 |
| 1:A:1085:U:H3' | 1:A:1086:U:C5 | 2.39 | 0.57 |
| 1:A:1117:G:N2 | 1:A:1180:A:H1' | 2.18 | 0.57 |
| 1:A:1306:A:N6 | 1:A:1331:G:H1' | 2.19 | 0.57 |
| 1:A:780:A:O2' | 1:A:781:A:H5'' | 2.04 | 0.57 |
| 20:T:59:ALA:O | 20:T:63:ILE:HG13 | 2.05 | 0.57 |
| 3:C:54:ARG:CG | 3:C:55:VAL:N | 2.67 | 0.57 |
| 8:H:112:LEU:HD23 | 8:H:112:LEU:N | 2.19 | 0.57 |
| 2:B:178:ARG:NH1 | 8:H:71:GLY:O | 2.37 | 0.57 |
| 9:I:32:ASP:O | 9:I:35:GLU:HB3 | 2.05 | 0.57 |
| 1:A:1129:C:OP1 | 9:I:62:TYR:OH | 2.14 | 0.57 |
| 1:A:269:C:H2' | 1:A:270:A:C8 | 2.40 | 0.57 |
| 2:B:196:LEU:H | 2:B:196:LEU:CD1 | 2.17 | 0.57 |
| 14:N:24:CYS:SG | 14:N:40:CYS:N | 2.77 | 0.57 |
| 6:F:92:LYS:NZ | 6:F:92:LYS:HB2 | 2.19 | 0.57 |
| 12:L:24:VAL:O | 12:L:26:ALA:N | 2.34 | 0.57 |
| 13:M:108:ARG:NE | 13:M:108:ARG:HA | 2.18 | 0.57 |
| 1:A:1178:G:C2 | 1:A:1180:A:C8 | 2.91 | 0.57 |
| 1:A:1397:C:H4' | 1:A:1398:A:OP2 | 2.03 | 0.57 |
| 1:A:1443:G:C5' | 1:A:1446:A:H3' | 2.34 | 0.57 |
| 1:A:580:U:H2' | 1:A:581:G:O4' | 2.05 | 0.57 |
| 3:C:14:ILE:O | 3:C:16:ARG:N | 2.37 | 0.57 |
| 4:D:173:TRP:CG | 4:D:189:PRO:HG3 | 2.40 | 0.57 |
| 7:G:146:GLU:CG | 7:G:149:ARG:HH21 | 2.14 | 0.57 |
| 7:G:26:PHE:CE2 | 7:G:30:ILE:HD11 | 2.40 | 0.57 |
| 13:M:19:LEU:HA | 13:M:22:ILE:HD13 | 1.87 | 0.57 |
| 13:M:5:ALA:HB3 | 13:M:8:GLU:CG | 2.35 | 0.57 |
| 1:A:1179:A:C2' | 1:A:1180:A:H5' | 2.35 | 0.57 |
| 2:B:114:ARG:HH12 | 2:B:118:LEU:HD21 | 1.69 | 0.57 |
| 3:C:126:ARG:O | 3:C:127:ARG:HB2 | 2.05 | 0.57 |
| 4:D:3:ARG:NE | 4:D:5:ILE:HD11 | 2.20 | 0.57 |
| 7:G:145:ALA:C | 7:G:147:ALA:H | 2.08 | 0.57 |
| 1:A:247:G:OP2 | 17:Q:99:SER:HB2 | 2.04 | 0.57 |
| 1:A:834:C:H2' | 1:A:835:U:H6 | 1.70 | 0.57 |
| 2:B:30:ARG:HD2 | 2:B:31:TYR:CE2 | 2.39 | 0.57 |
| 4:D:62:GLN:HE22 | 4:D:65:ARG:NH1 | 2.03 | 0.57 |
| 4:D:80:GLU:O | 4:D:84:LYS:HG3 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:23:VAL:O | 7:G:27:ILE:HG13 | 2.05 | 0.57 |
| 12:L:119:LYS:O | 12:L:120:TYR:HB2 | 2.05 | 0.57 |
| 15:O:78:TYR:CE1 | 15:O:82:ILE:HD11 | 2.39 | 0.57 |
| 1:A:1190:G:H3' | 3:C:3:ASN:HD22 | 1.69 | 0.57 |
| 1:A:1251:A:H5' | 9:I:12:GLU:OE1 | 2.04 | 0.57 |
| 6:F:45:LEU:HD12 | 6:F:45:LEU:O | 2.05 | 0.57 |
| 18:R:88:LYS:HG2 | 18:R:88:LYS:OXT | 2.03 | 0.57 |
| 1:A:1124:G:H2' | 1:A:1145:C:H5 | 1.69 | 0.57 |
| 1:A:1373:G:H5'' | 7:G:36:LYS:CB | 2.35 | 0.57 |
| 4:D:70:ILE:HG22 | 4:D:75:PHE:HB2 | 1.84 | 0.57 |
| 8:H:83:ILE:O | 8:H:83:ILE:HG23 | 2.05 | 0.57 |
| 1:A:254:G:O2' | 1:A:255:G:H5' | 2.04 | 0.56 |
| 1:A:491:G:H2' | 1:A:492:G:H8 | 1.70 | 0.56 |
| 1:A:877:C:O2' | 1:A:878:G:H5' | 2.05 | 0.56 |
| 2:B:69:LEU:HD22 | 2:B:155:LEU:HD11 | 1.87 | 0.56 |
| 2:B:25:ASN:ND2 | 2:B:25:ASN:C | 2.53 | 0.56 |
| 10:J:57:LYS:HD2 | 10:J:60:ARG:NH2 | 2.19 | 0.56 |
| 1:A:1178:G:N3 | 1:A:1180:A:C8 | 2.73 | 0.56 |
| 1:A:1326:C:H2' | 1:A:1327:C:C6 | 2.40 | 0.56 |
| 1:A:190(D):U:O2' | 1:A:190(E):U:H5' | 2.05 | 0.56 |
| 1:A:757:U:H2' | 1:A:758:G:O4' | 2.05 | 0.56 |
| 5:E:91:LEU:CD2 | 5:E:120:THR:HG22 | 2.34 | 0.56 |
| 6:F:43:LEU:HD12 | 6:F:46:ARG:HD2 | 1.85 | 0.56 |
| 9:I:108:VAL:HG12 | 9:I:109:VAL:N | 2.20 | 0.56 |
| 10:J:32:ALA:HB2 | 10:J:76:ASN:CG | 2.25 | 0.56 |
| 15:O:4:THR:HG1 | 15:O:7:GLU:HG3 | 1.69 | 0.56 |
| 19:S:51:VAL:HG21 | 19:S:71:LEU:HB3 | 1.87 | 0.56 |
| 1:A:1250:A:H2' | 1:A:1251:A:C8 | 2.39 | 0.56 |
| 3:C:130:VAL:HG21 | 3:C:157:ILE:HG23 | 1.87 | 0.56 |
| 13:M:9:ILE:N | 13:M:9:ILE:HD12 | 2.19 | 0.56 |
| 4:D:173:TRP:HB2 | 4:D:187:ARG:O | 2.04 | 0.56 |
| 8:H:121:ASP:O | 8:H:125:ARG:HB2 | 2.05 | 0.56 |
| 13:M:40:ASN:ND2 | 13:M:42:ALA:H | 2.03 | 0.56 |
| 17:Q:4:LYS:HE3 | 17:Q:6:LEU:HD21 | 1.86 | 0.56 |
| 1:A:1024:G:H2' | 1:A:1025:U:O4' | 2.05 | 0.56 |
| 3:C:95:THR:C | 3:C:97:LYS:H | 2.08 | 0.56 |
| 5:E:78:HIS:HD2 | 8:H:107:LEU:HD12 | 1.68 | 0.56 |
| 17:Q:63:ARG:HG2 | 17:Q:64:PRO:HD2 | 1.88 | 0.56 |
| 20:T:76:ALA:O | 20:T:80:ARG:HG3 | 2.06 | 0.56 |
| 2:B:91:PRO:HG2 | 2:B:155:LEU:HG | 1.86 | 0.56 |
| 3:C:172:ARG:HB3 | 3:C:172:ARG:HH11 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:20:GLN:NE2 | 5:E:21:ALA:O | 2.38 | 0.56 |
| 13:M:11:ARG:HG3 | 13:M:11:ARG:NH1 | 2.20 | 0.56 |
| 1:A:953:G:H1' | 13:M:125:ARG:CB | 2.34 | 0.56 |
| 17:Q:67:LYS:HA | 17:Q:70:ARG:NH1 | 2.13 | 0.56 |
| 1:A:1161:C:O2 | 1:A:1161:C:H2' | 2.05 | 0.56 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.53 | 0.56 |
| 1:A:547:A:H4' | 1:A:548:G:O5' | 2.05 | 0.56 |
| 1:A:818:G:H3' | 1:A:819:A:C5' | 2.36 | 0.56 |
| 1:A:973:G:H3' | 1:A:974:A:H5'' | 1.88 | 0.56 |
| 2:B:75:LYS:HA | 2:B:78:GLN:HB2 | 1.86 | 0.56 |
| 3:C:58:GLU:HB2 | 3:C:65:ALA:HB2 | 1.86 | 0.56 |
| 19:S:19:VAL:HG13 | 19:S:20:LEU:N | 2.20 | 0.56 |
| 21:U:14:TRP:CZ3 | 21:U:15:ARG:HD2 | 2.41 | 0.56 |
| 1:A:99:C:H2' | 1:A:101:A:C8 | 2.41 | 0.56 |
| 1:A:977:A:H2' | 1:A:978:A:H5' | 1.87 | 0.56 |
| 2:B:14:GLY:C | 2:B:15:VAL:HG22 | 2.26 | 0.56 |
| 6:F:13:ASN:O | 6:F:14:LEU:HD12 | 2.05 | 0.56 |
| 1:A:1034:G:N2 | 1:A:1035:A:H62 | 2.03 | 0.56 |
| 1:A:1347:G:H22 | 1:A:1373:G:H2' | 1.69 | 0.56 |
| 2:B:51:LEU:HD22 | 2:B:55:PHE:CE1 | 2.39 | 0.56 |
| 4:D:128:VAL:HG12 | 4:D:129:ASN:ND2 | 2.21 | 0.56 |
| 4:D:8:VAL:HB | 4:D:21:LEU:HD13 | 1.88 | 0.56 |
| 5:E:79:GLU:HG3 | 5:E:93:PRO:CD | 2.26 | 0.56 |
| 8:H:119:LEU:HD12 | 8:H:124:ALA:CA | 2.35 | 0.56 |
| 1:A:1228:C:OP1 | 13:M:115:LYS:HE3 | 2.05 | 0.56 |
| 20:T:99:LEU:O | 20:T:101:GLY:N | 2.39 | 0.56 |
| 2:B:54:THR:O | 2:B:57:PHE:HB3 | 2.06 | 0.56 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HG21 | 1.86 | 0.56 |
| 11:K:32:ILE:CD1 | 11:K:68:ALA:HB1 | 2.36 | 0.56 |
| 14:N:22:THR:HB | 14:N:33:VAL:CG2 | 2.34 | 0.56 |
| 9:I:111:ARG:HD2 | 14:N:61:TRP:OXT | 2.05 | 0.56 |
| 20:T:72:LEU:O | 20:T:73:HIS:O | 2.23 | 0.56 |
| 1:A:328:C:O2 | 1:A:328:C:C2' | 2.54 | 0.56 |
| 3:C:102:ASN:N | 3:C:102:ASN:ND2 | 2.52 | 0.56 |
| 4:D:189:PRO:CB | 4:D:194:LEU:HD21 | 2.35 | 0.56 |
| 12:L:55:VAL:CG1 | 12:L:56:ALA:H | 2.13 | 0.56 |
| 3:C:52:LEU:H | 3:C:52:LEU:HD23 | 1.69 | 0.55 |
| 7:G:65:ALA:O | 7:G:69:VAL:HG23 | 2.07 | 0.55 |
| 10:J:3:LYS:O | 10:J:101:VAL:N | 2.39 | 0.55 |
| 1:A:1020:U:H2' | 1:A:1021:G:H8 | 1.70 | 0.55 |
| 1:A:1053:G:C3' | 1:A:1054:C:H5' | 2.35 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1156:G:C3' | 1:A:1157:A:OP2 | 2.49 | 0.55 |
| 1:A:1288:A:H2' | 1:A:1289:A:C8 | 2.42 | 0.55 |
| 3:C:34:LEU:HG | 14:N:25:VAL:HG21 | 1.89 | 0.55 |
| 3:C:3:ASN:O | 3:C:4:LYS:HB2 | 2.06 | 0.55 |
| 6:F:39:LYS:HB3 | 6:F:64:GLN:HB3 | 1.87 | 0.55 |
| 10:J:34:VAL:HG13 | 10:J:74:ILE:HG12 | 1.88 | 0.55 |
| 14:N:8:GLU:O | 14:N:11:LYS:HB2 | 2.07 | 0.55 |
| 1:A:983:A:HO2' | 1:A:1049:U:HO2' | 1.54 | 0.55 |
| 1:A:1498:U:H4' | 1:A:1519:A:C2 | 2.41 | 0.55 |
| 1:A:1499:A:H1' | 1:A:1520:G:H5' | 1.88 | 0.55 |
| 1:A:371:G:C2' | 1:A:372:C:H5' | 2.35 | 0.55 |
| 1:A:730:G:N2 | 1:A:765:G:H5'' | 2.21 | 0.55 |
| 2:B:187:LEU:HD21 | 2:B:204:ASN:H | 1.71 | 0.55 |
| 3:C:70:VAL:O | 3:C:106:VAL:HG23 | 2.05 | 0.55 |
| 4:D:20:TYR:HD2 | 4:D:26:CYS:HB3 | 1.71 | 0.55 |
| 5:E:51:VAL:O | 5:E:54:ALA:HB3 | 2.06 | 0.55 |
| 11:K:104:GLN:OE1 | 11:K:106:LYS:HD3 | 2.06 | 0.55 |
| 1:A:1125:U:H5' | 1:A:1126:U:H5 | 1.72 | 0.55 |
| 1:A:629:G:H2' | 1:A:630:G:C4' | 2.36 | 0.55 |
| 7:G:38:LEU:HD12 | 7:G:38:LEU:O | 2.06 | 0.55 |
| 7:G:80:VAL:HG21 | 7:G:154:TYR:CE1 | 2.42 | 0.55 |
| 11:K:40:ILE:HG22 | 11:K:41:THR:HG23 | 1.88 | 0.55 |
| 18:R:53:ARG:HA | 18:R:56:THR:OG1 | 2.07 | 0.55 |
| 1:A:1053:G:H3' | 1:A:1054:C:H5' | 1.88 | 0.55 |
| 1:A:1208:C:H2' | 1:A:1209:C:C6 | 2.42 | 0.55 |
| 3:C:147:LYS:HD3 | 3:C:205:GLY:H | 1.72 | 0.55 |
| 8:H:20:TYR:CE1 | 8:H:76:PRO:HG2 | 2.41 | 0.55 |
| 10:J:7:LYS:HB3 | 10:J:97:GLU:HB2 | 1.88 | 0.55 |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:HA | 1.89 | 0.55 |
| 12:L:27:LEU:HG | 12:L:28:LYS:H | 1.70 | 0.55 |
| 1:A:1318:A:H1' | 19:S:37:ARG:NH1 | 2.22 | 0.55 |
| 1:A:1333:A:H2' | 1:A:1334:G:O4' | 2.06 | 0.55 |
| 1:A:190(L):U:C2 | 20:T:105:SER:HB2 | 2.41 | 0.55 |
| 1:A:287:U:O2' | 1:A:288:A:H5' | 2.05 | 0.55 |
| 2:B:204:ASN:C | 2:B:204:ASN:ND2 | 2.58 | 0.55 |
| 2:B:224:GLN:O | 2:B:224:GLN:HG2 | 2.06 | 0.55 |
| 4:D:2:GLY:O | 4:D:3:ARG:O | 2.25 | 0.55 |
| 1:A:974:A:OP2 | 14:N:41:ARG:NH1 | 2.39 | 0.55 |
| 1:A:337:C:H2' | 1:A:338:A:C8 | 2.42 | 0.55 |
| 1:A:629:G:H2' | 1:A:630:G:C5' | 2.35 | 0.55 |
| 1:A:750:G:N3 | 15:O:23:GLY:HA3 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:828:A:H2' | 1:A:829:G:O4' | 2.07 | 0.55 |
| 1:A:969:A:H61 | 13:M:126:LYS:HB2 | 1.72 | 0.55 |
| 2:B:8:LYS:N | 2:B:8:LYS:HD3 | 2.21 | 0.55 |
| 1:A:620:C:N1 | 4:D:135:LEU:HD13 | 2.22 | 0.55 |
| 5:E:147:ASP:OD1 | 5:E:147:ASP:N | 2.33 | 0.55 |
| 11:K:87:THR:HA | 11:K:91:ARG:HH21 | 1.72 | 0.55 |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:CB | 2.37 | 0.55 |
| 18:R:52:PRO:O | 18:R:56:THR:HG23 | 2.06 | 0.55 |
| 21:U:14:TRP:HZ3 | 21:U:15:ARG:HD2 | 1.72 | 0.55 |
| 1:A:915:A:H2' | 1:A:916:G:H5' | 1.89 | 0.55 |
| 3:C:39:ILE:HG22 | 3:C:40:ARG:N | 2.22 | 0.55 |
| 15:O:77:ARG:O | 15:O:80:ALA:HB3 | 2.07 | 0.55 |
| 1:A:457:C:H2' | 1:A:458:C:C6 | 2.41 | 0.55 |
| 1:A:940:C:H2' | 1:A:941:G:C8 | 2.42 | 0.55 |
| 2:B:122:PHE:O | 2:B:123:ALA:HB2 | 2.07 | 0.55 |
| 10:J:94:VAL:HG12 | 10:J:95:GLU:N | 2.22 | 0.55 |
| 12:L:83:VAL:CG2 | 12:L:100:ILE:HG23 | 2.36 | 0.55 |
| 20:T:53:LEU:HB2 | 20:T:100:ILE:HG21 | 1.88 | 0.55 |
| 1:A:1015:A:H2' | 1:A:1016:A:C8 | 2.42 | 0.55 |
| 1:A:411:A:O2' | 1:A:412:A:H5' | 2.07 | 0.55 |
| 2:B:139:LYS:C | 2:B:139:LYS:HD3 | 2.27 | 0.55 |
| 2:B:21:ARG:O | 2:B:39:ILE:HA | 2.07 | 0.55 |
| 2:B:85:ALA:HB3 | 2:B:92:TYR:HD2 | 1.72 | 0.55 |
| 3:C:8:ILE:HG23 | 3:C:16:ARG:HG2 | 1.88 | 0.55 |
| 16:P:26:ARG:NH2 | 16:P:31:LYS:NZ | 2.55 | 0.55 |
| 1:A:1007:C:H42 | 1:A:1022:G:H1 | 1.56 | 0.54 |
| 1:A:1152:A:H2' | 1:A:1153:C:H6 | 1.72 | 0.54 |
| 2:B:14:GLY:O | 2:B:15:VAL:HG13 | 2.07 | 0.54 |
| 3:C:20:SER:O | 14:N:54:PRO:HB3 | 2.06 | 0.54 |
| 1:A:404:U:H5' | 4:D:122:ARG:HD2 | 1.87 | 0.54 |
| 5:E:12:LEU:CD1 | 5:E:31:LEU:HB2 | 2.37 | 0.54 |
| 6:F:19:LEU:HD23 | 6:F:19:LEU:C | 2.28 | 0.54 |
| 13:M:11:ARG:HD3 | 13:M:12:ASN:N | 2.22 | 0.54 |
| 13:M:37:THR:HG23 | 13:M:55:ARG:CD | 2.34 | 0.54 |
| 16:P:43:LYS:HB3 | 16:P:48:TRP:CG | 2.42 | 0.54 |
| 1:A:1443:G:H5'' | 1:A:1446:A:H3' | 1.88 | 0.54 |
| 1:A:411:A:O2' | 1:A:413:G:H5' | 2.06 | 0.54 |
| 1:A:415:A:H2' | 1:A:416:G:C8 | 2.42 | 0.54 |
| 1:A:528:C:H5' | 1:A:535:A:C6 | 2.43 | 0.54 |
| 6:F:100:ASN:HD22 | 18:R:23:LYS:CG | 2.20 | 0.54 |
| 7:G:82:GLY:O | 7:G:83:ALA:HB2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:41:ARG:NH2 | 12:L:57:LYS:NZ | 2.56 | 0.54 |
| 1:A:1123:A:H2 | 10:J:39:PRO:HG2 | 1.72 | 0.54 |
| 1:A:1232:U:P | 9:I:124:GLN:HE21 | 2.30 | 0.54 |
| 1:A:357:G:O2' | 1:A:358:U:H5' | 2.07 | 0.54 |
| 2:B:162:ILE:HG22 | 2:B:164:VAL:HG23 | 1.88 | 0.54 |
| 2:B:22:LYS:HG3 | 2:B:35:GLU:OE2 | 2.08 | 0.54 |
| 7:G:20:ASP:OD2 | 7:G:22:LEU:HB3 | 2.07 | 0.54 |
| 19:S:33:THR:HG22 | 19:S:34:TRP:N | 2.22 | 0.54 |
| 1:A:959:A:C2 | 1:A:1222:G:O4' | 2.60 | 0.54 |
| 1:A:1230:C:O2' | 1:A:1231:G:H5' | 2.08 | 0.54 |
| 1:A:629:G:C2' | 1:A:630:G:H5'' | 2.36 | 0.54 |
| 2:B:55:PHE:HE2 | 2:B:218:ALA:HA | 1.72 | 0.54 |
| 2:B:73:THR:HG23 | 2:B:95:GLN:O | 2.07 | 0.54 |
| 4:D:127:THR:CG2 | 4:D:147:ALA:HB3 | 2.37 | 0.54 |
| 12:L:115:LYS:O | 12:L:117:ARG:N | 2.38 | 0.54 |
| 17:Q:75:ARG:HG3 | 17:Q:75:ARG:HH11 | 1.72 | 0.54 |
| 1:A:1175:G:C5 | 1:A:1176:A:N7 | 2.76 | 0.54 |
| 1:A:755:G:OP2 | 15:O:65:ARG:HD2 | 2.08 | 0.54 |
| 1:A:840:C:H4' | 1:A:848:C:O2 | 2.08 | 0.54 |
| 5:E:148:VAL:O | 5:E:152:ARG:HG3 | 2.07 | 0.54 |
| 5:E:80:ILE:HD11 | 5:E:91:LEU:HD12 | 1.89 | 0.54 |
| 6:F:36:ARG:NH2 | 6:F:38:GLU:HG2 | 2.22 | 0.54 |
| 10:J:22:LYS:HB2 | 10:J:22:LYS:NZ | 2.22 | 0.54 |
| 12:L:27:LEU:C | 12:L:29:GLY:N | 2.60 | 0.54 |
| 13:M:37:THR:O | 13:M:37:THR:HG22 | 2.08 | 0.54 |
| 1:A:1112:C:C4 | 3:C:178:LEU:HD23 | 2.43 | 0.54 |
| 1:A:149:A:H2' | 1:A:150:C:C6 | 2.42 | 0.54 |
| 2:B:229:VAL:O | 2:B:229:VAL:HG12 | 2.08 | 0.54 |
| 2:B:82:ARG:O | 2:B:86:GLU:HG3 | 2.08 | 0.54 |
| 6:F:33:TYR:HA | 6:F:71:ARG:CZ | 2.37 | 0.54 |
| 1:A:1532:U:O2' | 1:A:1533:C:H6 | 1.90 | 0.54 |
| 1:A:666:G:H5' | 1:A:726:C:H1' | 1.90 | 0.54 |
| 1:A:738:C:H5'' | 6:F:69:GLU:HB3 | 1.90 | 0.54 |
| 2:B:74:LYS:NZ | 2:B:206:ASP:HB2 | 2.21 | 0.54 |
| 3:C:25:GLY:O | 3:C:27:LYS:N | 2.40 | 0.54 |
| 5:E:121:LYS:HD2 | 5:E:122:GLU:H | 1.71 | 0.54 |
| 6:F:23:LYS:NZ | 6:F:42:GLU:OE2 | 2.39 | 0.54 |
| 7:G:143:ARG:O | 7:G:147:ALA:HB2 | 2.08 | 0.54 |
| 10:J:90:LEU:N | 10:J:91:PRO:HD2 | 2.23 | 0.54 |
| 17:Q:40:LYS:HG2 | 17:Q:42:TYR:CE1 | 2.43 | 0.54 |
| 20:T:86:ARG:HH11 | 20:T:86:ARG:HG3 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:1419:G:O2' | 1:A:1420:C:H5' | 2.08 | 0.54 |
| 1:A:421:U:H5' | 1:A:422:C:H5 | 1.73 | 0.54 |
| 11:K:57:THR:HG22 | 11:K:59:TYR:N | 2.18 | 0.54 |
| 17:Q:67:LYS:O | 17:Q:68:ARG:HB3 | 2.08 | 0.54 |
| 1:A:1001:A:H2' | 1:A:1002:G:H8 | 1.72 | 0.54 |
| 1:A:1035:A:H2' | 1:A:1036:G:C8 | 2.33 | 0.54 |
| 1:A:1060:C:O2 | 1:A:1198:G:C2 | 2.60 | 0.54 |
| 1:A:1179:A:N1 | 1:A:1180:A:C2 | 2.74 | 0.54 |
| 1:A:1277:C:O2' | 1:A:1279:A:H8 | 1.91 | 0.54 |
| 1:A:1498:U:H4' | 1:A:1519:A:H2 | 1.73 | 0.54 |
| 1:A:245:C:O2 | 1:A:283:C:N3 | 2.40 | 0.54 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.42 | 0.54 |
| 8:H:6:ILE:O | 8:H:10:LEU:HG | 2.08 | 0.54 |
| 1:A:1123:A:C2 | 10:J:39:PRO:HG2 | 2.42 | 0.54 |
| 16:P:20:VAL:CG1 | 16:P:21:VAL:N | 2.70 | 0.54 |
| 1:A:1002:G:H2' | 1:A:1003:G:C8 | 2.43 | 0.54 |
| 1:A:1091:U:O2 | 1:A:1093:A:H8 | 1.90 | 0.54 |
| 1:A:1179:A:C2' | 1:A:1180:A:C5' | 2.86 | 0.54 |
| 1:A:1211:U:H5' | 1:A:1212:U:OP1 | 2.08 | 0.54 |
| 1:A:392:G:H2' | 1:A:393:A:C8 | 2.43 | 0.54 |
| 3:C:188:LEU:O | 3:C:189:ALA:CB | 2.56 | 0.54 |
| 3:C:88:ARG:HG2 | 3:C:101:LEU:CD1 | 2.34 | 0.54 |
| 5:E:10:MET:O | 5:E:10:MET:HG3 | 2.08 | 0.54 |
| 1:A:1346:A:C4 | 7:G:10:ARG:NH2 | 2.76 | 0.54 |
| 19:S:80:TYR:CZ | 19:S:81:ARG:HB3 | 2.43 | 0.54 |
| 3:C:11:ARG:O | 3:C:14:ILE:O | 2.26 | 0.53 |
| 9:I:10:ARG:HG2 | 9:I:75:ASP:HB2 | 1.90 | 0.53 |
| 1:A:1005:A:H2' | 1:A:1006:C:H5' | 1.90 | 0.53 |
| 1:A:1091:U:O2 | 1:A:1093:A:C8 | 2.61 | 0.53 |
| 1:A:911:U:H2' | 1:A:912:C:C6 | 2.43 | 0.53 |
| 2:B:75:LYS:HD3 | 2:B:78:GLN:OE1 | 2.08 | 0.53 |
| 4:D:173:TRP:CD2 | 4:D:189:PRO:HG3 | 2.42 | 0.53 |
| 16:P:8:ARG:HH11 | 16:P:8:ARG:HG2 | 1.72 | 0.53 |
| 6:F:50:TYR:CE1 | 18:R:77:GLY:HA2 | 2.43 | 0.53 |
| 19:S:80:TYR:CG | 19:S:81:ARG:N | 2.76 | 0.53 |
| 1:A:1001:A:H2' | 1:A:1002:G:C8 | 2.44 | 0.53 |
| 1:A:433:C:C5' | 1:A:433:C:C6 | 2.87 | 0.53 |
| 1:A:984:C:H2' | 1:A:985:C:C6 | 2.42 | 0.53 |
| 2:B:172:ILE:H | 2:B:172:ILE:CD1 | 2.19 | 0.53 |
| 6:F:92:LYS:HZ2 | 6:F:92:LYS:HB2 | 1.73 | 0.53 |
| 15:O:33:THR:HG23 | 15:O:63:ARG:NH1 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:R:37:VAL:O | 18:R:41:LYS:HB2 | 2.08 | 0.53 |
| 6:F:60:PHE:CE2 | 18:R:78:LEU:HD21 | 2.44 | 0.53 |
| 1:A:1001:A:H2 | 1:A:1040:U:H3 | 1.54 | 0.53 |
| 10:J:22:LYS:C | 10:J:24:VAL:H | 2.12 | 0.53 |
| 11:K:99:GLN:HG2 | 11:K:105:VAL:HG21 | 1.90 | 0.53 |
| 1:A:235:C:C5' | 17:Q:70:ARG:HG2 | 2.35 | 0.53 |
| 19:S:39:THR:HG22 | 19:S:40:ILE:N | 2.23 | 0.53 |
| 1:A:1024:G:C3' | 1:A:1025:U:H5'' | 2.38 | 0.53 |
| 1:A:1229:A:O2' | 13:M:125:ARG:NE | 2.41 | 0.53 |
| 1:A:432:A:H3' | 1:A:433:C:C5' | 2.31 | 0.53 |
| 3:C:110:ASN:HD22 | 3:C:140:ARG:HB3 | 1.74 | 0.53 |
| 6:F:27:GLN:NE2 | 6:F:27:GLN:HA | 2.23 | 0.53 |
| 1:A:1373:G:C5' | 7:G:36:LYS:HB2 | 2.37 | 0.53 |
| 11:K:47:VAL:HG12 | 11:K:48:ILE:HD13 | 1.90 | 0.53 |
| 14:N:14:PRO:O | 14:N:15:LYS:CB | 2.56 | 0.53 |
| 16:P:10:GLY:HA3 | 16:P:14:ASN:O | 2.09 | 0.53 |
| 1:A:1262:C:O2' | 1:A:1263:C:H5' | 2.09 | 0.53 |
| 1:A:413:G:O6 | 4:D:35:ARG:HG3 | 2.08 | 0.53 |
| 2:B:122:PHE:CE2 | 2:B:139:LYS:HG2 | 2.43 | 0.53 |
| 4:D:165:MET:HA | 4:D:168:ARG:HG3 | 1.90 | 0.53 |
| 5:E:99:GLY:O | 5:E:117:ASP:HA | 2.08 | 0.53 |
| 2:B:178:ARG:HH21 | 8:H:68:ARG:HH22 | 1.54 | 0.53 |
| 9:I:17:VAL:HG11 | 9:I:81:ILE:N | 2.24 | 0.53 |
| 10:J:39:PRO:O | 10:J:69:ASN:O | 2.25 | 0.53 |
| 11:K:33:THR:HG22 | 11:K:39:PRO:CA | 2.37 | 0.53 |
| 1:A:192:U:C1' | 20:T:103:GLY:HA2 | 2.38 | 0.53 |
| 1:A:1121:U:H2' | 1:A:1122:U:C6 | 2.42 | 0.53 |
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.44 | 0.53 |
| 2:B:25:ASN:HD22 | 2:B:26:PRO:N | 2.06 | 0.53 |
| 4:D:18:LYS:HD3 | 4:D:20:TYR:CE2 | 2.44 | 0.53 |
| 9:I:14:VAL:HG22 | 9:I:66:ARG:O | 2.09 | 0.53 |
| 13:M:73:GLU:O | 13:M:76:ALA:HB3 | 2.09 | 0.53 |
| 14:N:36:PHE:O | 14:N:36:PHE:CD1 | 2.61 | 0.53 |
| 14:N:37:PHE:CE2 | 14:N:53:LEU:HD13 | 2.44 | 0.53 |
| 15:O:36:ILE:HA | 15:O:59:MET:HE3 | 1.91 | 0.53 |
| 1:A:192:U:H1' | 20:T:103:GLY:HA2 | 1.91 | 0.53 |
| 1:A:1330:U:OP1 | 13:M:23:TYR:O | 2.26 | 0.53 |
| 2:B:178:ARG:NH2 | 8:H:68:ARG:NH2 | 2.54 | 0.53 |
| 1:A:1232:U:OP1 | 9:I:124:GLN:HG2 | 2.08 | 0.53 |
| 16:P:34:GLU:OE2 | 16:P:55:ARG:HD3 | 2.08 | 0.53 |
| 17:Q:27:PHE:HB2 | 17:Q:28:PRO:HD2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1179:A:H2' | 1:A:1180:A:C5' | 2.39 | 0.53 |
| 1:A:1347:G:C2' | 1:A:1348:U:OP2 | 2.56 | 0.53 |
| 10:J:46:ARG:HH11 | 10:J:64:GLU:HB3 | 1.74 | 0.53 |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:HD2 | 1.72 | 0.53 |
| 10:J:49:VAL:HG21 | 14:N:41:ARG:O | 2.08 | 0.53 |
| 17:Q:75:ARG:NH1 | 17:Q:75:ARG:HG3 | 2.23 | 0.53 |
| 1:A:1347:G:O2' | 1:A:1348:U:OP2 | 2.27 | 0.53 |
| 1:A:730:G:H21 | 1:A:765:G:H5'' | 1.74 | 0.53 |
| 2:B:91:PRO:HG3 | 2:B:154:LEU:CB | 2.35 | 0.53 |
| 4:D:151:LYS:H | 4:D:151:LYS:CD | 2.22 | 0.53 |
| 1:A:761:G:O2' | 17:Q:105:ALA:HB2 | 2.09 | 0.53 |
| 1:A:1130:A:N9 | 1:A:1146:A:C2 | 2.76 | 0.52 |
| 1:A:475:G:H2' | 1:A:476:G:H8 | 1.74 | 0.52 |
| 2:B:209:ARG:HG2 | 2:B:239:VAL:HG13 | 1.91 | 0.52 |
| 3:C:155:GLY:CA | 3:C:164:ARG:H | 2.21 | 0.52 |
| 6:F:46:ARG:CA | 6:F:47:ARG:HH21 | 2.22 | 0.52 |
| 8:H:113:SER:HB2 | 8:H:134:ILE:HD11 | 1.90 | 0.52 |
| 10:J:90:LEU:H | 10:J:91:PRO:CD | 2.20 | 0.52 |
| 11:K:15:ALA:HA | 11:K:77:MET:HA | 1.90 | 0.52 |
| 1:A:166:G:H2' | 1:A:167:G:H8 | 1.74 | 0.52 |
| 1:A:269:C:H2' | 1:A:270:A:H8 | 1.75 | 0.52 |
| 3:C:107:GLN:NE2 | 3:C:107:GLN:H | 2.06 | 0.52 |
| 15:O:5:LYS:HD2 | 15:O:5:LYS:H | 1.73 | 0.52 |
| 16:P:20:VAL:HG13 | 16:P:32:TYR:HB2 | 1.92 | 0.52 |
| 6:F:94:GLN:NE2 | 18:R:32:ARG:HD3 | 2.24 | 0.52 |
| 22:X:3:G:H22 | 23:Y:34:TM2:C2 | 2.21 | 0.52 |
| 1:A:1179:A:N1 | 1:A:1180:A:N3 | 2.57 | 0.52 |
| 1:A:976:G:H5' | 1:A:1358:U:O2' | 2.09 | 0.52 |
| 1:A:1390:U:H2' | 1:A:1391:U:C6 | 2.44 | 0.52 |
| 2:B:78:GLN:O | 2:B:94:ASN:OD1 | 2.28 | 0.52 |
| 3:C:108:ASN:ND2 | 3:C:111:LEU:HG | 2.24 | 0.52 |
| 5:E:96:PRO:HA | 5:E:117:ASP:OD2 | 2.10 | 0.52 |
| 17:Q:40:LYS:HE3 | 17:Q:42:TYR:OH | 2.09 | 0.52 |
| 1:A:942:G:O2' | 1:A:943:U:H5' | 2.10 | 0.52 |
| 2:B:8:LYS:HE2 | 2:B:9:GLU:N | 2.20 | 0.52 |
| 3:C:134:ILE:HG22 | 3:C:168:ALA:HB3 | 1.90 | 0.52 |
| 5:E:92:LYS:HB3 | 5:E:119:LEU:HB2 | 1.90 | 0.52 |
| 5:E:121:LYS:HD2 | 5:E:122:GLU:N | 2.24 | 0.52 |
| 5:E:126:ARG:HG3 | 5:E:126:ARG:HH11 | 1.74 | 0.52 |
| 6:F:27:GLN:HE21 | 6:F:27:GLN:HA | 1.74 | 0.52 |
| 11:K:95:ILE:CG2 | 11:K:108:ILE:HD13 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:24:VAL:HG12 | 12:L:26:ALA:CB | 2.39 | 0.52 |
| 13:M:49:THR:HB | 13:M:52:GLU:HG3 | 1.90 | 0.52 |
| 20:T:67:ALA:HA | 20:T:73:HIS:N | 2.23 | 0.52 |
| 1:A:1048:G:H5'' | 14:N:3:ARG:HG3 | 1.92 | 0.52 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:CB | 2.40 | 0.52 |
| 1:A:490:G:H2' | 1:A:491:G:C8 | 2.44 | 0.52 |
| 3:C:127:ARG:HH11 | 3:C:127:ARG:HG3 | 1.73 | 0.52 |
| 6:F:22:GLU:HA | 6:F:22:GLU:OE2 | 2.09 | 0.52 |
| 9:I:9:ARG:HG2 | 9:I:14:VAL:HG12 | 1.91 | 0.52 |
| 10:J:30:SER:OG | 10:J:81:THR:HA | 2.09 | 0.52 |
| 12:L:41:ARG:HH22 | 12:L:57:LYS:NZ | 2.08 | 0.52 |
| 12:L:55:VAL:CG1 | 12:L:56:ALA:N | 2.73 | 0.52 |
| 14:N:29:ARG:HH11 | 14:N:29:ARG:HG2 | 1.75 | 0.52 |
| 1:A:1056:U:O2' | 1:A:1057:G:H5' | 2.10 | 0.52 |
| 1:A:157:G:O2' | 1:A:158:G:H5' | 2.08 | 0.52 |
| 1:A:382:A:H2' | 1:A:383:A:H8 | 1.71 | 0.52 |
| 2:B:33:TYR:HB2 | 2:B:43:ASP:HA | 1.90 | 0.52 |
| 3:C:137:ALA:HA | 3:C:140:ARG:HE | 1.75 | 0.52 |
| 13:M:22:ILE:HD12 | 13:M:22:ILE:N | 2.24 | 0.52 |
| 1:A:1130:A:C5 | 1:A:1146:A:C6 | 2.97 | 0.52 |
| 1:A:370:C:C2' | 1:A:371:G:H5' | 2.39 | 0.52 |
| 3:C:79:ARG:HG2 | 3:C:82:GLU:CG | 2.40 | 0.52 |
| 4:D:117:ALA:O | 4:D:121:VAL:HG23 | 2.09 | 0.52 |
| 4:D:148:VAL:HG11 | 4:D:158:ILE:HD13 | 1.92 | 0.52 |
| 10:J:28:ARG:HH11 | 10:J:28:ARG:HG2 | 1.74 | 0.52 |
| 1:A:1042:G:O2' | 1:A:1043:C:H5' | 2.09 | 0.52 |
| 1:A:1069:C:O2' | 1:A:1192:C:H1' | 2.10 | 0.52 |
| 1:A:961:U:C2' | 1:A:962:C:H5' | 2.40 | 0.52 |
| 2:B:156:LYS:O | 2:B:156:LYS:HG2 | 2.10 | 0.52 |
| 2:B:97:TRP:CH2 | 2:B:176:GLU:CD | 2.82 | 0.52 |
| 2:B:22:LYS:HE3 | 2:B:35:GLU:OE2 | 2.10 | 0.52 |
| 3:C:157:ILE:HG21 | 3:C:164:ARG:NH2 | 2.24 | 0.52 |
| 4:D:127:THR:HG23 | 4:D:147:ALA:HB3 | 1.92 | 0.52 |
| 8:H:84:ARG:O | 8:H:135:CYS:HB2 | 2.10 | 0.52 |
| 9:I:102:LEU:HD12 | 9:I:103:THR:H | 1.74 | 0.52 |
| 11:K:13:GLN:HA | 11:K:75:TYR:O | 2.09 | 0.52 |
| 16:P:75:ARG:HH11 | 16:P:75:ARG:HG3 | 1.74 | 0.52 |
| 1:A:1161:C:H2' | 1:A:1162:C:H5 | 1.71 | 0.52 |
| 1:A:26:A:H61 | 1:A:558:G:H1' | 1.75 | 0.52 |
| 1:A:818:G:C3' | 1:A:819:A:C5' | 2.88 | 0.52 |
| 2:B:103:THR:OG1 | 2:B:176:GLU:HB2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:70:ILE:HD11 | 4:D:100:ARG:CZ | 2.40 | 0.52 |
| 5:E:81:GLU:HG2 | 5:E:88:LYS:HE2 | 1.92 | 0.52 |
| 1:A:1003(A):G:C2' | 1:A:1004:A:H4' | 2.37 | 0.52 |
| 1:A:1124:G:HO2' | 1:A:1145:C:N4 | 2.08 | 0.52 |
| 1:A:1124:G:H2' | 1:A:1145:C:C5 | 2.45 | 0.52 |
| 1:A:1390:U:H2' | 1:A:1391:U:H6 | 1.75 | 0.52 |
| 1:A:417:C:O2' | 1:A:418:C:H5' | 2.10 | 0.52 |
| 6:F:45:LEU:HA | 6:F:58:GLY:O | 2.10 | 0.52 |
| 7:G:79:ARG:NH1 | 7:G:82:GLY:H | 2.05 | 0.52 |
| 10:J:30:SER:HA | 10:J:80:LYS:HG3 | 1.91 | 0.52 |
| 15:O:25:THR:HG21 | 15:O:70:LEU:HG | 1.92 | 0.52 |
| 1:A:791:G:C6 | 1:A:792:A:N7 | 2.77 | 0.51 |
| 5:E:33:VAL:HG11 | 5:E:109:ILE:HA | 1.93 | 0.51 |
| 10:J:46:ARG:HH12 | 10:J:64:GLU:HB3 | 1.71 | 0.51 |
| 13:M:102:ARG:HH11 | 13:M:102:ARG:HB2 | 1.75 | 0.51 |
| 1:A:1160:G:C6 | 1:A:1181:G:O6 | 2.63 | 0.51 |
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 2.09 | 0.51 |
| 1:A:46:G:O2' | 1:A:365:U:H1' | 2.10 | 0.51 |
| 9:I:107:ARG:HH11 | 9:I:107:ARG:HG2 | 1.75 | 0.51 |
| 15:O:10:LYS:HD2 | 15:O:10:LYS:O | 2.10 | 0.51 |
| 1:A:267:C:OP2 | 17:Q:67:LYS:HD2 | 2.11 | 0.51 |
| 19:S:3:ARG:O | 19:S:4:SER:HB3 | 2.10 | 0.51 |
| 20:T:50:GLU:HB2 | 20:T:99:LEU:HD12 | 1.92 | 0.51 |
| 22:X:2:U:H2' | 22:X:3:G:C8 | 2.45 | 0.51 |
| 23:Y:34:TM2:O2' | 23:Y:35:A:P | 2.68 | 0.51 |
| 1:A:1300:G:O2' | 1:A:1301:U:P | 2.68 | 0.51 |
| 1:A:131:C:H2' | 1:A:132:C:C6 | 2.45 | 0.51 |
| 1:A:1372:U:H2' | 1:A:1373:G:O4' | 2.11 | 0.51 |
| 1:A:662:G:H2' | 1:A:663:A:C8 | 2.45 | 0.51 |
| 5:E:101:ILE:HD12 | 5:E:119:LEU:HD23 | 1.92 | 0.51 |
| 16:P:43:LYS:HA | 16:P:48:TRP:CB | 2.40 | 0.51 |
| 1:A:1113:C:O2' | 1:A:1114:C:H5' | 2.08 | 0.51 |
| 1:A:1221:G:O2' | 1:A:1222:G:H5' | 2.09 | 0.51 |
| 2:B:111:ARG:HB3 | 2:B:149:LEU:HD11 | 1.91 | 0.51 |
| 2:B:60:ASP:CB | 2:B:64:ARG:HH12 | 2.10 | 0.51 |
| 3:C:100:ALA:O | 3:C:101:LEU:HB2 | 2.10 | 0.51 |
| 5:E:126:ARG:HG3 | 5:E:126:ARG:NH1 | 2.26 | 0.51 |
| 7:G:135:VAL:O | 7:G:139:GLU:HG3 | 2.10 | 0.51 |
| 1:A:1060:C:O2' | 1:A:1061:G:H5' | 2.10 | 0.51 |
| 1:A:1343:G:H1' | 9:I:121:ARG:NH1 | 2.23 | 0.51 |
| 1:A:532:A:O2' | 1:A:533:A:P | 2.69 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:736:C:OP2 | 18:R:68:LYS:HE2 | 2.11 | 0.51 |
| 1:A:860:A:H2' | 1:A:861:G:O4' | 2.11 | 0.51 |
| 2:B:92:TYR:C | 2:B:92:TYR:CD1 | 2.84 | 0.51 |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:CD1 | 2.40 | 0.51 |
| 1:A:1020:U:H2' | 1:A:1021:G:C8 | 2.45 | 0.51 |
| 1:A:1381:U:O2' | 1:A:1382:C:H5' | 2.11 | 0.51 |
| 1:A:432:A:C2' | 1:A:433:C:H5'' | 2.40 | 0.51 |
| 1:A:818:G:H3' | 1:A:819:A:H5'' | 1.93 | 0.51 |
| 2:B:98:LEU:O | 2:B:101:MET:HG3 | 2.11 | 0.51 |
| 2:B:178:ARG:HB3 | 2:B:178:ARG:NH1 | 2.25 | 0.51 |
| 9:I:99:LEU:HB3 | 9:I:101:PHE:CE1 | 2.45 | 0.51 |
| 15:O:4:THR:HB | 15:O:6:GLU:OE2 | 2.10 | 0.51 |
| 1:A:250:A:O5' | 1:A:250:A:H8 | 1.92 | 0.51 |
| 1:A:392:G:H2' | 1:A:393:A:H8 | 1.76 | 0.51 |
| 1:A:560:U:H5' | 1:A:566:G:N2 | 2.25 | 0.51 |
| 1:A:619:U:O2 | 4:D:133:VAL:HA | 2.11 | 0.51 |
| 7:G:15:ASP:HB3 | 7:G:19:GLY:N | 2.26 | 0.51 |
| 13:M:31:LYS:O | 13:M:35:GLU:HG3 | 2.10 | 0.51 |
| 13:M:84:ILE:O | 13:M:85:GLY:C | 2.49 | 0.51 |
| 20:T:83:ARG:O | 20:T:87:LYS:HG3 | 2.11 | 0.51 |
| 1:A:1505:G:H3' | 1:A:1505:G:C8 | 2.46 | 0.51 |
| 1:A:407:G:O2' | 4:D:116:GLN:HG3 | 2.10 | 0.51 |
| 4:D:121:VAL:O | 4:D:134:ASP:HA | 2.11 | 0.51 |
| 10:J:75:ILE:HG22 | 10:J:76:ASN:N | 2.26 | 0.51 |
| 1:A:1249:C:H6 | 1:A:1249:C:H5'' | 1.76 | 0.51 |
| 1:A:1355:G:O2' | 1:A:1356:G:H5' | 2.10 | 0.51 |
| 1:A:1427:U:H2' | 1:A:1428:A:C8 | 2.45 | 0.51 |
| 1:A:629:G:C3' | 1:A:630:G:H5'' | 2.41 | 0.51 |
| 4:D:61:LYS:HE3 | 4:D:207:TYR:OH | 2.10 | 0.51 |
| 4:D:36:ARG:HB2 | 4:D:38:TYR:CZ | 2.45 | 0.51 |
| 6:F:62:TRP:C | 6:F:63:TYR:CD2 | 2.83 | 0.51 |
| 9:I:78:LYS:HD3 | 9:I:101:PHE:HD2 | 1.76 | 0.51 |
| 9:I:58:ARG:HD2 | 9:I:59:PHE:CE1 | 2.46 | 0.51 |
| 10:J:6:ILE:HG23 | 10:J:98:ILE:HD11 | 1.92 | 0.51 |
| 22:X:1:U:H2' | 22:X:2:U:H5' | 1.93 | 0.51 |
| 23:Y:34:TM2:O2' | 23:Y:35:A:O5' | 2.23 | 0.51 |
| 1:A:178:C:O2' | 1:A:179:A:H5' | 2.11 | 0.51 |
| 1:A:397:A:N3 | 1:A:397:A:H3' | 2.25 | 0.51 |
| 1:A:629:G:H2' | 1:A:630:G:O4' | 2.11 | 0.51 |
| 3:C:91:LEU:HD21 | 3:C:99:VAL:N | 2.17 | 0.51 |
| 6:F:82:ARG:HB2 | 6:F:85:VAL:CG2 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:103:VAL:HG21 | 8:H:109:ILE:C | 2.31 | 0.51 |
| 1:A:1347:G:OP2 | 9:I:107:ARG:HG2 | 2.10 | 0.51 |
| 11:K:87:THR:HG22 | 11:K:88:GLY:N | 2.26 | 0.51 |
| 12:L:47:LYS:HG2 | 12:L:48:PRO:HD3 | 1.92 | 0.51 |
| 12:L:75:HIS:CD2 | 12:L:77:LEU:H | 2.27 | 0.51 |
| 1:A:1026:G:C3' | 1:A:1027:C:H5'' | 2.40 | 0.50 |
| 1:A:1160:G:O6 | 1:A:1181:G:O6 | 2.28 | 0.50 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.46 | 0.50 |
| 1:A:697:U:H2' | 1:A:698:G:H5' | 1.93 | 0.50 |
| 20:T:43:LEU:CD1 | 20:T:55:ILE:HD12 | 2.40 | 0.50 |
| 1:A:582:U:OP1 | 15:O:64:ARG:NH2 | 2.41 | 0.50 |
| 5:E:78:HIS:CE1 | 5:E:142:LEU:HD23 | 2.46 | 0.50 |
| 11:K:24:SER:HB3 | 11:K:27:ASN:O | 2.11 | 0.50 |
| 9:I:128:ARG:HA | 13:M:126:LYS:CE | 2.41 | 0.50 |
| 15:O:17:ARG:NH1 | 15:O:77:ARG:NH1 | 2.59 | 0.50 |
| 1:A:1014:A:C2 | 1:A:1219:U:H1' | 2.47 | 0.50 |
| 1:A:1063:C:H2' | 1:A:1064:G:C8 | 2.47 | 0.50 |
| 1:A:1159:U:C4 | 1:A:1182:G:C6 | 2.98 | 0.50 |
| 2:B:211:ILE:O | 2:B:215:LEU:HB2 | 2.11 | 0.50 |
| 3:C:47:LEU:CD1 | 3:C:47:LEU:H | 2.24 | 0.50 |
| 3:C:54:ARG:HG2 | 3:C:55:VAL:N | 2.27 | 0.50 |
| 8:H:24:THR:HG22 | 8:H:63:LEU:HD21 | 1.92 | 0.50 |
| 12:L:27:LEU:C | 12:L:29:GLY:H | 2.15 | 0.50 |
| 12:L:86:ARG:HG3 | 12:L:86:ARG:HH11 | 1.77 | 0.50 |
| 20:T:69:GLY:O | 20:T:73:HIS:CD2 | 2.64 | 0.50 |
| 1:A:1133:G:H2' | 1:A:1134:G:C8 | 2.41 | 0.50 |
| 1:A:1143:G:H2' | 1:A:1144:G:C8 | 2.46 | 0.50 |
| 2:B:123:ALA:H | 2:B:127:ILE:HG12 | 1.76 | 0.50 |
| 3:C:167:TRP:O | 3:C:168:ALA:HB3 | 2.10 | 0.50 |
| 1:A:1112:C:O2 | 3:C:179:ARG:HG2 | 2.11 | 0.50 |
| 6:F:45:LEU:HB3 | 6:F:59:TYR:HD1 | 1.77 | 0.50 |
| 12:L:26:ALA:O | 12:L:27:LEU:O | 2.30 | 0.50 |
| 1:A:521:G:OP1 | 12:L:73:GLU:O | 2.27 | 0.50 |
| 16:P:45:THR:HB | 16:P:46:PRO:HD2 | 1.92 | 0.50 |
| 19:S:28:LYS:CG | 19:S:29:ARG:H | 2.04 | 0.50 |
| 20:T:39:LYS:HD3 | 20:T:55:ILE:HD13 | 1.93 | 0.50 |
| 22:X:3:G:H22 | 23:Y:34:TM2:H3 | 1.59 | 0.50 |
| 1:A:1201:A:O2' | 1:A:1202:G:OP2 | 2.26 | 0.50 |
| 1:A:1425:U:H2' | 1:A:1426:C:C6 | 2.46 | 0.50 |
| 1:A:337:C:H2' | 1:A:338:A:H8 | 1.76 | 0.50 |
| 1:A:942:G:H2' | 1:A:943:U:C6 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:150:GLU:HG3 | 4:D:153:ARG:NH1 | 2.26 | 0.50 |
| 9:I:87:GLN:O | 9:I:88:TYR:C | 2.49 | 0.50 |
| 20:T:39:LYS:CD | 20:T:55:ILE:HD13 | 2.41 | 0.50 |
| 1:A:1513:A:H2' | 1:A:1514:C:C6 | 2.46 | 0.50 |
| 2:B:116:GLU:HG2 | 2:B:153:ARG:HH11 | 1.77 | 0.50 |
| 2:B:51:LEU:CD2 | 2:B:55:PHE:HE1 | 2.22 | 0.50 |
| 3:C:119:ARG:O | 3:C:122:GLU:HB3 | 2.12 | 0.50 |
| 5:E:146:ALA:O | 5:E:150:ARG:HB2 | 2.12 | 0.50 |
| 9:I:53:VAL:HG23 | 9:I:55:ALA:H | 1.77 | 0.50 |
| 12:L:8:ASN:O | 12:L:12:ARG:HG3 | 2.10 | 0.50 |
| 1:A:438:G:C4' | 1:A:439:A:OP1 | 2.57 | 0.50 |
| 1:A:539:A:H2' | 1:A:540:G:H8 | 1.75 | 0.50 |
| 1:A:895:G:H2' | 1:A:896:C:C6 | 2.46 | 0.50 |
| 2:B:25:ASN:HD22 | 2:B:27:LYS:H | 1.57 | 0.50 |
| 3:C:91:LEU:HD23 | 3:C:92:ALA:N | 2.27 | 0.50 |
| 7:G:62:PHE:HD1 | 7:G:124:LEU:HD21 | 1.76 | 0.50 |
| 9:I:97:LYS:HA | 9:I:102:LEU:HD21 | 1.93 | 0.50 |
| 10:J:15:THR:O | 10:J:15:THR:HG22 | 2.12 | 0.50 |
| 1:A:537:G:OP1 | 12:L:113:ARG:NH2 | 2.45 | 0.50 |
| 15:O:17:ARG:HG3 | 15:O:17:ARG:NH1 | 2.25 | 0.50 |
| 17:Q:10:VAL:HG13 | 17:Q:19:VAL:HB | 1.94 | 0.50 |
| 21:U:5:ASP:HB3 | 21:U:8:THR:OG1 | 2.12 | 0.50 |
| 1:A:1054:C:H5 | 1:A:1196:U:C5 | 2.30 | 0.50 |
| 1:A:1223:C:P | 19:S:78:ARG:NH1 | 2.85 | 0.50 |
| 1:A:978:A:O2' | 1:A:1322:C:N3 | 2.44 | 0.50 |
| 1:A:538:G:OP2 | 12:L:115:LYS:HD2 | 2.11 | 0.50 |
| 1:A:861:G:O2' | 1:A:862:C:H5' | 2.11 | 0.50 |
| 2:B:102:LEU:CD1 | 2:B:102:LEU:N | 2.75 | 0.50 |
| 2:B:72:GLY:HA3 | 2:B:165:VAL:HG21 | 1.93 | 0.50 |
| 4:D:83:SER:HA | 4:D:89:THR:HG23 | 1.94 | 0.50 |
| 9:I:105:ASP:OD2 | 9:I:107:ARG:HD3 | 2.11 | 0.50 |
| 9:I:33:PHE:C | 9:I:35:GLU:H | 2.15 | 0.50 |
| 1:A:1227:A:OP2 | 13:M:96:LEU:HD21 | 2.11 | 0.50 |
| 1:A:1399:C:C2 | 1:A:1502:A:N6 | 2.80 | 0.50 |
| 1:A:543:C:O2' | 1:A:544:G:H5' | 2.12 | 0.50 |
| 6:F:33:TYR:HA | 6:F:71:ARG:NH1 | 2.27 | 0.50 |
| 10:J:80:LYS:O | 10:J:80:LYS:HD3 | 2.12 | 0.50 |
| 17:Q:10:VAL:HG23 | 17:Q:55:ASP:O | 2.12 | 0.50 |
| 17:Q:96:GLN:HB3 | 17:Q:103:GLY:CA | 2.38 | 0.50 |
| 1:A:110:C:H2' | 1:A:111:G:O4' | 2.12 | 0.49 |
| 1:A:1360:A:O2' | 1:A:1361:G:H5' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1365:G:O2' | 1:A:1366:C:H5' | 2.11 | 0.49 |
| 1:A:633:G:H2' | 1:A:634:C:C6 | 2.46 | 0.49 |
| 2:B:24:TRP:HB3 | 2:B:40:HIS:NE2 | 2.27 | 0.49 |
| 3:C:87:LEU:C | 3:C:89:GLU:H | 2.16 | 0.49 |
| 1:A:1123:A:O3' | 10:J:36:GLY:HA3 | 2.12 | 0.49 |
| 15:O:21:ASP:OD2 | 15:O:24:SER:HB3 | 2.11 | 0.49 |
| 16:P:4:ILE:HG13 | 16:P:64:ALA:HB1 | 1.93 | 0.49 |
| 17:Q:68:ARG:H | 17:Q:70:ARG:HH11 | 1.56 | 0.49 |
| 1:A:1154:G:O2' | 1:A:1155:G:H5' | 2.12 | 0.49 |
| 1:A:141:A:O2' | 1:A:142:G:H5' | 2.12 | 0.49 |
| 1:A:478:A:O2' | 1:A:479:C:H5' | 2.12 | 0.49 |
| 1:A:738:C:OP2 | 6:F:92:LYS:NZ | 2.40 | 0.49 |
| 2:B:192:SER:O | 2:B:194:PRO:HD3 | 2.12 | 0.49 |
| 2:B:16:HIS:HE1 | 2:B:214:ILE:HG12 | 1.76 | 0.49 |
| 3:C:23:TYR:C | 3:C:23:TYR:CD2 | 2.86 | 0.49 |
| 10:J:30:SER:HB2 | 10:J:80:LYS:O | 2.13 | 0.49 |
| 10:J:9:ARG:HH11 | 10:J:9:ARG:CB | 2.24 | 0.49 |
| 18:R:87:ARG:HG2 | 18:R:87:ARG:NH1 | 2.26 | 0.49 |
| 1:A:631:G:H5' | 1:A:632:A:OP1 | 2.12 | 0.49 |
| 1:A:644:G:O2' | 1:A:645:C:H5' | 2.12 | 0.49 |
| 1:A:947:G:H2' | 1:A:948:C:O4' | 2.13 | 0.49 |
| 2:B:223:ILE:HG22 | 2:B:226:ARG:HH21 | 1.78 | 0.49 |
| 3:C:172:ARG:HH12 | 3:C:174:PRO:HG3 | 1.77 | 0.49 |
| 3:C:62:ASP:O | 3:C:99:VAL:HG12 | 2.13 | 0.49 |
| 4:D:64:LEU:HD23 | 4:D:64:LEU:O | 2.12 | 0.49 |
| 5:E:149:GLU:O | 5:E:153:LYS:HG2 | 2.12 | 0.49 |
| 9:I:36:TYR:HD2 | 9:I:37:PHE:CE2 | 2.30 | 0.49 |
| 14:N:9:LYS:HD3 | 14:N:9:LYS:C | 2.33 | 0.49 |
| 1:A:1127:G:N2 | 1:A:1146:A:H62 | 2.10 | 0.49 |
| 1:A:1152:A:H5' | 10:J:70:ARG:NH2 | 2.25 | 0.49 |
| 3:C:155:GLY:HA3 | 3:C:164:ARG:H | 1.78 | 0.49 |
| 7:G:113:GLU:HG2 | 7:G:119:ARG:HG2 | 1.95 | 0.49 |
| 2:B:181:PHE:CD2 | 8:H:70:GLN:HB3 | 2.48 | 0.49 |
| 12:L:50:SER:O | 12:L:51:ALA:HB2 | 2.13 | 0.49 |
| 1:A:1006:C:H2' | 1:A:1007:C:C6 | 2.45 | 0.49 |
| 1:A:129(A):G:O2' | 1:A:130:A:OP2 | 2.31 | 0.49 |
| 1:A:556:C:C2' | 1:A:557:G:H5' | 2.41 | 0.49 |
| 1:A:639:G:O2' | 1:A:640:A:H5' | 2.13 | 0.49 |
| 1:A:919:A:O2' | 1:A:920:U:H5' | 2.12 | 0.49 |
| 2:B:121:LEU:HA | 2:B:124:SER:OG | 2.13 | 0.49 |
| 4:D:180:GLY:O | 4:D:182:LYS:HG2 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:45:PRO:HD3 | 12:L:51:ALA:O | 2.12 | 0.49 |
| 12:L:47:LYS:CG | 12:L:48:PRO:HD3 | 2.43 | 0.49 |
| 12:L:92:ASP:O | 12:L:94:PRO:HD3 | 2.12 | 0.49 |
| 16:P:57:ARG:NH1 | 16:P:79:VAL:O | 2.46 | 0.49 |
| 1:A:1054:C:C5 | 1:A:1196:U:C6 | 3.00 | 0.49 |
| 1:A:1313:U:H5 | 19:S:4:SER:HB2 | 1.78 | 0.49 |
| 1:A:1503:A:HO2' | 1:A:1504:G:P | 2.36 | 0.49 |
| 2:B:184:VAL:O | 2:B:184:VAL:HG12 | 2.12 | 0.49 |
| 2:B:69:LEU:HB3 | 2:B:162:ILE:HD13 | 1.94 | 0.49 |
| 3:C:206:GLU:O | 3:C:208:ILE:N | 2.46 | 0.49 |
| 3:C:83:ARG:C | 3:C:85:ARG:H | 2.15 | 0.49 |
| 3:C:64:VAL:CG2 | 3:C:99:VAL:HG11 | 2.28 | 0.49 |
| 8:H:51:VAL:HG11 | 8:H:60:ARG:NH1 | 2.28 | 0.49 |
| 1:A:689:C:P | 11:K:46:GLY:HA3 | 2.53 | 0.49 |
| 1:A:1424:C:O2' | 1:A:1425:U:H5' | 2.13 | 0.49 |
| 1:A:338:A:H2 | 1:A:351:G:H22 | 1.58 | 0.49 |
| 1:A:77:G:O2' | 1:A:78:G:H5' | 2.13 | 0.49 |
| 2:B:178:ARG:HB3 | 2:B:178:ARG:HH11 | 1.76 | 0.49 |
| 3:C:53:ALA:O | 3:C:54:ARG:CB | 2.60 | 0.49 |
| 4:D:102:ASP:HB3 | 4:D:136:PRO:HB3 | 1.95 | 0.49 |
| 6:F:74:ASP:O | 6:F:77:ARG:HB3 | 2.13 | 0.49 |
| 1:A:972:C:P | 10:J:57:LYS:HE2 | 2.53 | 0.49 |
| 12:L:43:VAL:HG12 | 12:L:44:THR:H | 1.77 | 0.49 |
| 1:A:1381:U:H2' | 1:A:1382:C:H6 | 1.77 | 0.49 |
| 4:D:33:MET:CE | 4:D:37:PRO:HA | 2.43 | 0.49 |
| 6:F:14:LEU:HD13 | 6:F:19:LEU:HB2 | 1.95 | 0.49 |
| 7:G:115:ARG:HB2 | 7:G:118:VAL:HG23 | 1.95 | 0.49 |
| 9:I:104:ARG:CD | 9:I:105:ASP:H | 2.17 | 0.49 |
| 14:N:23:ARG:HG2 | 14:N:23:ARG:HH11 | 1.77 | 0.49 |
| 14:N:6:LEU:C | 14:N:8:GLU:H | 2.16 | 0.49 |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:CD1 | 2.48 | 0.49 |
| 1:A:130:A:C8 | 17:Q:63:ARG:HG3 | 2.48 | 0.49 |
| 1:A:1051:C:H2' | 1:A:1052:U:C6 | 2.48 | 0.49 |
| 1:A:1106:G:OP1 | 3:C:172:ARG:HD3 | 2.13 | 0.49 |
| 1:A:1454:G:H2' | 1:A:1455:G:H8 | 1.78 | 0.49 |
| 1:A:180:U:H2' | 1:A:181:G:H5' | 1.94 | 0.49 |
| 1:A:92:C:O2' | 1:A:93:G:H5' | 2.13 | 0.49 |
| 2:B:118:LEU:HB2 | 2:B:142:LEU:HD13 | 1.95 | 0.49 |
| 2:B:51:LEU:O | 2:B:55:PHE:HD1 | 1.95 | 0.49 |
| 4:D:3:ARG:HD2 | 4:D:118:ARG:NE | 2.28 | 0.49 |
| 6:F:36:ARG:HH21 | 6:F:38:GLU:HG2 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:31:GLN:HE21 | 9:I:35:GLU:HG3 | 1.77 | 0.49 |
| 10:J:22:LYS:HZ1 | 10:J:89:ASP:HA | 1.78 | 0.49 |
| 15:O:8:LYS:O | 15:O:11:VAL:HB | 2.13 | 0.49 |
| 22:X:1:U:C2' | 22:X:2:U:H5' | 2.43 | 0.49 |
| 1:A:1052:U:H2' | 1:A:1055:A:OP1 | 2.13 | 0.49 |
| 1:A:1288:A:H2' | 1:A:1289:A:H8 | 1.77 | 0.49 |
| 1:A:431:A:O2' | 1:A:432:A:H5' | 2.13 | 0.49 |
| 1:A:601:C:O2' | 1:A:602:A:H5' | 2.13 | 0.49 |
| 1:A:867:G:O2' | 1:A:868:C:H5' | 2.12 | 0.49 |
| 3:C:43:LEU:HD23 | 3:C:43:LEU:C | 2.33 | 0.49 |
| 3:C:46:GLU:C | 3:C:48:TYR:H | 2.16 | 0.49 |
| 3:C:91:LEU:HD11 | 3:C:99:VAL:O | 2.13 | 0.49 |
| 11:K:91:ARG:NH1 | 18:R:88:LYS:HE3 | 2.27 | 0.49 |
| 12:L:43:VAL:CG1 | 12:L:44:THR:N | 2.76 | 0.49 |
| 13:M:23:TYR:HB2 | 13:M:67:GLU:OE2 | 2.12 | 0.49 |
| 4:D:173:TRP:CD1 | 4:D:189:PRO:HG3 | 2.49 | 0.48 |
| 11:K:101:SER:O | 11:K:103:LEU:N | 2.38 | 0.48 |
| 12:L:19:ARG:HH11 | 12:L:19:ARG:HG3 | 1.78 | 0.48 |
| 1:A:127:G:HO2' | 17:Q:2:PRO:N | 2.11 | 0.48 |
| 20:T:94:ALA:O | 20:T:95:ALA:HB2 | 2.13 | 0.48 |
| 1:A:977:A:C2' | 1:A:978:A:H5' | 2.43 | 0.48 |
| 2:B:118:LEU:HD11 | 2:B:141:GLU:OE2 | 2.12 | 0.48 |
| 2:B:204:ASN:HD22 | 2:B:206:ASP:H | 1.61 | 0.48 |
| 2:B:230:VAL:HG12 | 2:B:231:GLU:N | 2.28 | 0.48 |
| 2:B:86:GLU:C | 2:B:88:ALA:H | 2.17 | 0.48 |
| 3:C:60:ALA:O | 3:C:61:ALA:CB | 2.61 | 0.48 |
| 8:H:20:TYR:CE2 | 8:H:75:ARG:HD2 | 2.47 | 0.48 |
| 13:M:14:ARG:NH1 | 13:M:16:ASP:OD2 | 2.46 | 0.48 |
| 19:S:22:LEU:HD21 | 19:S:28:LYS:HD2 | 1.94 | 0.48 |
| 1:A:1175:G:C2 | 1:A:1176:A:N9 | 2.81 | 0.48 |
| 3:C:15:THR:O | 3:C:16:ARG:CB | 2.58 | 0.48 |
| 3:C:195:VAL:O | 3:C:196:LEU:HD22 | 2.13 | 0.48 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:CG2 | 2.29 | 0.48 |
| 14:N:46:GLU:O | 14:N:49:HIS:HB2 | 2.13 | 0.48 |
| 16:P:20:VAL:CG1 | 16:P:32:TYR:HB2 | 2.44 | 0.48 |
| 16:P:42:ARG:O | 16:P:43:LYS:C | 2.52 | 0.48 |
| 1:A:633:G:H2' | 1:A:634:C:H6 | 1.78 | 0.48 |
| 1:A:740:U:O2' | 1:A:741:G:H5' | 2.13 | 0.48 |
| 2:B:130:ARG:HB3 | 2:B:131:PRO:HD2 | 1.95 | 0.48 |
| 2:B:161:ALA:HB1 | 2:B:185:ILE:CD1 | 2.42 | 0.48 |
| 2:B:7:VAL:CG1 | 2:B:221:LEU:HD23 | 2.40 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:C:28:GLN:O | 3:C:31:HIS:HB2 | 2.13 | 0.48 |
| 3:C:58:GLU:O | 3:C:64:VAL:HA | 2.13 | 0.48 |
| 6:F:46:ARG:HA | 6:F:47:ARG:HH21 | 1.79 | 0.48 |
| 7:G:129:GLU:OE2 | 7:G:131:LYS:HE2 | 2.14 | 0.48 |
| 12:L:59:ARG:HB2 | 12:L:59:ARG:NH1 | 2.18 | 0.48 |
| 12:L:60:LEU:HD21 | 12:L:66:VAL:HG22 | 1.95 | 0.48 |
| 18:R:74:ARG:HB3 | 18:R:81:PHE:CE1 | 2.48 | 0.48 |
| 18:R:73:ALA:HB3 | 18:R:79:LEU:HD12 | 1.95 | 0.48 |
| 19:S:44:MET:O | 19:S:47:HIS:HB2 | 2.13 | 0.48 |
| 1:A:1014:A:H2' | 1:A:1015:A:C8 | 2.48 | 0.48 |
| 1:A:1168:A:C6 | 1:A:1169:A:C6 | 3.01 | 0.48 |
| 1:A:409:G:H1 | 1:A:433:C:N4 | 2.11 | 0.48 |
| 1:A:954:G:H2' | 1:A:955:U:C6 | 2.49 | 0.48 |
| 4:D:17:VAL:CG1 | 4:D:18:LYS:N | 2.76 | 0.48 |
| 1:A:923:A:OP1 | 5:E:21:ALA:HB2 | 2.12 | 0.48 |
| 1:A:1129:C:OP1 | 9:I:62:TYR:CE2 | 2.66 | 0.48 |
| 12:L:37:CYS:O | 12:L:79:GLU:O | 2.32 | 0.48 |
| 13:M:40:ASN:HB3 | 13:M:43:THR:CG2 | 2.41 | 0.48 |
| 16:P:26:ARG:CD | 16:P:31:LYS:O | 2.62 | 0.48 |
| 16:P:81:ARG:NH1 | 16:P:81:ARG:HB2 | 2.29 | 0.48 |
| 17:Q:68:ARG:HH11 | 17:Q:68:ARG:HG2 | 1.79 | 0.48 |
| 6:F:101:ALA:CB | 18:R:28:GLU:HB2 | 2.41 | 0.48 |
| 1:A:1127:G:H2' | 1:A:1128:C:C6 | 2.48 | 0.48 |
| 1:A:1191:A:C3' | 1:A:1192:C:OP2 | 2.51 | 0.48 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:HB2 | 1.96 | 0.48 |
| 24:A:1601:PAR:H642 | 24:A:1601:PAR:H43 | 1.95 | 0.48 |
| 2:B:116:GLU:HG2 | 2:B:153:ARG:NH1 | 2.28 | 0.48 |
| 2:B:98:LEU:N | 2:B:98:LEU:HD23 | 2.29 | 0.48 |
| 4:D:8:VAL:HB | 4:D:21:LEU:CD1 | 2.43 | 0.48 |
| 10:J:38:ILE:HB | 10:J:71:LEU:CB | 2.43 | 0.48 |
| 10:J:9:ARG:CB | 10:J:9:ARG:NH1 | 2.77 | 0.48 |
| 1:A:1056:U:H5' | 3:C:163:ALA:CB | 2.44 | 0.48 |
| 1:A:1371:G:OP1 | 9:I:11:LYS:O | 2.32 | 0.48 |
| 1:A:325:A:H2' | 1:A:326:G:O4' | 2.14 | 0.48 |
| 1:A:866:C:H2' | 1:A:867:G:O4' | 2.13 | 0.48 |
| 1:A:975:A:H4' | 1:A:976:G:C5' | 2.37 | 0.48 |
| 3:C:134:ILE:CG2 | 3:C:168:ALA:HB3 | 2.44 | 0.48 |
| 3:C:63:ASN:HA | 3:C:99:VAL:HG12 | 1.94 | 0.48 |
| 1:A:8:A:N6 | 4:D:205:GLU:O | 2.47 | 0.48 |
| 5:E:24:ARG:HH11 | 5:E:24:ARG:HG2 | 1.78 | 0.48 |
| 6:F:45:LEU:HA | 6:F:59:TYR:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:1343:G:C1' | 9:I:121:ARG:HH12 | 2.22 | 0.48 |
| 11:K:99:GLN:CG | 11:K:105:VAL:HG21 | 2.43 | 0.48 |
| 18:R:68:LYS:O | 18:R:72:ARG:HG3 | 2.14 | 0.48 |
| 1:A:1216:G:O2' | 1:A:1217:C:H5' | 2.13 | 0.48 |
| 1:A:1227:A:H3' | 1:A:1227:A:H8 | 1.78 | 0.48 |
| 1:A:1272:G:O2' | 1:A:1273:G:H5' | 2.14 | 0.48 |
| 1:A:1251:A:H1' | 1:A:1369:C:HO2' | 1.78 | 0.48 |
| 1:A:1521:G:H2' | 1:A:1522:U:C6 | 2.49 | 0.48 |
| 1:A:16:A:C2' | 1:A:17:U:H5' | 2.44 | 0.48 |
| 1:A:123:C:OP1 | 1:A:312:C:H5' | 2.14 | 0.48 |
| 3:C:95:THR:O | 3:C:97:LYS:N | 2.46 | 0.48 |
| 9:I:53:VAL:CG1 | 9:I:96:LEU:HD11 | 2.44 | 0.48 |
| 10:J:50:ILE:HA | 10:J:60:ARG:HA | 1.94 | 0.48 |
| 20:T:86:ARG:NH1 | 20:T:86:ARG:HG3 | 2.28 | 0.48 |
| 1:A:1054:C:C2' | 1:A:1055:A:H5'' | 2.44 | 0.48 |
| 1:A:1376:U:H2' | 1:A:1377:A:C8 | 2.49 | 0.48 |
| 1:A:1532:U:O2' | 1:A:1533:C:C6 | 2.66 | 0.48 |
| 1:A:343:U:H2' | 1:A:345:C:C5 | 2.49 | 0.48 |
| 1:A:409:G:H1 | 1:A:433:C:H42 | 1.62 | 0.48 |
| 1:A:723:U:O2 | 1:A:723:U:H2' | 2.12 | 0.48 |
| 2:B:97:TRP:CH2 | 2:B:176:GLU:OE2 | 2.66 | 0.48 |
| 4:D:70:ILE:HD11 | 4:D:100:ARG:NH2 | 2.29 | 0.48 |
| 6:F:67:MET:SD | 6:F:75:LEU:HD12 | 2.54 | 0.48 |
| 10:J:7:LYS:HD2 | 10:J:71:LEU:CD2 | 2.44 | 0.48 |
| 22:X:3:G:H2' | 22:X:4:A:C5' | 2.43 | 0.48 |
| 1:A:1127:G:H21 | 1:A:1146:A:H61 | 1.59 | 0.48 |
| 1:A:1244:C:O2' | 1:A:1245:A:H5' | 2.14 | 0.48 |
| 1:A:1306:A:H61 | 1:A:1331:G:H1' | 1.79 | 0.48 |
| 1:A:513:C:H2' | 1:A:514:C:C6 | 2.49 | 0.48 |
| 2:B:18:GLY:CA | 2:B:41:ILE:HA | 2.35 | 0.48 |
| 3:C:56:ASP:O | 3:C:57:ILE:HG13 | 2.14 | 0.48 |
| 9:I:9:ARG:CG | 9:I:14:VAL:HG12 | 2.43 | 0.48 |
| 1:A:1007:C:O2' | 1:A:1008:C:H5' | 2.14 | 0.47 |
| 1:A:1407:C:O2' | 1:A:1408:A:H5' | 2.14 | 0.47 |
| 1:A:145:G:O2' | 1:A:146:G:H5' | 2.14 | 0.47 |
| 1:A:961:U:O2' | 1:A:962:C:H5' | 2.14 | 0.47 |
| 1:A:974:A:P | 14:N:41:ARG:HH12 | 2.35 | 0.47 |
| 3:C:154:SER:HB3 | 3:C:197:GLY:H | 1.79 | 0.47 |
| 4:D:63:LYS:HD2 | 4:D:198:VAL:HG22 | 1.96 | 0.47 |
| 5:E:81:GLU:HG3 | 5:E:90:VAL:HG22 | 1.96 | 0.47 |
| 7:G:15:ASP:HB2 | 7:G:20:ASP:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:119:LEU:CD1 | 8:H:124:ALA:HA | 2.44 | 0.47 |
| 8:H:88:LYS:O | 8:H:89:PRO:C | 2.52 | 0.47 |
| 9:I:65:VAL:HG11 | 9:I:77:ILE:HD11 | 1.96 | 0.47 |
| 10:J:63:PHE:HE1 | 14:N:45:ARG:HG3 | 1.79 | 0.47 |
| 19:S:55:LYS:HG2 | 19:S:56:GLN:HG3 | 1.96 | 0.47 |
| 1:A:1113:C:H6 | 1:A:1113:C:O5' | 1.97 | 0.47 |
| 1:A:1228:C:H4' | 13:M:116:THR:HA | 1.96 | 0.47 |
| 1:A:1470:G:O2' | 1:A:1471:G:H5' | 2.14 | 0.47 |
| 1:A:432:A:H2' | 1:A:433:C:H5'' | 1.96 | 0.47 |
| 2:B:55:PHE:CE2 | 2:B:218:ALA:HA | 2.49 | 0.47 |
| 5:E:57:LYS:HG2 | 5:E:61:TYR:CE2 | 2.49 | 0.47 |
| 10:J:48:THR:HG1 | 10:J:62:HIS:CD2 | 2.31 | 0.47 |
| 10:J:49:VAL:O | 10:J:60:ARG:O | 2.32 | 0.47 |
| 12:L:83:VAL:HG23 | 12:L:100:ILE:HG23 | 1.95 | 0.47 |
| 13:M:85:GLY:O | 13:M:86:CYS:O | 2.33 | 0.47 |
| 16:P:3:LYS:O | 16:P:21:VAL:HA | 2.14 | 0.47 |
| 1:A:101:A:O2' | 1:A:102:G:H5' | 2.14 | 0.47 |
| 1:A:848:C:H2' | 1:A:849:C:H6 | 1.79 | 0.47 |
| 1:A:879:C:O2' | 1:A:880:C:H5' | 2.14 | 0.47 |
| 2:B:15:VAL:HB | 2:B:210:SER:HB2 | 1.96 | 0.47 |
| 3:C:31:HIS:C | 3:C:33:LEU:H | 2.17 | 0.47 |
| 4:D:20:TYR:CD2 | 4:D:26:CYS:HB3 | 2.49 | 0.47 |
| 10:J:30:SER:CB | 10:J:80:LYS:HG3 | 2.44 | 0.47 |
| 10:J:80:LYS:O | 10:J:83:GLU:HB2 | 2.13 | 0.47 |
| 11:K:115:PRO:C | 11:K:117:ASN:H | 2.18 | 0.47 |
| 1:A:1347:G:C6 | 9:I:107:ARG:NH2 | 2.82 | 0.47 |
| 3:C:47:LEU:N | 3:C:47:LEU:CD1 | 2.77 | 0.47 |
| 3:C:52:LEU:HD23 | 3:C:52:LEU:N | 2.29 | 0.47 |
| 3:C:54:ARG:O | 3:C:55:VAL:HG23 | 2.14 | 0.47 |
| 3:C:6:HIS:NE2 | 3:C:8:ILE:HD12 | 2.30 | 0.47 |
| 7:G:137:LYS:O | 7:G:141:VAL:HG12 | 2.14 | 0.47 |
| 8:H:60:ARG:NH1 | 8:H:60:ARG:HG3 | 2.28 | 0.47 |
| 12:L:19:ARG:NH1 | 12:L:19:ARG:HG3 | 2.30 | 0.47 |
| 13:M:102:ARG:HB2 | 13:M:102:ARG:NH1 | 2.30 | 0.47 |
| 14:N:44:LEU:C | 14:N:44:LEU:HD12 | 2.34 | 0.47 |
| 1:A:1161:C:H2' | 1:A:1162:C:C6 | 2.50 | 0.47 |
| 1:A:1250:A:O3' | 9:I:67:GLY:HA2 | 2.15 | 0.47 |
| 1:A:167:G:O2' | 1:A:168:G:H5' | 2.14 | 0.47 |
| 1:A:586:C:H5'' | 8:H:90:GLY:CA | 2.45 | 0.47 |
| 3:C:112:SER:OG | 3:C:115:LEU:HD12 | 2.15 | 0.47 |
| 3:C:120:VAL:O | 3:C:124:ILE:HG13 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:62:GLN:HA | 4:D:62:GLN:NE2 | 2.29 | 0.47 |
| 1:A:545:C:H5'' | 4:D:72:GLU:HG2 | 1.97 | 0.47 |
| 5:E:82:VAL:HG11 | 5:E:137:GLU:HB3 | 1.96 | 0.47 |
| 20:T:16:HIS:CE1 | 20:T:20:LEU:HD11 | 2.50 | 0.47 |
| 1:A:1005:A:C2' | 1:A:1006:C:H5' | 2.44 | 0.47 |
| 1:A:1038:C:H2' | 1:A:1039:C:C6 | 2.46 | 0.47 |
| 1:A:1095:U:H2' | 1:A:1096:C:H6 | 1.73 | 0.47 |
| 1:A:1116:C:H2' | 1:A:1117:G:C5' | 2.33 | 0.47 |
| 1:A:1149:C:O2' | 1:A:1280:A:N1 | 2.45 | 0.47 |
| 1:A:1505:G:H2' | 1:A:1541:U:OP2 | 2.14 | 0.47 |
| 1:A:327:A:O3' | 1:A:328:C:H4' | 2.15 | 0.47 |
| 1:A:96:G:O2' | 1:A:97:G:H5' | 2.15 | 0.47 |
| 5:E:7:GLU:OE2 | 5:E:37:ARG:NE | 2.45 | 0.47 |
| 7:G:145:ALA:O | 7:G:147:ALA:N | 2.45 | 0.47 |
| 7:G:45:ASP:O | 7:G:49:ILE:HG13 | 2.15 | 0.47 |
| 10:J:71:LEU:O | 10:J:72:VAL:HB | 2.14 | 0.47 |
| 1:A:1063:C:H2' | 1:A:1064:G:H8 | 1.77 | 0.47 |
| 1:A:279:A:H5'' | 1:A:281:G:O4' | 2.15 | 0.47 |
| 2:B:27:LYS:HD2 | 2:B:193:ASP:OD2 | 2.15 | 0.47 |
| 4:D:157:LEU:HD11 | 4:D:161:ASN:HD21 | 1.80 | 0.47 |
| 6:F:2:ARG:NE | 6:F:69:GLU:CG | 2.74 | 0.47 |
| 10:J:31:GLY:HA3 | 10:J:78:ASN:ND2 | 2.30 | 0.47 |
| 11:K:48:ILE:HD13 | 11:K:48:ILE:N | 2.30 | 0.47 |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:HB2 | 1.97 | 0.47 |
| 16:P:1:MET:O | 16:P:24:ALA:HB2 | 2.14 | 0.47 |
| 20:T:57:ARG:HE | 20:T:102:GLY:HA3 | 1.79 | 0.47 |
| 1:A:1112:C:N3 | 3:C:178:LEU:HD23 | 2.29 | 0.47 |
| 1:A:1249:C:H2' | 1:A:1250:A:H5' | 1.95 | 0.47 |
| 1:A:309:G:H1' | 1:A:608:A:C2 | 2.49 | 0.47 |
| 1:A:780:A:C2 | 1:A:801:U:C5 | 3.03 | 0.47 |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:NH2 | 2.30 | 0.47 |
| 4:D:19:LEU:HD22 | 4:D:67:ILE:HG12 | 1.97 | 0.47 |
| 8:H:10:LEU:HD22 | 8:H:83:ILE:HD11 | 1.97 | 0.47 |
| 12:L:89:ARG:NH2 | 12:L:91:LYS:HG2 | 2.28 | 0.47 |
| 15:O:39:LEU:CD1 | 15:O:56:LEU:HB2 | 2.45 | 0.47 |
| 15:O:87:ILE:CG2 | 15:O:88:ARG:H | 2.15 | 0.47 |
| 1:A:1038:C:C6 | 1:A:1039:C:H5 | 2.33 | 0.47 |
| 1:A:1429:C:O2' | 1:A:1430:C:H5' | 2.15 | 0.47 |
| 1:A:463:A:H4' | 16:P:80:PHE:O | 2.15 | 0.47 |
| 2:B:10:LEU:O | 2:B:12:GLU:N | 2.46 | 0.47 |
| 3:C:155:GLY:O | 3:C:156:ARG:CB | 2.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:32:ARG:O | 7:G:33:ASP:HB2 | 2.15 | 0.47 |
| 7:G:80:VAL:HG12 | 7:G:80:VAL:O | 2.15 | 0.47 |
| 10:J:30:SER:HB2 | 10:J:80:LYS:HG3 | 1.97 | 0.47 |
| 10:J:57:LYS:HD2 | 10:J:60:ARG:HH21 | 1.80 | 0.47 |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:CB | 2.44 | 0.47 |
| 16:P:81:ARG:HG3 | 16:P:83:GLU:HG2 | 1.97 | 0.47 |
| 17:Q:67:LYS:CA | 17:Q:70:ARG:NH1 | 2.75 | 0.47 |
| 17:Q:81:ARG:O | 17:Q:81:ARG:HG3 | 2.15 | 0.47 |
| 6:F:62:TRP:CG | 18:R:35:ARG:NH1 | 2.82 | 0.47 |
| 19:S:22:LEU:HD13 | 19:S:28:LYS:HB3 | 1.97 | 0.47 |
| 1:A:105:G:H2' | 1:A:106:C:C6 | 2.49 | 0.47 |
| 1:A:1320:C:O2' | 1:A:1321:C:H5' | 2.15 | 0.47 |
| 1:A:458:C:H2' | 1:A:459:G:H8 | 1.80 | 0.47 |
| 5:E:45:PHE:CE2 | 5:E:47:LYS:HD2 | 2.50 | 0.47 |
| 5:E:79:GLU:CD | 5:E:79:GLU:H | 2.19 | 0.47 |
| 8:H:20:TYR:HE2 | 8:H:75:ARG:HD2 | 1.78 | 0.47 |
| 12:L:52:LEU:O | 12:L:54:LYS:HD2 | 2.15 | 0.47 |
| 14:N:44:LEU:O | 14:N:44:LEU:HD12 | 2.15 | 0.47 |
| 19:S:15:LEU:HD12 | 19:S:16:LEU:N | 2.30 | 0.47 |
| 20:T:10:LEU:O | 20:T:12:ALA:N | 2.48 | 0.47 |
| 3:C:19:GLU:O | 3:C:40:ARG:NH2 | 2.48 | 0.47 |
| 1:A:921:U:O2 | 5:E:19:MET:HB2 | 2.15 | 0.47 |
| 8:H:4:ASP:OD1 | 8:H:85:ARG:NH1 | 2.48 | 0.47 |
| 9:I:100:GLY:HA2 | 9:I:102:LEU:HD11 | 1.97 | 0.47 |
| 9:I:127:LYS:O | 9:I:128:ARG:CB | 2.63 | 0.47 |
| 9:I:46:ALA:HB2 | 9:I:74:ILE:HG23 | 1.97 | 0.47 |
| 9:I:97:LYS:N | 9:I:98:PRO:CD | 2.77 | 0.47 |
| 10:J:6:ILE:HD13 | 10:J:73:ASP:N | 2.28 | 0.47 |
| 14:N:53:LEU:HB3 | 14:N:56:VAL:HG21 | 1.96 | 0.47 |
| 19:S:15:LEU:HD12 | 19:S:16:LEU:H | 1.80 | 0.47 |
| 1:A:1157:A:H4' | 1:A:1158:C:O5' | 2.15 | 0.46 |
| 1:A:1182:G:O2' | 1:A:1183:A:P | 2.72 | 0.46 |
| 1:A:16:A:H2' | 1:A:17:U:H5' | 1.97 | 0.46 |
| 1:A:406:G:H5'' | 4:D:5:ILE:HG23 | 1.96 | 0.46 |
| 3:C:113:ALA:N | 3:C:114:PRO:CD | 2.78 | 0.46 |
| 6:F:46:ARG:HH11 | 6:F:46:ARG:CB | 2.27 | 0.46 |
| 7:G:16:LEU:HD22 | 7:G:16:LEU:N | 2.30 | 0.46 |
| 7:G:58:PRO:HG2 | 7:G:59:LEU:H | 1.80 | 0.46 |
| 8:H:11:THR:HA | 8:H:14:ARG:NH1 | 2.30 | 0.46 |
| 11:K:12:ARG:O | 11:K:12:ARG:HD2 | 2.14 | 0.46 |
| 12:L:46:LYS:O | 12:L:47:LYS:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 18:R:36:ASN:ND2 | 18:R:38:GLU:HG2 | 2.30 | 0.46 |
| 1:A:1060:C:H2' | 1:A:1061:G:C8 | 2.47 | 0.46 |
| 1:A:1300:G:O2' | 1:A:1301:U:H6 | 1.98 | 0.46 |
| 1:A:1498:U:C4' | 1:A:1519:A:H2 | 2.29 | 0.46 |
| 1:A:814:A:H2' | 1:A:816:A:H5'' | 1.96 | 0.46 |
| 2:B:196:LEU:N | 2:B:196:LEU:CD1 | 2.77 | 0.46 |
| 2:B:77:ALA:HB1 | 2:B:211:ILE:HG21 | 1.97 | 0.46 |
| 2:B:223:ILE:CG2 | 2:B:226:ARG:HH21 | 2.28 | 0.46 |
| 3:C:64:VAL:HB | 3:C:99:VAL:CG2 | 2.30 | 0.46 |
| 7:G:120:ILE:H | 7:G:120:ILE:CD1 | 2.26 | 0.46 |
| 7:G:62:PHE:HA | 7:G:124:LEU:HD22 | 1.96 | 0.46 |
| 8:H:138:TRP:OXT | 8:H:138:TRP:HE3 | 1.98 | 0.46 |
| 10:J:40:LEU:HD11 | 10:J:71:LEU:HD23 | 1.97 | 0.46 |
| 12:L:38:THR:HB | 12:L:57:LYS:HB3 | 1.96 | 0.46 |
| 14:N:9:LYS:HE3 | 14:N:21:TYR:O | 2.16 | 0.46 |
| 18:R:42:ARG:HH11 | 18:R:42:ARG:HB3 | 1.79 | 0.46 |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:HD13 | 1.96 | 0.46 |
| 1:A:1116:C:C3' | 1:A:1117:G:H5'' | 2.45 | 0.46 |
| 1:A:1129:C:O2' | 1:A:1130:A:P | 2.74 | 0.46 |
| 1:A:339:C:H2' | 1:A:340:U:C6 | 2.49 | 0.46 |
| 1:A:965:A:C2 | 1:A:969:A:C2 | 3.04 | 0.46 |
| 4:D:168:ARG:CB | 4:D:168:ARG:HH11 | 2.13 | 0.46 |
| 4:D:5:ILE:HG22 | 4:D:5:ILE:O | 2.13 | 0.46 |
| 8:H:119:LEU:HD23 | 8:H:119:LEU:N | 2.31 | 0.46 |
| 9:I:50:LEU:O | 9:I:53:VAL:HG22 | 2.15 | 0.46 |
| 10:J:57:LYS:O | 10:J:57:LYS:HD2 | 2.14 | 0.46 |
| 10:J:38:ILE:HB | 10:J:71:LEU:HB3 | 1.96 | 0.46 |
| 13:M:84:ILE:O | 13:M:84:ILE:HG13 | 2.15 | 0.46 |
| 15:O:5:LYS:N | 15:O:5:LYS:HD2 | 2.30 | 0.46 |
| 16:P:63:GLY:O | 16:P:64:ALA:C | 2.54 | 0.46 |
| 20:T:100:ILE:O | 20:T:101:GLY:C | 2.54 | 0.46 |
| 1:A:1065:U:H5'' | 1:A:1190:G:H21 | 1.77 | 0.46 |
| 1:A:1075:C:OP1 | 2:B:179:LYS:NZ | 2.49 | 0.46 |
| 1:A:1120:G:O2' | 1:A:1121:U:H5' | 2.15 | 0.46 |
| 1:A:1370:G:C2 | 1:A:1371:G:C8 | 3.04 | 0.46 |
| 1:A:147:G:O2' | 1:A:148:G:H5' | 2.15 | 0.46 |
| 1:A:52:G:O2' | 1:A:53:A:H5' | 2.15 | 0.46 |
| 1:A:912:C:O2' | 1:A:913:A:H5' | 2.14 | 0.46 |
| 3:C:119:ARG:NE | 3:C:140:ARG:HH12 | 2.12 | 0.46 |
| 7:G:138:LYS:C | 7:G:138:LYS:HD3 | 2.36 | 0.46 |
| 2:B:181:PHE:HD2 | 8:H:70:GLN:HB3 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:3:LYS:HB3 | 10:J:75:ILE:HA | 1.96 | 0.46 |
| 13:M:37:THR:HG22 | 13:M:39:ILE:HG13 | 1.96 | 0.46 |
| 22:X:2:U:H2' | 22:X:3:G:H8 | 1.78 | 0.46 |
| 1:A:1074:G:O3' | 2:B:103:THR:CG2 | 2.63 | 0.46 |
| 1:A:1227:A:H3' | 1:A:1227:A:C8 | 2.51 | 0.46 |
| 2:B:19:HIS:O | 2:B:20:GLU:O | 2.34 | 0.46 |
| 8:H:86:ILE:HG12 | 8:H:135:CYS:HA | 1.97 | 0.46 |
| 9:I:100:GLY:HA2 | 9:I:102:LEU:CD1 | 2.46 | 0.46 |
| 9:I:42:ARG:NH2 | 9:I:71:SER:O | 2.49 | 0.46 |
| 9:I:92:TYR:O | 9:I:96:LEU:HD13 | 2.15 | 0.46 |
| 11:K:32:ILE:HD13 | 11:K:68:ALA:HB1 | 1.96 | 0.46 |
| 12:L:24:VAL:CG1 | 12:L:26:ALA:HB2 | 2.43 | 0.46 |
| 17:Q:51:TYR:C | 17:Q:52:LYS:HD2 | 2.36 | 0.46 |
| 1:A:1504:G:H3' | 1:A:1504:G:OP2 | 2.15 | 0.46 |
| 1:A:414:A:H2' | 1:A:415:A:C8 | 2.51 | 0.46 |
| 1:A:945:G:H2' | 1:A:945:G:N3 | 2.30 | 0.46 |
| 1:A:986:A:H2' | 1:A:987:G:O4' | 2.16 | 0.46 |
| 7:G:115:ARG:HB2 | 7:G:118:VAL:CG2 | 2.45 | 0.46 |
| 12:L:85:ILE:HG23 | 12:L:98:TYR:HB3 | 1.96 | 0.46 |
| 1:A:1286:A:C2 | 21:U:18:TYR:OH | 2.69 | 0.46 |
| 1:A:1130:A:C2 | 1:A:1146:A:N3 | 2.83 | 0.46 |
| 1:A:1321:C:H5'' | 13:M:87:TYR:CE2 | 2.51 | 0.46 |
| 1:A:1505:G:H8 | 1:A:1505:G:H3' | 1.81 | 0.46 |
| 1:A:200:G:H2' | 1:A:201:C:O4' | 2.16 | 0.46 |
| 1:A:834:C:H2' | 1:A:835:U:C6 | 2.50 | 0.46 |
| 1:A:882:C:O2' | 1:A:883:C:H5' | 2.16 | 0.46 |
| 2:B:76:GLN:HG3 | 2:B:206:ASP:OD1 | 2.16 | 0.46 |
| 3:C:5:ILE:H | 3:C:5:ILE:HD12 | 1.80 | 0.46 |
| 3:C:64:VAL:N | 3:C:99:VAL:HB | 2.29 | 0.46 |
| 4:D:163:GLU:C | 4:D:165:MET:H | 2.19 | 0.46 |
| 4:D:17:VAL:HG12 | 4:D:18:LYS:N | 2.30 | 0.46 |
| 5:E:82:VAL:CG2 | 5:E:138:ALA:HA | 2.41 | 0.46 |
| 6:F:13:ASN:O | 6:F:14:LEU:O | 2.33 | 0.46 |
| 6:F:21:LEU:O | 6:F:24:GLU:HB3 | 2.16 | 0.46 |
| 9:I:48:GLU:N | 9:I:49:PRO:CD | 2.79 | 0.46 |
| 1:A:261:U:OP2 | 20:T:79:ARG:NH2 | 2.49 | 0.46 |
| 1:A:1127:G:H4' | 9:I:66:ARG:NH1 | 2.30 | 0.46 |
| 1:A:369:C:O2' | 1:A:370:C:H5' | 2.16 | 0.46 |
| 1:A:627:G:H2' | 1:A:628:G:H8 | 1.81 | 0.46 |
| 1:A:994:A:N3 | 1:A:994:A:H2' | 2.31 | 0.46 |
| 3:C:36:ASP:OD2 | 3:C:36:ASP:N | 2.42 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:51:VAL:HB | 5:E:52:PRO:CD | 2.41 | 0.46 |
| 10:J:6:ILE:HG23 | 10:J:98:ILE:CD1 | 2.46 | 0.46 |
| 10:J:98:ILE:CG2 | 10:J:99:LYS:N | 2.78 | 0.46 |
| 1:A:954:G:H5'' | 13:M:120:LYS:HD3 | 1.97 | 0.46 |
| 19:S:12:ASP:O | 19:S:15:LEU:HD12 | 2.15 | 0.46 |
| 1:A:1130:A:OP2 | 1:A:1130:A:H3' | 2.16 | 0.46 |
| 1:A:551:U:H2' | 1:A:552:U:C6 | 2.51 | 0.46 |
| 1:A:701:C:O2' | 1:A:702:A:OP2 | 2.27 | 0.46 |
| 1:A:961:U:H2' | 1:A:962:C:H5' | 1.98 | 0.46 |
| 2:B:132:LYS:C | 2:B:134:GLU:N | 2.67 | 0.46 |
| 2:B:24:TRP:HZ3 | 2:B:29:ALA:HB2 | 1.81 | 0.46 |
| 10:J:75:ILE:O | 10:J:76:ASN:HB2 | 2.16 | 0.46 |
| 12:L:68:ALA:HB3 | 12:L:100:ILE:HD11 | 1.98 | 0.46 |
| 16:P:20:VAL:CG1 | 16:P:32:TYR:CB | 2.93 | 0.46 |
| 1:A:1053:G:C3' | 1:A:1054:C:C5' | 2.94 | 0.46 |
| 1:A:1154:G:H2' | 1:A:1155:G:H8 | 1.81 | 0.46 |
| 1:A:459:G:C6 | 1:A:461:C:H5'' | 2.50 | 0.46 |
| 3:C:3:ASN:O | 3:C:4:LYS:CB | 2.64 | 0.46 |
| 4:D:192:GLU:OE1 | 4:D:192:GLU:HA | 2.15 | 0.46 |
| 2:B:178:ARG:HH22 | 8:H:68:ARG:HH22 | 1.61 | 0.46 |
| 10:J:60:ARG:HA | 10:J:60:ARG:HD3 | 1.89 | 0.46 |
| 11:K:124:LYS:HD2 | 11:K:125:PHE:CZ | 2.50 | 0.46 |
| 12:L:11:VAL:HG13 | 17:Q:29:HIS:CD2 | 2.50 | 0.46 |
| 12:L:46:LYS:HG3 | 12:L:47:LYS:N | 2.31 | 0.46 |
| 14:N:9:LYS:C | 14:N:11:LYS:H | 2.20 | 0.46 |
| 19:S:67:VAL:HG12 | 19:S:68:GLY:N | 2.30 | 0.46 |
| 1:A:1227:A:C4 | 19:S:81:ARG:NH1 | 2.83 | 0.46 |
| 1:A:999:C:H2' | 1:A:1000:U:C6 | 2.50 | 0.45 |
| 1:A:1018:C:H6 | 1:A:1018:C:O5' | 1.99 | 0.45 |
| 1:A:1405:G:O2' | 1:A:1406:U:H5' | 2.16 | 0.45 |
| 1:A:1423:G:O2' | 1:A:1424:C:H5' | 2.16 | 0.45 |
| 1:A:1427:U:H2' | 1:A:1428:A:H8 | 1.81 | 0.45 |
| 2:B:38:GLY:C | 2:B:39:ILE:HG13 | 2.36 | 0.45 |
| 3:C:87:LEU:C | 3:C:89:GLU:N | 2.69 | 0.45 |
| 4:D:151:LYS:N | 4:D:151:LYS:HD2 | 2.31 | 0.45 |
| 8:H:14:ARG:O | 8:H:18:ARG:HD3 | 2.16 | 0.45 |
| 10:J:16:LEU:HD21 | 10:J:94:VAL:HG13 | 1.97 | 0.45 |
| 1:A:103:C:P | 20:T:17:ARG:HH11 | 2.40 | 0.45 |
| 21:U:6:ARG:CD | 21:U:15:ARG:NH1 | 2.79 | 0.45 |
| 1:A:1533:C:H2' | 1:A:1534:A:C5' | 2.42 | 0.45 |
| 1:A:383:A:C2' | 1:A:384:G:H5' | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:831:U:H2' | 1:A:832:C:C6 | 2.51 | 0.45 |
| 2:B:208:ILE:HD12 | 2:B:208:ILE:N | 2.06 | 0.45 |
| 3:C:32:LEU:HD22 | 3:C:59:ARG:NH1 | 2.31 | 0.45 |
| 6:F:48:LEU:HD13 | 6:F:52:ILE:CD1 | 2.44 | 0.45 |
| 8:H:91:ARG:HG3 | 12:L:7:ILE:HG13 | 1.99 | 0.45 |
| 11:K:32:ILE:HD12 | 11:K:32:ILE:N | 2.31 | 0.45 |
| 11:K:43:SER:O | 11:K:44:SER:HB3 | 2.16 | 0.45 |
| 1:A:1313:U:C5 | 19:S:4:SER:HB2 | 2.52 | 0.45 |
| 1:A:7:G:H21 | 5:E:121:LYS:HG2 | 1.81 | 0.45 |
| 2:B:83:MET:HA | 2:B:83:MET:HE2 | 1.97 | 0.45 |
| 3:C:83:ARG:C | 3:C:85:ARG:N | 2.70 | 0.45 |
| 5:E:76:ILE:HG13 | 5:E:142:LEU:HD13 | 1.98 | 0.45 |
| 10:J:23:ILE:CD1 | 10:J:23:ILE:N | 2.78 | 0.45 |
| 10:J:30:SER:CA | 10:J:80:LYS:HG3 | 2.46 | 0.45 |
| 11:K:29:ILE:HG22 | 11:K:44:SER:HB2 | 1.98 | 0.45 |
| 12:L:119:LYS:O | 12:L:120:TYR:CB | 2.64 | 0.45 |
| 14:N:25:VAL:HG12 | 14:N:38:GLY:O | 2.15 | 0.45 |
| 1:A:1090:U:H2' | 1:A:1091:U:H6 | 1.81 | 0.45 |
| 1:A:1141:C:O2' | 1:A:1142:G:H5' | 2.16 | 0.45 |
| 1:A:1313:U:OP2 | 19:S:6:LYS:HA | 2.17 | 0.45 |
| 1:A:1288:A:H1' | 1:A:1352:C:O2' | 2.17 | 0.45 |
| 1:A:1486:G:H2' | 1:A:1487:G:O4' | 2.16 | 0.45 |
| 1:A:443:C:H2' | 1:A:444:C:H6 | 1.82 | 0.45 |
| 2:B:157:ARG:HH11 | 2:B:157:ARG:HG3 | 1.80 | 0.45 |
| 5:E:143:ARG:HD3 | 5:E:143:ARG:HA | 1.57 | 0.45 |
| 5:E:51:VAL:O | 5:E:55:VAL:HG23 | 2.16 | 0.45 |
| 1:A:1152:A:C5' | 10:J:13:HIS:HD2 | 2.16 | 0.45 |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:C8 | 2.52 | 0.45 |
| 1:A:1544:U:O3' | 22:X:1:U:C5' | 2.65 | 0.45 |
| 1:A:67:C:O2' | 1:A:171:A:H1' | 2.16 | 0.45 |
| 1:A:630:G:H8 | 1:A:630:G:H5' | 1.82 | 0.45 |
| 1:A:792:A:H1' | 1:A:794:A:N7 | 2.32 | 0.45 |
| 1:A:979:C:H2' | 1:A:980:C:H5' | 1.98 | 0.45 |
| 4:D:10:ARG:CG | 4:D:10:ARG:HH11 | 2.30 | 0.45 |
| 5:E:40:ARG:HH11 | 5:E:40:ARG:HG2 | 1.82 | 0.45 |
| 15:O:7:GLU:O | 15:O:11:VAL:HG23 | 2.16 | 0.45 |
| 1:A:1060:C:H5'' | 10:J:51:ARG:HB3 | 1.98 | 0.45 |
| 1:A:106:C:O2 | 1:A:379:C:H4' | 2.17 | 0.45 |
| 1:A:1125:U:H5' | 1:A:1126:U:C5 | 2.51 | 0.45 |
| 1:A:1226:C:N4 | 13:M:104:ARG:HG3 | 2.32 | 0.45 |
| 1:A:1296:C:H4' | 1:A:1302:U:C5 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1394:A:C5 | 1:A:1501:C:H4' | 2.51 | 0.45 |
| 1:A:1437:C:H2' | 1:A:1438:G:H8 | 1.82 | 0.45 |
| 1:A:718:G:H5' | 11:K:117:ASN:ND2 | 2.20 | 0.45 |
| 1:A:960:U:H2' | 1:A:960:U:O2 | 2.16 | 0.45 |
| 2:B:184:VAL:N | 2:B:198:ASP:OD2 | 2.50 | 0.45 |
| 2:B:92:TYR:C | 2:B:92:TYR:HD1 | 2.19 | 0.45 |
| 3:C:5:ILE:N | 3:C:5:ILE:HD12 | 2.32 | 0.45 |
| 4:D:64:LEU:HD22 | 4:D:75:PHE:CZ | 2.51 | 0.45 |
| 5:E:77:PRO:HG2 | 5:E:142:LEU:HD22 | 1.98 | 0.45 |
| 7:G:99:LEU:HD22 | 7:G:103:TRP:CZ2 | 2.52 | 0.45 |
| 16:P:20:VAL:HG13 | 16:P:21:VAL:N | 2.32 | 0.45 |
| 1:A:1431:C:C2' | 1:A:1432:G:H5' | 2.47 | 0.45 |
| 1:A:129(A):G:O2' | 1:A:190(E):U:C6 | 2.70 | 0.45 |
| 1:A:627:G:H2' | 1:A:628:G:C8 | 2.51 | 0.45 |
| 4:D:102:ASP:HB3 | 4:D:136:PRO:HA | 1.99 | 0.45 |
| 5:E:144:THR:CG2 | 5:E:145:LYS:N | 2.79 | 0.45 |
| 9:I:79:LEU:HD21 | 9:I:102:LEU:O | 2.17 | 0.45 |
| 13:M:33:ALA:O | 13:M:37:THR:HB | 2.17 | 0.45 |
| 16:P:43:LYS:HB3 | 16:P:48:TRP:CD2 | 2.51 | 0.45 |
| 16:P:4:ILE:HG23 | 16:P:36:ILE:HD11 | 1.99 | 0.45 |
| 17:Q:17:LYS:HA | 17:Q:46:ASP:O | 2.17 | 0.45 |
| 20:T:45:GLN:NE2 | 20:T:45:GLN:O | 2.50 | 0.45 |
| 1:A:1202:G:O2' | 1:A:1203:C:H5' | 2.17 | 0.45 |
| 1:A:1251:A:H2' | 1:A:1252:A:C8 | 2.51 | 0.45 |
| 1:A:579:G:C5' | 1:A:728:A:H1' | 2.30 | 0.45 |
| 2:B:69:LEU:HD22 | 2:B:155:LEU:CD1 | 2.45 | 0.45 |
| 2:B:48:MET:O | 2:B:51:LEU:HB2 | 2.16 | 0.45 |
| 4:D:108:LEU:HD21 | 4:D:174:LEU:HD13 | 1.99 | 0.45 |
| 5:E:28:PHE:O | 5:E:47:LYS:HA | 2.17 | 0.45 |
| 5:E:83:GLU:HG3 | 5:E:88:LYS:HG3 | 1.99 | 0.45 |
| 6:F:30:LEU:HB3 | 6:F:35:ALA:HB3 | 1.98 | 0.45 |
| 11:K:14:VAL:O | 11:K:15:ALA:HB3 | 2.17 | 0.45 |
| 19:S:43:GLU:H | 19:S:43:GLU:CD | 2.20 | 0.45 |
| 20:T:49:ALA:O | 20:T:53:LEU:HD13 | 2.17 | 0.45 |
| 1:A:1147:C:H4' | 9:I:5:TYR:CE2 | 2.52 | 0.45 |
| 1:A:1191:A:H3' | 1:A:1192:C:OP2 | 2.17 | 0.45 |
| 1:A:250:A:O4' | 1:A:252:U:C6 | 2.70 | 0.45 |
| 1:A:266:G:O2' | 1:A:267:C:OP2 | 2.32 | 0.45 |
| 1:A:335:C:H2' | 1:A:336:C:C6 | 2.51 | 0.45 |
| 1:A:445:G:O2' | 1:A:446:G:H5' | 2.17 | 0.45 |
| 1:A:491:G:H2' | 1:A:492:G:C8 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:594:G:O2' | 1:A:595:G:H5' | 2.17 | 0.45 |
| 1:A:659:U:O2' | 1:A:660:G:H5' | 2.17 | 0.45 |
| 1:A:953:G:H2' | 1:A:954:G:O4' | 2.17 | 0.45 |
| 2:B:132:LYS:C | 2:B:134:GLU:H | 2.19 | 0.45 |
| 2:B:60:ASP:C | 2:B:64:ARG:NH1 | 2.70 | 0.45 |
| 3:C:14:ILE:O | 3:C:15:THR:C | 2.55 | 0.45 |
| 3:C:195:VAL:C | 3:C:196:LEU:HD22 | 2.37 | 0.45 |
| 4:D:146:ILE:N | 4:D:146:ILE:CD1 | 2.78 | 0.45 |
| 4:D:58:LEU:CD2 | 4:D:62:GLN:HG2 | 2.47 | 0.45 |
| 5:E:43:LEU:HD23 | 5:E:43:LEU:HA | 1.83 | 0.45 |
| 7:G:12:LEU:H | 7:G:12:LEU:HD12 | 1.82 | 0.45 |
| 10:J:46:ARG:HG2 | 10:J:46:ARG:NH1 | 2.29 | 0.45 |
| 11:K:21:ILE:HD12 | 11:K:95:ILE:HD13 | 1.99 | 0.45 |
| 15:O:2:PRO:O | 15:O:3:ILE:HG13 | 2.16 | 0.45 |
| 17:Q:40:LYS:HE3 | 17:Q:42:TYR:CZ | 2.51 | 0.45 |
| 6:F:91:VAL:HG11 | 18:R:72:ARG:NH1 | 2.32 | 0.45 |
| 1:A:1055:A:C2 | 1:A:1056:U:H1' | 2.52 | 0.45 |
| 2:B:24:TRP:CG | 2:B:25:ASN:N | 2.85 | 0.45 |
| 5:E:31:LEU:HD23 | 5:E:31:LEU:HA | 1.78 | 0.45 |
| 6:F:26:ILE:HG21 | 6:F:63:TYR:OH | 2.16 | 0.45 |
| 8:H:17:THR:HG22 | 8:H:63:LEU:HG | 1.99 | 0.45 |
| 1:A:1232:U:H5'' | 9:I:124:GLN:O | 2.17 | 0.45 |
| 10:J:3:LYS:CB | 10:J:75:ILE:HA | 2.46 | 0.45 |
| 11:K:15:ALA:CA | 11:K:77:MET:HA | 2.47 | 0.45 |
| 1:A:1061:G:H2' | 1:A:1062:U:C6 | 2.53 | 0.44 |
| 1:A:1129:C:OP1 | 9:I:62:TYR:CZ | 2.69 | 0.44 |
| 1:A:1179:A:H2' | 1:A:1180:A:O4' | 2.16 | 0.44 |
| 2:B:69:LEU:HD12 | 2:B:70:PHE:N | 2.32 | 0.44 |
| 2:B:7:VAL:HG11 | 2:B:221:LEU:CD2 | 2.44 | 0.44 |
| 3:C:9:GLY:HA2 | 3:C:12:LEU:HG | 1.99 | 0.44 |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:CA | 2.46 | 0.44 |
| 13:M:6:GLY:O | 13:M:8:GLU:HG2 | 2.16 | 0.44 |
| 17:Q:59:ILE:CG2 | 17:Q:71:PHE:CD1 | 3.00 | 0.44 |
| 19:S:23:ASN:HA | 19:S:26:GLY:O | 2.17 | 0.44 |
| 1:A:1129:C:O2' | 1:A:1130:A:OP2 | 2.34 | 0.44 |
| 1:A:1178:G:N3 | 1:A:1180:A:N7 | 2.65 | 0.44 |
| 1:A:1181:G:O2' | 1:A:1184:G:H5' | 2.16 | 0.44 |
| 1:A:1472:U:O2' | 1:A:1473:A:H5' | 2.17 | 0.44 |
| 1:A:402:G:O2' | 1:A:403:C:H5' | 2.17 | 0.44 |
| 1:A:45:U:H2' | 1:A:46:G:H8 | 1.80 | 0.44 |
| 1:A:693:G:C8 | 1:A:1539:C:H1' | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:974:A:P | 14:N:29:ARG:HH22 | 2.39 | 0.44 |
| 2:B:126:GLU:HG2 | 2:B:129:GLU:OE1 | 2.17 | 0.44 |
| 2:B:44:LEU:H | 2:B:44:LEU:HG | 1.45 | 0.44 |
| 2:B:92:TYR:CD1 | 2:B:151:GLY:HA3 | 2.52 | 0.44 |
| 3:C:70:VAL:HG12 | 3:C:71:ALA:H | 1.82 | 0.44 |
| 6:F:63:TYR:CD2 | 6:F:63:TYR:N | 2.85 | 0.44 |
| 8:H:60:ARG:NH1 | 8:H:60:ARG:CG | 2.80 | 0.44 |
| 9:I:37:PHE:CD1 | 9:I:43:ALA:HB1 | 2.52 | 0.44 |
| 13:M:106:ASN:O | 13:M:107:ALA:HB3 | 2.18 | 0.44 |
| 13:M:19:LEU:C | 13:M:22:ILE:HD13 | 2.36 | 0.44 |
| 15:O:5:LYS:CD | 15:O:5:LYS:H | 2.30 | 0.44 |
| 1:A:1051:C:H2' | 1:A:1052:U:H6 | 1.82 | 0.44 |
| 1:A:304:U:H2' | 1:A:305:G:C8 | 2.53 | 0.44 |
| 1:A:384:G:O2' | 1:A:385:C:H5' | 2.17 | 0.44 |
| 1:A:499:A:H4' | 1:A:500:G:OP1 | 2.17 | 0.44 |
| 1:A:862:C:O2' | 1:A:863:U:H5' | 2.18 | 0.44 |
| 1:A:930:C:C2' | 1:A:931:C:H5' | 2.47 | 0.44 |
| 1:A:969:A:C2' | 1:A:970:C:H5' | 2.48 | 0.44 |
| 3:C:15:THR:HG21 | 3:C:179:ARG:HA | 2.00 | 0.44 |
| 4:D:35:ARG:HH11 | 4:D:35:ARG:HG2 | 1.83 | 0.44 |
| 8:H:118:VAL:C | 8:H:119:LEU:HD23 | 2.37 | 0.44 |
| 11:K:27:ASN:OD1 | 11:K:28:THR:N | 2.50 | 0.44 |
| 16:P:43:LYS:HA | 16:P:48:TRP:HB3 | 1.98 | 0.44 |
| 17:Q:63:ARG:HG2 | 17:Q:64:PRO:CD | 2.46 | 0.44 |
| 1:A:1220:G:H2' | 1:A:1221:G:C8 | 2.53 | 0.44 |
| 1:A:1474:G:O2' | 1:A:1475:G:H5' | 2.18 | 0.44 |
| 1:A:1487:G:O2' | 1:A:1488:G:H5' | 2.17 | 0.44 |
| 1:A:262:A:C6 | 1:A:263:A:C6 | 3.05 | 0.44 |
| 1:A:596:C:O2' | 1:A:597:G:H5' | 2.17 | 0.44 |
| 1:A:644:G:C5 | 1:A:645:C:C5 | 3.05 | 0.44 |
| 3:C:70:VAL:C | 3:C:106:VAL:HG23 | 2.37 | 0.44 |
| 7:G:8:GLU:HG3 | 7:G:8:GLU:H | 1.59 | 0.44 |
| 9:I:33:PHE:CE2 | 9:I:47:LEU:HD11 | 2.53 | 0.44 |
| 11:K:110:ASP:OD2 | 18:R:88:LYS:NZ | 2.42 | 0.44 |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:H | 1.82 | 0.44 |
| 13:M:14:ARG:N | 13:M:44:ARG:HH12 | 2.15 | 0.44 |
| 1:A:1054:C:H5 | 1:A:1196:U:C6 | 2.36 | 0.44 |
| 1:A:190(H):G:O2' | 1:A:190(I):G:H5' | 2.17 | 0.44 |
| 1:A:858:G:O6 | 1:A:869:G:H3' | 2.18 | 0.44 |
| 3:C:40:ARG:HB3 | 3:C:44:GLU:HG3 | 1.99 | 0.44 |
| 4:D:111:ALA:HB3 | 4:D:117:ALA:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:142:PRO:HA | 4:D:185:PHE:HD2 | 1.83 | 0.44 |
| 4:D:173:TRP:O | 4:D:186:LEU:HB2 | 2.17 | 0.44 |
| 4:D:60:GLU:O | 4:D:63:LYS:HB3 | 2.17 | 0.44 |
| 4:D:76:ARG:HH11 | 4:D:76:ARG:HG3 | 1.83 | 0.44 |
| 5:E:20:GLN:HB3 | 5:E:20:GLN:HE21 | 1.60 | 0.44 |
| 6:F:69:GLU:O | 6:F:71:ARG:N | 2.50 | 0.44 |
| 10:J:26:ALA:HB1 | 10:J:84:GLN:HB3 | 1.99 | 0.44 |
| 12:L:73:GLU:CD | 12:L:74:GLY:N | 2.71 | 0.44 |
| 13:M:40:ASN:C | 13:M:40:ASN:HD22 | 2.18 | 0.44 |
| 16:P:26:ARG:HD2 | 16:P:31:LYS:O | 2.17 | 0.44 |
| 18:R:87:ARG:O | 18:R:88:LYS:HB3 | 2.18 | 0.44 |
| 19:S:20:LEU:HD12 | 19:S:21:GLU:HG3 | 2.00 | 0.44 |
| 1:A:1222:G:C2' | 1:A:1223:C:H5' | 2.47 | 0.44 |
| 5:E:53:LEU:H | 5:E:53:LEU:CD2 | 2.23 | 0.44 |
| 7:G:126:ASP:HA | 7:G:131:LYS:HE3 | 2.00 | 0.44 |
| 10:J:28:ARG:NH1 | 10:J:28:ARG:HG2 | 2.32 | 0.44 |
| 11:K:26:ASN:O | 11:K:27:ASN:HB2 | 2.18 | 0.44 |
| 12:L:48:PRO:C | 12:L:49:ASN:HD22 | 2.20 | 0.44 |
| 19:S:40:ILE:HD13 | 19:S:62:ILE:HD13 | 1.98 | 0.44 |
| 1:A:1120:G:H2' | 1:A:1121:U:C6 | 2.52 | 0.44 |
| 1:A:1263:C:H2' | 1:A:1264:C:C6 | 2.53 | 0.44 |
| 1:A:1406:U:O2' | 1:A:1407:C:H5' | 2.18 | 0.44 |
| 1:A:1443:G:H5' | 1:A:1446:A:H3' | 1.98 | 0.44 |
| 1:A:458:C:H2' | 1:A:459:G:C8 | 2.51 | 0.44 |
| 1:A:528:C:H5' | 1:A:535:A:N6 | 2.33 | 0.44 |
| 1:A:620:C:C2 | 4:D:135:LEU:HD13 | 2.53 | 0.44 |
| 2:B:54:THR:O | 2:B:58:ILE:HG13 | 2.18 | 0.44 |
| 3:C:193:TYR:HE1 | 3:C:196:LEU:HD21 | 1.83 | 0.44 |
| 3:C:29:TYR:C | 3:C:29:TYR:CD2 | 2.90 | 0.44 |
| 4:D:100:ARG:O | 4:D:103:ASN:HB3 | 2.18 | 0.44 |
| 4:D:78:LEU:HD22 | 4:D:96:LEU:HB3 | 2.00 | 0.44 |
| 7:G:120:ILE:HG22 | 7:G:124:LEU:HD12 | 1.98 | 0.44 |
| 1:A:160:A:H1' | 1:A:344:A:N7 | 2.33 | 0.44 |
| 1:A:437:U:O2' | 4:D:123:HIS:CD2 | 2.71 | 0.44 |
| 1:A:689:C:H2' | 1:A:690:G:O4' | 2.18 | 0.44 |
| 4:D:163:GLU:C | 4:D:165:MET:N | 2.71 | 0.44 |
| 4:D:4:TYR:O | 4:D:5:ILE:HB | 2.18 | 0.44 |
| 5:E:76:ILE:HG22 | 5:E:78:HIS:O | 2.18 | 0.44 |
| 5:E:93:PRO:HG2 | 8:H:105:ARG:NH2 | 2.33 | 0.44 |
| 6:F:40:VAL:HG22 | 6:F:41:GLU:N | 2.32 | 0.44 |
| 10:J:29:ARG:O | 10:J:84:GLN:NE2 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:K:93:GLN:HE21 | 11:K:96:ARG:HH21 | 1.65 | 0.44 |
| 12:L:126:LYS:HD2 | 12:L:126:LYS:C | 2.38 | 0.44 |
| 1:A:1367:C:H5' | 10:J:60:ARG:HH11 | 1.75 | 0.44 |
| 1:A:1450:U:H2' | 1:A:1452:C:C5 | 2.53 | 0.44 |
| 1:A:112:G:H4' | 1:A:389:A:H5'' | 1.99 | 0.44 |
| 2:B:71:VAL:O | 2:B:165:VAL:HG23 | 2.17 | 0.44 |
| 2:B:75:LYS:HE2 | 2:B:96:ARG:NH2 | 2.32 | 0.44 |
| 1:A:542:G:H5' | 4:D:41:GLY:HA3 | 1.99 | 0.44 |
| 4:D:81:GLU:O | 4:D:85:LYS:HG3 | 2.17 | 0.44 |
| 7:G:38:LEU:HD11 | 7:G:42:ILE:HD11 | 1.99 | 0.44 |
| 10:J:23:ILE:O | 10:J:23:ILE:CG2 | 2.63 | 0.44 |
| 1:A:1367:C:H4' | 10:J:48:THR:HG21 | 2.00 | 0.44 |
| 10:J:3:LYS:HA | 10:J:74:ILE:O | 2.18 | 0.44 |
| 12:L:25:PRO:C | 12:L:27:LEU:N | 2.61 | 0.44 |
| 16:P:82:GLN:O | 16:P:83:GLU:C | 2.56 | 0.44 |
| 20:T:74:LYS:HB3 | 20:T:74:LYS:HE3 | 1.77 | 0.44 |
| 1:A:1047:G:O2' | 1:A:1048:G:H5' | 2.17 | 0.43 |
| 1:A:1194:U:O2' | 1:A:1195:C:H5' | 2.17 | 0.43 |
| 1:A:1298:C:H4' | 1:A:1299:A:O4' | 2.18 | 0.43 |
| 1:A:1238:A:N7 | 1:A:1303:C:H1' | 2.33 | 0.43 |
| 1:A:1425:U:H3 | 1:A:1475:G:H1 | 1.65 | 0.43 |
| 1:A:51:A:H4' | 1:A:52:G:C5' | 2.47 | 0.43 |
| 1:A:9:G:N7 | 1:A:558:G:O2' | 2.48 | 0.43 |
| 3:C:3:ASN:N | 3:C:3:ASN:OD1 | 2.51 | 0.43 |
| 3:C:47:LEU:HD12 | 3:C:47:LEU:H | 1.82 | 0.43 |
| 5:E:72:GLN:O | 5:E:73:ASN:HB3 | 2.18 | 0.43 |
| 5:E:80:ILE:CD1 | 5:E:91:LEU:HD12 | 2.48 | 0.43 |
| 7:G:145:ALA:C | 7:G:147:ALA:N | 2.71 | 0.43 |
| 10:J:89:ASP:CB | 10:J:91:PRO:HD2 | 2.46 | 0.43 |
| 11:K:11:LYS:O | 11:K:12:ARG:HB2 | 2.18 | 0.43 |
| 12:L:104:VAL:O | 12:L:105:TYR:HB2 | 2.18 | 0.43 |
| 18:R:54:ARG:H | 18:R:54:ARG:HD3 | 1.82 | 0.43 |
| 1:A:1010:G:H2' | 1:A:1011:G:H8 | 1.83 | 0.43 |
| 1:A:1222:G:O2' | 1:A:1223:C:H5' | 2.18 | 0.43 |
| 1:A:1505:G:H4' | 1:A:1506:U:O5' | 2.18 | 0.43 |
| 1:A:603:U:H2' | 1:A:604:G:C8 | 2.53 | 0.43 |
| 2:B:74:LYS:O | 2:B:76:GLN:N | 2.43 | 0.43 |
| 3:C:112:SER:C | 3:C:114:PRO:HD2 | 2.37 | 0.43 |
| 3:C:150:LYS:CG | 3:C:169:ALA:HB2 | 2.45 | 0.43 |
| 3:C:91:LEU:C | 3:C:91:LEU:HD23 | 2.38 | 0.43 |
| 12:L:40:VAL:HG21 | 12:L:78:GLN:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1156:G:H3' | 1:A:1157:A:OP2 | 2.17 | 0.43 |
| 1:A:613:C:O2' | 1:A:614:A:H5' | 2.18 | 0.43 |
| 1:A:983:A:H2 | 1:A:984:C:C6 | 2.36 | 0.43 |
| 2:B:157:ARG:HG2 | 2:B:158:LEU:N | 2.31 | 0.43 |
| 3:C:157:ILE:CG2 | 3:C:164:ARG:HH21 | 2.31 | 0.43 |
| 4:D:58:LEU:HD22 | 4:D:62:GLN:HG2 | 1.99 | 0.43 |
| 9:I:4:TYR:O | 9:I:18:PHE:HA | 2.17 | 0.43 |
| 9:I:81:ILE:HG22 | 9:I:81:ILE:O | 2.17 | 0.43 |
| 12:L:47:LYS:HB3 | 12:L:48:PRO:HD2 | 1.91 | 0.43 |
| 12:L:58:VAL:O | 12:L:65:GLU:HA | 2.17 | 0.43 |
| 16:P:67:THR:CG2 | 16:P:68:ASP:N | 2.81 | 0.43 |
| 17:Q:52:LYS:O | 17:Q:55:ASP:HB2 | 2.18 | 0.43 |
| 17:Q:63:ARG:O | 17:Q:65:ILE:HD12 | 2.18 | 0.43 |
| 1:A:1171:G:H2' | 1:A:1172:C:C6 | 2.54 | 0.43 |
| 1:A:1495:U:H2' | 1:A:1496:C:C6 | 2.53 | 0.43 |
| 1:A:149:A:H2' | 1:A:150:C:H6 | 1.82 | 0.43 |
| 1:A:382:A:C2 | 1:A:383:A:C4 | 3.07 | 0.43 |
| 1:A:424:G:H2' | 1:A:425:G:H8 | 1.83 | 0.43 |
| 1:A:487:A:H2' | 1:A:488:C:O4' | 2.19 | 0.43 |
| 1:A:976:G:N7 | 1:A:1358:U:C2 | 2.87 | 0.43 |
| 1:A:993:G:O2' | 1:A:994:A:P | 2.76 | 0.43 |
| 2:B:107:THR:C | 2:B:109:SER:N | 2.71 | 0.43 |
| 2:B:187:LEU:HD21 | 2:B:203:GLY:HA3 | 1.99 | 0.43 |
| 3:C:108:ASN:ND2 | 3:C:144:SER:HB3 | 2.33 | 0.43 |
| 3:C:164:ARG:NH1 | 3:C:166:GLU:OE1 | 2.52 | 0.43 |
| 1:A:620:C:C1' | 4:D:135:LEU:HD13 | 2.49 | 0.43 |
| 4:D:42:GLN:CG | 4:D:42:GLN:O | 2.65 | 0.43 |
| 5:E:142:LEU:O | 5:E:143:ARG:HD3 | 2.19 | 0.43 |
| 6:F:21:LEU:O | 6:F:25:ILE:HG13 | 2.18 | 0.43 |
| 5:E:93:PRO:HG2 | 8:H:105:ARG:CZ | 2.48 | 0.43 |
| 9:I:9:ARG:HD3 | 9:I:14:VAL:HG12 | 2.01 | 0.43 |
| 1:A:718:G:C4' | 11:K:117:ASN:HD22 | 2.30 | 0.43 |
| 12:L:60:LEU:N | 12:L:64:TYR:O | 2.48 | 0.43 |
| 17:Q:82:MET:O | 17:Q:86:GLU:HG2 | 2.18 | 0.43 |
| 1:A:1059:C:O2' | 1:A:1060:C:H5' | 2.18 | 0.43 |
| 1:A:1193:G:HO2' | 1:A:1194:U:H5' | 1.83 | 0.43 |
| 1:A:1217:C:O2' | 1:A:1218:C:H5' | 2.18 | 0.43 |
| 1:A:475:G:H2' | 1:A:476:G:C8 | 2.53 | 0.43 |
| 1:A:646:U:H2' | 1:A:647:C:C6 | 2.53 | 0.43 |
| 1:A:952:U:O2' | 1:A:953:G:H5' | 2.18 | 0.43 |
| 2:B:185:ILE:H | 2:B:185:ILE:HD12 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:74:LYS:HD3 | 2:B:205:ASP:O | 2.18 | 0.43 |
| 3:C:54:ARG:HG3 | 3:C:55:VAL:H | 1.82 | 0.43 |
| 4:D:64:LEU:HD21 | 4:D:97:LEU:CD1 | 2.48 | 0.43 |
| 9:I:8:GLY:HA3 | 9:I:76:ALA:O | 2.18 | 0.43 |
| 11:K:14:VAL:HG21 | 11:K:40:ILE:CD1 | 2.48 | 0.43 |
| 11:K:91:ARG:HD2 | 11:K:92:GLU:OE1 | 2.18 | 0.43 |
| 12:L:41:ARG:NH2 | 12:L:57:LYS:HZ3 | 2.15 | 0.43 |
| 17:Q:79:SER:O | 17:Q:80:GLY:O | 2.36 | 0.43 |
| 19:S:63:THR:OG1 | 19:S:66:MET:HG2 | 2.19 | 0.43 |
| 1:A:476:G:O2' | 1:A:477:G:H5' | 2.19 | 0.43 |
| 2:B:10:LEU:HD23 | 2:B:10:LEU:C | 2.39 | 0.43 |
| 2:B:157:ARG:HG3 | 2:B:157:ARG:NH1 | 2.33 | 0.43 |
| 3:C:53:ALA:HB2 | 3:C:115:LEU:HG | 2.00 | 0.43 |
| 3:C:11:ARG:O | 3:C:13:GLY:N | 2.52 | 0.43 |
| 1:A:1191:A:H5'' | 3:C:4:LYS:NZ | 2.33 | 0.43 |
| 4:D:3:ARG:CZ | 4:D:5:ILE:HD11 | 2.48 | 0.43 |
| 6:F:25:ILE:HD13 | 6:F:82:ARG:HD3 | 2.01 | 0.43 |
| 10:J:6:ILE:CD1 | 10:J:73:ASP:H | 2.26 | 0.43 |
| 13:M:121:LYS:C | 13:M:123:ALA:H | 2.22 | 0.43 |
| 21:U:15:ARG:CG | 21:U:15:ARG:HH11 | 2.26 | 0.43 |
| 1:A:1072:G:H2' | 1:A:1073:U:C6 | 2.54 | 0.43 |
| 1:A:1223:C:OP2 | 1:A:1224:G:H2' | 2.18 | 0.43 |
| 1:A:1226:C:H5' | 19:S:80:TYR:CE1 | 2.54 | 0.43 |
| 1:A:1236:A:H2' | 1:A:1237:C:C6 | 2.54 | 0.43 |
| 1:A:1312:G:N7 | 19:S:3:ARG:O | 2.52 | 0.43 |
| 1:A:1337:G:H5'' | 1:A:1338:G:OP1 | 2.19 | 0.43 |
| 1:A:1351:U:O2' | 1:A:1352:C:H5' | 2.19 | 0.43 |
| 1:A:1518:A:H2' | 1:A:1519:A:C8 | 2.53 | 0.43 |
| 1:A:163:C:O2' | 1:A:164:U:H5' | 2.18 | 0.43 |
| 1:A:404:U:H2' | 1:A:405:U:H6 | 1.83 | 0.43 |
| 1:A:518:C:H2' | 1:A:530:G:N3 | 2.33 | 0.43 |
| 1:A:838:G:N2 | 1:A:849:C:C2 | 2.87 | 0.43 |
| 1:A:895:G:H2' | 1:A:896:C:H6 | 1.82 | 0.43 |
| 1:A:941:G:C2 | 1:A:942:G:C8 | 3.07 | 0.43 |
| 2:B:24:TRP:HB3 | 2:B:40:HIS:CD2 | 2.53 | 0.43 |
| 3:C:14:ILE:CG2 | 3:C:15:THR:H | 1.98 | 0.43 |
| 1:A:1112:C:C2 | 3:C:178:LEU:HB2 | 2.54 | 0.43 |
| 4:D:121:VAL:HG12 | 4:D:134:ASP:HA | 1.99 | 0.43 |
| 4:D:126:ILE:HG22 | 4:D:127:THR:H | 1.81 | 0.43 |
| 6:F:71:ARG:O | 6:F:72:VAL:C | 2.57 | 0.43 |
| 5:E:152:ARG:HA | 8:H:64:LYS:NZ | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:75:ASP:O | 9:I:78:LYS:HB3 | 2.19 | 0.43 |
| 20:T:26:ASN:O | 20:T:29:LYS:N | 2.51 | 0.43 |
| 20:T:73:HIS:O | 20:T:74:LYS:CB | 2.67 | 0.43 |
| 1:A:184:G:O2' | 1:A:185:A:H5' | 2.19 | 0.43 |
| 1:A:832:C:O2' | 1:A:833:U:H5' | 2.19 | 0.43 |
| 2:B:53:ARG:NH1 | 2:B:199:TYR:CD2 | 2.87 | 0.43 |
| 2:B:74:LYS:HD2 | 2:B:166:ASP:HB2 | 2.00 | 0.43 |
| 2:B:74:LYS:O | 2:B:75:LYS:HB2 | 2.18 | 0.43 |
| 3:C:5:ILE:H | 3:C:5:ILE:CD1 | 2.32 | 0.43 |
| 3:C:95:THR:C | 3:C:97:LYS:N | 2.72 | 0.43 |
| 19:S:42:PRO:O | 19:S:45:VAL:HG23 | 2.19 | 0.43 |
| 21:U:23:PRO:C | 21:U:25:LYS:H | 2.22 | 0.43 |
| 1:A:1505:G:C2' | 1:A:1541:U:OP2 | 2.67 | 0.43 |
| 1:A:242:C:H2' | 1:A:243:A:H5' | 2.01 | 0.43 |
| 1:A:41:G:H2' | 1:A:42:G:C8 | 2.53 | 0.43 |
| 1:A:909:A:H2' | 1:A:910:C:O4' | 2.19 | 0.43 |
| 1:A:915:A:C2' | 1:A:916:G:H5' | 2.49 | 0.43 |
| 2:B:82:ARG:HD3 | 2:B:83:MET:HE2 | 2.01 | 0.43 |
| 4:D:33:MET:O | 4:D:37:PRO:HB3 | 2.18 | 0.43 |
| 5:E:24:ARG:O | 5:E:25:ARG:HG2 | 2.19 | 0.43 |
| 6:F:43:LEU:HD13 | 6:F:43:LEU:O | 2.18 | 0.43 |
| 7:G:146:GLU:C | 7:G:148:ASN:H | 2.20 | 0.43 |
| 10:J:81:THR:C | 10:J:83:GLU:N | 2.72 | 0.43 |
| 12:L:93:LEU:HD23 | 12:L:93:LEU:N | 2.34 | 0.43 |
| 12:L:6:THR:OG1 | 12:L:9:GLN:HG3 | 2.18 | 0.43 |
| 13:M:19:LEU:CA | 13:M:22:ILE:HD13 | 2.49 | 0.43 |
| 13:M:37:THR:HG23 | 13:M:55:ARG:CG | 2.49 | 0.43 |
| 19:S:33:THR:CG2 | 19:S:34:TRP:N | 2.82 | 0.43 |
| 1:A:1138:G:N1 | 1:A:1140:C:C2 | 2.87 | 0.43 |
| 1:A:1237:C:H2' | 1:A:1336:C:H5 | 1.84 | 0.43 |
| 1:A:1453:G:H2' | 1:A:1454:G:O4' | 2.19 | 0.43 |
| 1:A:706:A:H4' | 11:K:29:ILE:HD11 | 2.00 | 0.43 |
| 6:F:101:ALA:HB2 | 18:R:28:GLU:CB | 2.42 | 0.43 |
| 8:H:4:ASP:OD2 | 8:H:7:ALA:CB | 2.66 | 0.43 |
| 17:Q:57:VAL:HG23 | 17:Q:59:ILE:HD13 | 2.00 | 0.43 |
| 23:Y:34:TM2:H6 | 23:Y:34:TM2:O5' | 2.19 | 0.43 |
| 1:A:1320:C:O2 | 19:S:72:GLY:HA3 | 2.18 | 0.42 |
| 1:A:339:C:H2' | 1:A:340:U:H6 | 1.84 | 0.42 |
| 1:A:384:G:H2' | 1:A:385:C:C6 | 2.54 | 0.42 |
| 6:F:41:GLU:HB2 | 6:F:62:TRP:HB3 | 2.00 | 0.42 |
| 10:J:47:PHE:CZ | 14:N:37:PHE:HE1 | 2.36 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1221:G:C2' | 1:A:1222:G:H5' | 2.49 | 0.42 |
| 1:A:1281:U:H4' | 1:A:1282:C:OP2 | 2.20 | 0.42 |
| 1:A:1329:A:P | 13:M:28:ALA:HB3 | 2.59 | 0.42 |
| 1:A:1251:A:H1' | 1:A:1369:C:O2' | 2.18 | 0.42 |
| 1:A:151:A:H2' | 1:A:152:A:O4' | 2.18 | 0.42 |
| 1:A:586:C:O3' | 8:H:89:PRO:HB2 | 2.20 | 0.42 |
| 2:B:107:THR:C | 2:B:109:SER:H | 2.22 | 0.42 |
| 1:A:1056:U:C5' | 3:C:163:ALA:HB2 | 2.49 | 0.42 |
| 3:C:79:ARG:C | 3:C:81:GLY:H | 2.22 | 0.42 |
| 4:D:98:GLU:HG2 | 4:D:189:PRO:HG2 | 2.01 | 0.42 |
| 7:G:18:TYR:CE2 | 7:G:59:LEU:HB2 | 2.54 | 0.42 |
| 9:I:3:GLN:HE22 | 9:I:20:ARG:NH2 | 2.12 | 0.42 |
| 9:I:96:LEU:HD12 | 9:I:96:LEU:N | 2.33 | 0.42 |
| 10:J:8:LEU:CD2 | 10:J:96:ILE:HG12 | 2.48 | 0.42 |
| 12:L:113:ARG:NH1 | 12:L:116:SER:H | 2.16 | 0.42 |
| 12:L:46:LYS:CG | 12:L:47:LYS:N | 2.82 | 0.42 |
| 13:M:9:ILE:HD12 | 13:M:9:ILE:H | 1.84 | 0.42 |
| 19:S:74:PHE:N | 19:S:74:PHE:CD1 | 2.86 | 0.42 |
| 1:A:1175:G:C2 | 1:A:1176:A:N7 | 2.86 | 0.42 |
| 1:A:1305:G:O2' | 1:A:1331:G:N2 | 2.53 | 0.42 |
| 1:A:1330:U:H5'' | 1:A:1331:G:OP2 | 2.18 | 0.42 |
| 1:A:1351:U:H4' | 7:G:33:ASP:OD2 | 2.18 | 0.42 |
| 1:A:1385:G:O2' | 1:A:1386:G:H5' | 2.20 | 0.42 |
| 1:A:335:C:H2' | 1:A:336:C:H6 | 1.83 | 0.42 |
| 1:A:393:A:C2' | 1:A:394:G:H5' | 2.50 | 0.42 |
| 1:A:456:C:O2' | 1:A:457:C:H5' | 2.19 | 0.42 |
| 1:A:778:G:O2' | 1:A:779:C:H5' | 2.19 | 0.42 |
| 1:A:792:A:C4 | 1:A:794:A:C6 | 3.07 | 0.42 |
| 2:B:124:SER:CB | 2:B:125:PRO:HD2 | 2.41 | 0.42 |
| 2:B:79:ASP:C | 2:B:81:VAL:N | 2.71 | 0.42 |
| 4:D:126:ILE:CG2 | 4:D:127:THR:N | 2.79 | 0.42 |
| 4:D:24:GLU:C | 4:D:26:CYS:H | 2.23 | 0.42 |
| 4:D:61:LYS:NZ | 4:D:62:GLN:NE2 | 2.67 | 0.42 |
| 10:J:6:ILE:O | 10:J:71:LEU:HD13 | 2.19 | 0.42 |
| 12:L:54:LYS:CD | 12:L:54:LYS:N | 2.81 | 0.42 |
| 13:M:11:ARG:HD3 | 13:M:11:ARG:C | 2.40 | 0.42 |
| 13:M:3:ARG:CZ | 13:M:7:VAL:HA | 2.48 | 0.42 |
| 15:O:70:LEU:HD13 | 15:O:78:TYR:HA | 2.01 | 0.42 |
| 1:A:1388:C:H2' | 1:A:1389:C:C6 | 2.55 | 0.42 |
| 1:A:247:G:OP1 | 17:Q:100:LYS:HE3 | 2.19 | 0.42 |
| 1:A:413:G:H1' | 1:A:428:G:H21 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:594:G:C2' | 1:A:595:G:H5' | 2.49 | 0.42 |
| 1:A:840:C:H4' | 1:A:848:C:C2 | 2.55 | 0.42 |
| 1:A:939:G:H2' | 1:A:940:C:H6 | 1.78 | 0.42 |
| 1:A:998:G:O2' | 1:A:999:C:H5' | 2.19 | 0.42 |
| 9:I:10:ARG:CD | 9:I:105:ASP:HB3 | 2.49 | 0.42 |
| 12:L:10:LEU:HD21 | 12:L:15:ARG:NE | 2.34 | 0.42 |
| 13:M:4:ILE:HG22 | 13:M:5:ALA:H | 1.80 | 0.42 |
| 17:Q:65:ILE:N | 17:Q:65:ILE:CD1 | 2.79 | 0.42 |
| 1:A:1212:U:H4' | 1:A:1213:A:C8 | 2.55 | 0.42 |
| 1:A:1256:A:H2 | 1:A:1277:C:C5 | 2.38 | 0.42 |
| 1:A:1508:G:O2' | 1:A:1509:C:H5' | 2.19 | 0.42 |
| 1:A:197:A:N1 | 1:A:220:G:O2' | 2.46 | 0.42 |
| 1:A:490:G:O2' | 1:A:491:G:H5' | 2.20 | 0.42 |
| 2:B:135:GLN:C | 2:B:137:ARG:H | 2.23 | 0.42 |
| 2:B:85:ALA:CB | 2:B:92:TYR:HD2 | 2.32 | 0.42 |
| 8:H:117:GLY:O | 8:H:119:LEU:HD23 | 2.19 | 0.42 |
| 8:H:72:PRO:O | 8:H:73:ASP:HB3 | 2.20 | 0.42 |
| 10:J:49:VAL:HG22 | 14:N:41:ARG:HD2 | 2.00 | 0.42 |
| 1:A:1058:G:C6 | 1:A:1059:C:N3 | 2.88 | 0.42 |
| 1:A:794:A:H2' | 1:A:795:C:C6 | 2.54 | 0.42 |
| 1:A:833:U:H2' | 1:A:834:C:H6 | 1.81 | 0.42 |
| 2:B:123:ALA:N | 2:B:127:ILE:HG12 | 2.34 | 0.42 |
| 2:B:204:ASN:HD21 | 2:B:206:ASP:H | 1.62 | 0.42 |
| 2:B:216:SER:O | 2:B:219:VAL:N | 2.50 | 0.42 |
| 2:B:85:ALA:HB3 | 2:B:92:TYR:CD2 | 2.53 | 0.42 |
| 5:E:20:GLN:O | 5:E:21:ALA:C | 2.58 | 0.42 |
| 9:I:40:LEU:O | 9:I:42:ARG:N | 2.53 | 0.42 |
| 10:J:30:SER:HB2 | 10:J:80:LYS:C | 2.39 | 0.42 |
| 12:L:111:LYS:O | 12:L:112:ASP:HB2 | 2.19 | 0.42 |
| 13:M:108:ARG:CA | 13:M:108:ARG:HE | 2.21 | 0.42 |
| 13:M:6:GLY:O | 13:M:7:VAL:HG22 | 2.20 | 0.42 |
| 20:T:56:MET:CE | 20:T:88:VAL:HG11 | 2.50 | 0.42 |
| 1:A:1034:G:N2 | 1:A:1035:A:N6 | 2.66 | 0.42 |
| 1:A:1279:A:H5'' | 1:A:1280:A:OP1 | 2.19 | 0.42 |
| 1:A:1314:C:OP2 | 19:S:6:LYS:CD | 2.68 | 0.42 |
| 1:A:1422:G:O2' | 1:A:1423:G:H5' | 2.19 | 0.42 |
| 1:A:838:G:C2' | 1:A:839:U:H5'' | 2.47 | 0.42 |
| 4:D:12:CYS:SG | 4:D:19:LEU:HB2 | 2.59 | 0.42 |
| 4:D:64:LEU:CD2 | 4:D:64:LEU:C | 2.87 | 0.42 |
| 5:E:101:ILE:HD12 | 5:E:119:LEU:CD2 | 2.50 | 0.42 |
| 6:F:63:TYR:N | 6:F:63:TYR:HD2 | 2.16 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:102:LEU:CD1 | 9:I:102:LEU:H | 2.33 | 0.42 |
| 9:I:37:PHE:HD1 | 9:I:43:ALA:HB1 | 1.84 | 0.42 |
| 13:M:60:VAL:HG12 | 13:M:66:LEU:HD11 | 2.01 | 0.42 |
| 13:M:94:ARG:NH1 | 13:M:94:ARG:HG3 | 2.34 | 0.42 |
| 23:Y:35:A:H2' | 23:Y:36:A:O4' | 2.20 | 0.42 |
| 1:A:1130:A:H1' | 1:A:1146:A:H2 | 1.83 | 0.42 |
| 1:A:1167:A:H2' | 1:A:1168:A:H8 | 1.83 | 0.42 |
| 1:A:1285:A:H4' | 1:A:1286:A:O5' | 2.20 | 0.42 |
| 1:A:1503:A:O2' | 1:A:1504:G:O5' | 2.37 | 0.42 |
| 1:A:21:G:H2' | 1:A:22:G:C8 | 2.55 | 0.42 |
| 2:B:144:ARG:C | 2:B:146:GLN:H | 2.23 | 0.42 |
| 2:B:185:ILE:HD12 | 2:B:185:ILE:N | 2.34 | 0.42 |
| 2:B:80:ILE:HD11 | 2:B:208:ILE:CG2 | 2.47 | 0.42 |
| 2:B:96:ARG:O | 2:B:98:LEU:HD23 | 2.19 | 0.42 |
| 3:C:130:VAL:O | 3:C:134:ILE:HG13 | 2.20 | 0.42 |
| 4:D:33:MET:HE3 | 4:D:37:PRO:HA | 2.01 | 0.42 |
| 4:D:98:GLU:OE2 | 4:D:103:ASN:ND2 | 2.42 | 0.42 |
| 9:I:24:GLY:HA2 | 9:I:59:PHE:O | 2.19 | 0.42 |
| 10:J:21:GLN:O | 10:J:25:GLU:HG3 | 2.20 | 0.42 |
| 10:J:4:ILE:O | 10:J:73:ASP:HA | 2.19 | 0.42 |
| 10:J:94:VAL:CG1 | 10:J:95:GLU:N | 2.82 | 0.42 |
| 12:L:41:ARG:HH22 | 12:L:57:LYS:HZ3 | 1.68 | 0.42 |
| 12:L:61:THR:C | 12:L:63:GLY:H | 2.23 | 0.42 |
| 12:L:83:VAL:CG2 | 12:L:84:LEU:N | 2.83 | 0.42 |
| 16:P:75:ARG:HG3 | 16:P:75:ARG:NH1 | 2.35 | 0.42 |
| 1:A:1010:G:H2' | 1:A:1011:G:C8 | 2.55 | 0.42 |
| 1:A:1225:A:N3 | 1:A:1225:A:H2' | 2.35 | 0.42 |
| 1:A:1305:G:OP1 | 21:U:2:GLY:N | 2.53 | 0.42 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 3.07 | 0.42 |
| 1:A:741:G:H2' | 1:A:742:G:O4' | 2.20 | 0.42 |
| 1:A:782:A:H2' | 1:A:783:C:O4' | 2.20 | 0.42 |
| 1:A:817:C:C2 | 1:A:819:A:O4' | 2.72 | 0.42 |
| 2:B:20:GLU:HB2 | 2:B:190:THR:HB | 2.02 | 0.42 |
| 3:C:11:ARG:O | 3:C:12:LEU:C | 2.58 | 0.42 |
| 1:A:8:A:H5' | 5:E:101:ILE:HG22 | 2.02 | 0.42 |
| 6:F:34:GLY:N | 6:F:71:ARG:NH2 | 2.68 | 0.42 |
| 7:G:51:GLN:O | 7:G:53:LYS:N | 2.44 | 0.42 |
| 8:H:11:THR:O | 8:H:12:ARG:C | 2.57 | 0.42 |
| 11:K:69:ALA:O | 11:K:73:MET:HG2 | 2.20 | 0.42 |
| 12:L:53:ARG:HH11 | 12:L:53:ARG:HG2 | 1.84 | 0.42 |
| 13:M:32:GLU:O | 13:M:35:GLU:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:70:LEU:HB3 | 15:O:78:TYR:HB2 | 2.01 | 0.42 |
| 17:Q:66:SER:OG | 17:Q:69:LYS:HB2 | 2.20 | 0.42 |
| 18:R:87:ARG:HB3 | 18:R:88:LYS:H | 1.45 | 0.42 |
| 22:X:3:G:O2' | 22:X:4:A:C5' | 2.33 | 0.42 |
| 1:A:1175:G:N3 | 1:A:1176:A:N9 | 2.67 | 0.42 |
| 1:A:1475:G:H2' | 1:A:1476:G:C8 | 2.55 | 0.42 |
| 1:A:184:G:H2' | 1:A:185:A:H8 | 1.84 | 0.42 |
| 1:A:197:A:H4' | 1:A:198:G:O5' | 2.19 | 0.42 |
| 1:A:338:A:H2' | 1:A:339:C:O4' | 2.20 | 0.42 |
| 1:A:513:C:H2' | 1:A:514:C:H6 | 1.83 | 0.42 |
| 1:A:930:C:H2' | 1:A:931:C:H5' | 2.02 | 0.42 |
| 2:B:100:GLY:O | 2:B:104:ASN:N | 2.46 | 0.42 |
| 2:B:20:GLU:O | 2:B:21:ARG:O | 2.38 | 0.42 |
| 6:F:69:GLU:C | 6:F:71:ARG:H | 2.24 | 0.42 |
| 9:I:55:ALA:O | 9:I:56:LEU:CB | 2.65 | 0.42 |
| 9:I:114:TYR:HD2 | 10:J:60:ARG:HB2 | 1.76 | 0.42 |
| 10:J:15:THR:CG2 | 10:J:94:VAL:HG23 | 2.48 | 0.42 |
| 7:G:149:ARG:HD2 | 11:K:59:TYR:CE1 | 2.54 | 0.42 |
| 11:K:59:TYR:O | 11:K:62:GLN:N | 2.53 | 0.42 |
| 17:Q:82:MET:HA | 17:Q:85:VAL:HG23 | 2.02 | 0.42 |
| 20:T:57:ARG:NE | 20:T:102:GLY:HA3 | 2.34 | 0.42 |
| 1:A:107:G:H2' | 1:A:108:G:C5' | 2.50 | 0.41 |
| 1:A:1279:A:O2' | 1:A:1282:C:N4 | 2.53 | 0.41 |
| 1:A:1499:A:C1' | 1:A:1520:G:H5' | 2.49 | 0.41 |
| 1:A:806:C:O2' | 1:A:807:A:H5' | 2.20 | 0.41 |
| 1:A:920:U:H2' | 1:A:921:U:C6 | 2.55 | 0.41 |
| 2:B:184:VAL:HG12 | 2:B:197:VAL:HA | 2.02 | 0.41 |
| 2:B:236:TYR:O | 2:B:236:TYR:CD2 | 2.73 | 0.41 |
| 2:B:73:THR:O | 2:B:75:LYS:N | 2.53 | 0.41 |
| 4:D:60:GLU:OE2 | 4:D:198:VAL:HA | 2.20 | 0.41 |
| 5:E:36:ASP:O | 5:E:37:ARG:HB2 | 2.20 | 0.41 |
| 14:N:35:ARG:C | 14:N:37:PHE:H | 2.24 | 0.41 |
| 1:A:1029:C:H2' | 1:A:1030:C:C6 | 2.55 | 0.41 |
| 1:A:1153:C:C2 | 1:A:1154:G:C8 | 3.09 | 0.41 |
| 1:A:1299:A:C5 | 1:A:1301:U:C2 | 3.08 | 0.41 |
| 1:A:1363:A:H1' | 1:A:1365:G:N7 | 2.35 | 0.41 |
| 2:B:197:VAL:CB | 2:B:200:ILE:HG12 | 2.43 | 0.41 |
| 2:B:88:ALA:HB2 | 2:B:219:VAL:CG1 | 2.45 | 0.41 |
| 3:C:25:GLY:HA3 | 3:C:26:LYS:NZ | 2.36 | 0.41 |
| 5:E:42:GLY:HA2 | 5:E:65:ASN:O | 2.20 | 0.41 |
| 6:F:46:ARG:HB3 | 6:F:46:ARG:HH11 | 1.78 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:15:ASP:OD2 | 7:G:44:TYR:OH | 2.37 | 0.41 |
| 8:H:77:GLU:CG | 8:H:78:GLN:N | 2.83 | 0.41 |
| 12:L:46:LYS:CG | 12:L:47:LYS:H | 2.32 | 0.41 |
| 9:I:128:ARG:HG2 | 13:M:126:LYS:HD3 | 2.03 | 0.41 |
| 13:M:96:LEU:O | 13:M:97:PRO:C | 2.56 | 0.41 |
| 16:P:81:ARG:CG | 16:P:83:GLU:HG2 | 2.50 | 0.41 |
| 1:A:1294:G:O2' | 1:A:1295:G:H5' | 2.21 | 0.41 |
| 1:A:1347:G:H3' | 9:I:108:VAL:O | 2.19 | 0.41 |
| 1:A:1396:A:H2 | 5:E:19:MET:HG3 | 1.85 | 0.41 |
| 1:A:1527:C:C2' | 1:A:1528:U:H5' | 2.50 | 0.41 |
| 1:A:190(I):G:O2' | 1:A:190(J):U:H5' | 2.20 | 0.41 |
| 1:A:448:A:H2' | 1:A:449:C:H6 | 1.82 | 0.41 |
| 2:B:173:ALA:O | 2:B:174:VAL:C | 2.58 | 0.41 |
| 2:B:209:ARG:HG2 | 2:B:239:VAL:CG1 | 2.50 | 0.41 |
| 3:C:157:ILE:HG21 | 3:C:164:ARG:HH21 | 1.85 | 0.41 |
| 3:C:180:ALA:HB1 | 3:C:182:ILE:HG13 | 2.01 | 0.41 |
| 4:D:175:SER:HB3 | 4:D:186:LEU:HD11 | 2.00 | 0.41 |
| 6:F:14:LEU:HD12 | 6:F:14:LEU:O | 2.20 | 0.41 |
| 6:F:40:VAL:HA | 6:F:63:TYR:HA | 2.01 | 0.41 |
| 1:A:1298:C:H2' | 7:G:114:ARG:NH2 | 2.36 | 0.41 |
| 13:M:67:GLU:O | 13:M:69:GLU:N | 2.53 | 0.41 |
| 20:T:24:LEU:O | 20:T:24:LEU:HD12 | 2.19 | 0.41 |
| 1:A:1189:C:OP1 | 10:J:51:ARG:NH2 | 2.44 | 0.41 |
| 1:A:1262:C:H42 | 1:A:1273:G:H1 | 1.68 | 0.41 |
| 1:A:1305:G:H5'' | 21:U:4:GLY:C | 2.41 | 0.41 |
| 1:A:1360:A:H8 | 1:A:1360:A:OP1 | 2.04 | 0.41 |
| 2:B:124:SER:C | 2:B:126:GLU:H | 2.23 | 0.41 |
| 2:B:140:HIS:HA | 2:B:143:GLU:OE1 | 2.20 | 0.41 |
| 2:B:184:VAL:HB | 2:B:198:ASP:OD2 | 2.21 | 0.41 |
| 2:B:27:LYS:O | 2:B:194:PRO:HG2 | 2.20 | 0.41 |
| 3:C:70:VAL:CG1 | 3:C:71:ALA:N | 2.82 | 0.41 |
| 7:G:78:ARG:NH1 | 7:G:156:TRP:HB2 | 2.35 | 0.41 |
| 7:G:15:ASP:OD2 | 7:G:16:LEU:N | 2.53 | 0.41 |
| 7:G:26:PHE:HD1 | 7:G:101:LEU:HD22 | 1.85 | 0.41 |
| 8:H:68:ARG:HH11 | 8:H:68:ARG:HG2 | 1.86 | 0.41 |
| 9:I:50:LEU:O | 9:I:51:ARG:C | 2.57 | 0.41 |
| 10:J:48:THR:OG1 | 10:J:62:HIS:CD2 | 2.74 | 0.41 |
| 15:O:74:ASP:CG | 15:O:77:ARG:HG3 | 2.41 | 0.41 |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:CD1 | 2.55 | 0.41 |
| 19:S:5:LEU:O | 19:S:6:LYS:CB | 2.64 | 0.41 |
| 20:T:100:ILE:HG13 | 20:T:100:ILE:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1197:G:O2' | 1:A:1198:G:H5' | 2.21 | 0.41 |
| 1:A:976:G:C8 | 1:A:1358:U:O2 | 2.73 | 0.41 |
| 1:A:222:U:H2' | 1:A:223:U:C6 | 2.55 | 0.41 |
| 1:A:375:U:C2 | 1:A:376:G:C8 | 3.09 | 0.41 |
| 1:A:429:U:H1' | 1:A:430:A:H5'' | 2.01 | 0.41 |
| 3:C:111:LEU:HD23 | 3:C:111:LEU:HA | 1.93 | 0.41 |
| 7:G:141:VAL:HG13 | 7:G:142:GLU:N | 2.36 | 0.41 |
| 9:I:102:LEU:HD12 | 9:I:102:LEU:H | 1.85 | 0.41 |
| 13:M:65:LYS:HG3 | 13:M:69:GLU:HG2 | 2.03 | 0.41 |
| 1:A:377:G:OP1 | 16:P:3:LYS:HD3 | 2.21 | 0.41 |
| 19:S:20:LEU:O | 19:S:23:ASN:HB2 | 2.20 | 0.41 |
| 1:A:1157:A:C6 | 1:A:1180:A:N7 | 2.89 | 0.41 |
| 1:A:1194:U:H2' | 1:A:1195:C:C6 | 2.55 | 0.41 |
| 1:A:1207:G:O2' | 1:A:1208:C:H5' | 2.20 | 0.41 |
| 1:A:1253:G:H2' | 1:A:1254:C:C6 | 2.55 | 0.41 |
| 1:A:1283:G:O2' | 1:A:1284:C:H5' | 2.20 | 0.41 |
| 1:A:260:G:H2' | 1:A:261:U:C6 | 2.56 | 0.41 |
| 1:A:620:C:H2' | 1:A:621:A:O4' | 2.21 | 0.41 |
| 1:A:795:C:H5'' | 1:A:796:C:OP2 | 2.21 | 0.41 |
| 2:B:223:ILE:C | 2:B:225:ALA:N | 2.73 | 0.41 |
| 2:B:51:LEU:O | 2:B:54:THR:HB | 2.21 | 0.41 |
| 2:B:60:ASP:HB3 | 2:B:64:ARG:CZ | 2.46 | 0.41 |
| 3:C:180:ALA:O | 3:C:181:ASN:HB3 | 2.21 | 0.41 |
| 4:D:39:PRO:O | 4:D:44:GLY:HA3 | 2.20 | 0.41 |
| 7:G:116:ALA:O | 7:G:120:ILE:CD1 | 2.69 | 0.41 |
| 9:I:11:LYS:O | 9:I:12:GLU:HB3 | 2.20 | 0.41 |
| 10:J:86:MET:HE3 | 10:J:86:MET:O | 2.21 | 0.41 |
| 11:K:22:HIS:HB3 | 11:K:29:ILE:HG12 | 2.02 | 0.41 |
| 1:A:585:G:H4' | 12:L:8:ASN:OD1 | 2.21 | 0.41 |
| 13:M:23:TYR:HB2 | 13:M:67:GLU:CD | 2.41 | 0.41 |
| 14:N:9:LYS:C | 14:N:11:LYS:N | 2.74 | 0.41 |
| 19:S:17:GLU:CA | 19:S:20:LEU:HG | 2.40 | 0.41 |
| 1:A:263:A:OP2 | 20:T:79:ARG:NH1 | 2.53 | 0.41 |
| 20:T:79:ARG:O | 20:T:83:ARG:HG3 | 2.21 | 0.41 |
| 22:X:2:U:C2' | 22:X:3:G:H5' | 2.50 | 0.41 |
| 22:X:3:G:N2 | 23:Y:34:TM2:O2 | 2.50 | 0.41 |
| 1:A:989:C:O2' | 1:A:990:C:H5' | 2.21 | 0.41 |
| 2:B:207:ALA:HB3 | 2:B:210:SER:HB3 | 2.02 | 0.41 |
| 3:C:134:ILE:HG22 | 3:C:168:ALA:CB | 2.51 | 0.41 |
| 3:C:46:GLU:O | 3:C:48:TYR:N | 2.52 | 0.41 |
| 4:D:29:PRO:O | 4:D:35:ARG:NH1 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:18:TYR:OH | 7:G:58:PRO:HG3 | 2.20 | 0.41 |
| 7:G:65:ALA:HB1 | 7:G:127:ALA:CB | 2.51 | 0.41 |
| 1:A:587:G:OP1 | 8:H:89:PRO:HB3 | 2.21 | 0.41 |
| 9:I:11:LYS:O | 9:I:12:GLU:CB | 2.67 | 0.41 |
| 9:I:27:THR:HG22 | 9:I:28:VAL:N | 2.35 | 0.41 |
| 12:L:20:LYS:HA | 12:L:20:LYS:HD3 | 1.85 | 0.41 |
| 12:L:43:VAL:CG1 | 12:L:44:THR:H | 2.34 | 0.41 |
| 13:M:14:ARG:HB3 | 13:M:16:ASP:OD1 | 2.20 | 0.41 |
| 17:Q:79:SER:OG | 17:Q:80:GLY:N | 2.53 | 0.41 |
| 1:A:1003(A):G:C6 | 1:A:1004:A:N3 | 2.89 | 0.41 |
| 1:A:1206:G:H4' | 3:C:192:THR:O | 2.21 | 0.41 |
| 1:A:1525:G:P | 11:K:120:ARG:HH22 | 2.44 | 0.41 |
| 1:A:555:C:H2' | 1:A:556:C:C6 | 2.56 | 0.41 |
| 1:A:768:A:H2' | 1:A:769:G:O4' | 2.21 | 0.41 |
| 2:B:22:LYS:HE3 | 2:B:35:GLU:CD | 2.41 | 0.41 |
| 3:C:108:ASN:HD21 | 3:C:144:SER:CB | 2.33 | 0.41 |
| 3:C:52:LEU:N | 3:C:52:LEU:CD2 | 2.79 | 0.41 |
| 7:G:21:VAL:HG23 | 7:G:22:LEU:N | 2.35 | 0.41 |
| 12:L:41:ARG:HG2 | 12:L:42:THR:N | 2.27 | 0.41 |
| 13:M:77:ASN:O | 13:M:80:ARG:HB3 | 2.21 | 0.41 |
| 13:M:81:LEU:HD11 | 13:M:88:ARG:HH21 | 1.86 | 0.41 |
| 11:K:92:GLU:OE2 | 18:R:88:LYS:OXT | 2.38 | 0.41 |
| 21:U:6:ARG:CG | 21:U:15:ARG:NH1 | 2.84 | 0.41 |
| 1:A:1223:C:P | 19:S:78:ARG:HH12 | 2.43 | 0.41 |
| 1:A:1369:C:H2' | 1:A:1370:G:H8 | 1.73 | 0.41 |
| 1:A:1399:C:C2 | 1:A:1401:G:C5 | 3.08 | 0.41 |
| 1:A:1402:C:H2' | 1:A:1403:C:O4' | 2.21 | 0.41 |
| 1:A:380:G:C2 | 1:A:384:G:C6 | 3.09 | 0.41 |
| 1:A:567:G:H2' | 1:A:568:G:O4' | 2.21 | 0.41 |
| 1:A:837:G:O2' | 1:A:838:G:H5' | 2.21 | 0.41 |
| 2:B:12:GLU:C | 2:B:14:GLY:N | 2.71 | 0.41 |
| 2:B:26:PRO:C | 2:B:28:PHE:H | 2.25 | 0.41 |
| 3:C:79:ARG:NE | 3:C:82:GLU:HG2 | 2.36 | 0.41 |
| 4:D:173:TRP:CE2 | 4:D:189:PRO:HG3 | 2.55 | 0.41 |
| 4:D:22:LYS:HB2 | 4:D:26:CYS:SG | 2.61 | 0.41 |
| 7:G:9:VAL:HG11 | 7:G:94:ARG:NH1 | 2.36 | 0.41 |
| 10:J:30:SER:CB | 10:J:81:THR:HA | 2.50 | 0.41 |
| 11:K:87:THR:HG22 | 11:K:88:GLY:H | 1.85 | 0.41 |
| 13:M:8:GLU:C | 13:M:9:ILE:HG13 | 2.40 | 0.41 |
| 19:S:62:ILE:HA | 19:S:66:MET:HE2 | 2.02 | 0.41 |
| 1:A:1163:C:O2' | 1:A:1164:G:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1227:A:C8 | 1:A:1227:A:C3' | 3.04 | 0.41 |
| 1:A:1347:G:H2' | 1:A:1373:G:H1 | 1.85 | 0.41 |
| 1:A:1426:C:H2' | 1:A:1427:U:C6 | 2.56 | 0.41 |
| 1:A:254:G:H21 | 17:Q:16:GLN:HE22 | 1.65 | 0.41 |
| 1:A:828:A:H5'' | 1:A:859:A:C2 | 2.55 | 0.41 |
| 2:B:209:ARG:NH1 | 2:B:239:VAL:HG11 | 2.35 | 0.41 |
| 2:B:7:VAL:C | 2:B:8:LYS:HG3 | 2.41 | 0.41 |
| 6:F:10:LEU:HD23 | 6:F:85:VAL:HA | 2.02 | 0.41 |
| 7:G:116:ALA:HA | 7:G:119:ARG:NH2 | 2.36 | 0.41 |
| 9:I:16:ARG:HG3 | 9:I:16:ARG:HH11 | 1.86 | 0.41 |
| 11:K:40:ILE:HG23 | 11:K:75:TYR:CD2 | 2.56 | 0.41 |
| 11:K:67:ASP:OD1 | 11:K:71:LYS:HE3 | 2.21 | 0.41 |
| 1:A:363:A:N6 | 12:L:28:LYS:HE3 | 2.25 | 0.41 |
| 12:L:60:LEU:CD2 | 12:L:66:VAL:HG22 | 2.51 | 0.41 |
| 13:M:97:PRO:HB3 | 13:M:101:GLN:OE1 | 2.21 | 0.41 |
| 19:S:22:LEU:CD2 | 19:S:28:LYS:HD2 | 2.51 | 0.41 |
| 20:T:92:LEU:O | 20:T:94:ALA:N | 2.44 | 0.41 |
| 21:U:9:ARG:HH11 | 21:U:9:ARG:HG3 | 1.86 | 0.41 |
| 1:A:1105:A:H2' | 1:A:1106:G:H8 | 1.85 | 0.41 |
| 1:A:412:A:H4' | 1:A:413:G:H8 | 1.86 | 0.41 |
| 1:A:514:C:O2' | 1:A:515:G:H5' | 2.21 | 0.41 |
| 1:A:671:G:H2' | 1:A:672:U:O4' | 2.20 | 0.41 |
| 1:A:674:G:O2' | 1:A:675:A:H5' | 2.21 | 0.41 |
| 1:A:701:C:O2' | 1:A:702:A:P | 2.79 | 0.41 |
| 2:B:124:SER:HB2 | 2:B:125:PRO:CD | 2.43 | 0.41 |
| 4:D:100:ARG:NH1 | 4:D:137:SER:HA | 2.37 | 0.41 |
| 4:D:64:LEU:HD22 | 4:D:75:PHE:CE1 | 2.56 | 0.41 |
| 6:F:76:ALA:O | 6:F:80:ARG:HG3 | 2.20 | 0.41 |
| 8:H:19:VAL:CG2 | 8:H:21:LYS:HD3 | 2.48 | 0.41 |
| 9:I:56:LEU:HD23 | 9:I:56:LEU:C | 2.41 | 0.41 |
| 10:J:87:THR:HG22 | 10:J:87:THR:O | 2.20 | 0.41 |
| 10:J:98:ILE:HG22 | 10:J:99:LYS:H | 1.86 | 0.41 |
| 11:K:26:ASN:O | 11:K:27:ASN:CB | 2.68 | 0.41 |
| 11:K:29:ILE:HG21 | 11:K:29:ILE:HD13 | 1.82 | 0.41 |
| 11:K:91:ARG:CD | 18:R:88:LYS:HE2 | 2.34 | 0.41 |
| 19:S:27:GLU:HB3 | 19:S:28:LYS:H | 1.76 | 0.41 |
| 1:A:191:G:C4 | 20:T:105:SER:HB3 | 2.55 | 0.41 |
| 1:A:1047:G:O5' | 1:A:1047:G:H8 | 2.04 | 0.40 |
| 1:A:1053:G:H3' | 1:A:1054:C:C5' | 2.51 | 0.40 |
| 1:A:1257:U:H5'' | 1:A:1258:G:OP2 | 2.21 | 0.40 |
| 1:A:1288:A:O4' | 1:A:1353:G:H4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1392:G:N2 | 1:A:1502:A:C8 | 2.88 | 0.40 |
| 1:A:642:A:C8 | 8:H:115:SER:HA | 2.55 | 0.40 |
| 2:B:189:ASP:CB | 2:B:205:ASP:OD2 | 2.68 | 0.40 |
| 5:E:50:GLU:HB3 | 5:E:53:LEU:HG | 2.03 | 0.40 |
| 6:F:46:ARG:HB3 | 6:F:46:ARG:CZ | 2.51 | 0.40 |
| 8:H:51:VAL:HG21 | 8:H:60:ARG:HG2 | 2.03 | 0.40 |
| 9:I:127:LYS:O | 9:I:127:LYS:CD | 2.69 | 0.40 |
| 10:J:81:THR:C | 10:J:83:GLU:H | 2.23 | 0.40 |
| 13:M:23:TYR:CB | 13:M:67:GLU:HA | 2.52 | 0.40 |
| 1:A:1126:U:H2' | 1:A:1127:G:C8 | 2.56 | 0.40 |
| 1:A:1460:A:H2' | 1:A:1461:G:O4' | 2.21 | 0.40 |
| 1:A:583:A:H2' | 1:A:584:G:O4' | 2.21 | 0.40 |
| 1:A:603:U:H2' | 1:A:604:G:H8 | 1.85 | 0.40 |
| 3:C:188:LEU:HB3 | 3:C:189:ALA:H | 1.59 | 0.40 |
| 4:D:61:LYS:HD3 | 4:D:62:GLN:HE21 | 1.86 | 0.40 |
| 5:E:36:ASP:OD2 | 5:E:40:ARG:HB2 | 2.21 | 0.40 |
| 7:G:48:LYS:O | 7:G:51:GLN:HB2 | 2.21 | 0.40 |
| 7:G:37:ASN:ND2 | 9:I:41:VAL:HG12 | 2.36 | 0.40 |
| 6:F:97:PHE:HB2 | 18:R:32:ARG:NH2 | 2.36 | 0.40 |
| 23:Y:34:TM2:O3S | 23:Y:36:A:N6 | 2.54 | 0.40 |
| 1:A:1019:C:O2' | 1:A:1020:U:H5' | 2.22 | 0.40 |
| 1:A:1058:G:O2' | 1:A:1059:C:H5' | 2.21 | 0.40 |
| 1:A:1202:G:C2' | 1:A:1203:C:H5' | 2.51 | 0.40 |
| 1:A:1292:U:H2' | 1:A:1293:G:C8 | 2.56 | 0.40 |
| 1:A:1237:C:H3' | 1:A:1336:C:H41 | 1.86 | 0.40 |
| 1:A:1368:G:O2' | 1:A:1369:C:H5' | 2.22 | 0.40 |
| 1:A:174:C:H2' | 1:A:175:C:H6 | 1.85 | 0.40 |
| 1:A:389:A:H2' | 1:A:390:C:C5' | 2.52 | 0.40 |
| 1:A:397:A:H5' | 1:A:398:C:P | 2.62 | 0.40 |
| 1:A:502:G:H2' | 1:A:503:C:O4' | 2.21 | 0.40 |
| 1:A:718:G:C5' | 11:K:117:ASN:ND2 | 2.76 | 0.40 |
| 2:B:130:ARG:CB | 2:B:131:PRO:HD2 | 2.51 | 0.40 |
| 4:D:102:ASP:HB3 | 4:D:136:PRO:CA | 2.51 | 0.40 |
| 5:E:76:ILE:CG2 | 5:E:78:HIS:O | 2.69 | 0.40 |
| 7:G:114:ARG:N | 7:G:114:ARG:HD2 | 2.24 | 0.40 |
| 9:I:108:VAL:CG1 | 9:I:109:VAL:N | 2.83 | 0.40 |
| 9:I:120:ARG:O | 9:I:121:ARG:C | 2.58 | 0.40 |
| 17:Q:52:LYS:HD2 | 17:Q:52:LYS:N | 2.36 | 0.40 |
| 19:S:19:VAL:CG1 | 19:S:20:LEU:N | 2.84 | 0.40 |
| 1:A:1439:C:P | 20:T:38:LYS:HZ3 | 2.44 | 0.40 |
| 1:A:1202:G:C2 | 14:N:42:ILE:HG21 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.56 | 0.40 |
| 1:A:1474:G:H2' | 1:A:1475:G:H8 | 1.86 | 0.40 |
| 1:A:267:C:H2' | 1:A:268:C:C6 | 2.56 | 0.40 |
| 1:A:716:A:H1' | 11:K:118:GLY:HA2 | 2.03 | 0.40 |
| 3:C:127:ARG:NH1 | 3:C:127:ARG:HG3 | 2.35 | 0.40 |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:HB | 2.02 | 0.40 |
| 3:C:113:ALA:N | 3:C:202:ILE:HD12 | 2.36 | 0.40 |
| 5:E:135:THR:O | 5:E:138:ALA:N | 2.55 | 0.40 |
| 12:L:26:ALA:C | 12:L:27:LEU:O | 2.59 | 0.40 |
| 13:M:108:ARG:NH1 | 13:M:114:ARG:HG2 | 2.37 | 0.40 |
| 1:A:1206:G:C6 | 1:A:1207:G:C5 | 3.10 | 0.40 |
| 1:A:1263:C:H2' | 1:A:1264:C:H6 | 1.85 | 0.40 |
| 1:A:1299:A:C5 | 1:A:1301:U:O2 | 2.75 | 0.40 |
| 1:A:1317:C:H2' | 1:A:1318:A:O4' | 2.22 | 0.40 |
| 1:A:1413:A:C2 | 1:A:1488:G:C2 | 3.09 | 0.40 |
| 1:A:1499:A:O2' | 1:A:1500:A:H5' | 2.22 | 0.40 |
| 1:A:590:C:O2' | 1:A:591:U:H5' | 2.21 | 0.40 |
| 1:A:663:A:O2' | 1:A:664:G:H5' | 2.21 | 0.40 |
| 1:A:807:A:H2' | 1:A:808:C:H6 | 1.82 | 0.40 |
| 7:G:18:TYR:HD2 | 7:G:59:LEU:HD22 | 1.87 | 0.40 |
| 10:J:9:ARG:C | 10:J:16:LEU:HD11 | 2.41 | 0.40 |
| 12:L:29:GLY:O | 12:L:30:ALA:C | 2.60 | 0.40 |
| 12:L:41:ARG:NH2 | 12:L:57:LYS:HZ2 | 2.18 | 0.40 |
| 1:A:1226:C:C4 | 13:M:104:ARG:HG3 | 2.57 | 0.40 |
| 14:N:33:VAL:HG23 | 14:N:33:VAL:O | 2.21 | 0.40 |
| 10:J:63:PHE:CE1 | 14:N:45:ARG:HG3 | 2.56 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 233/256 (91%) | 147 (63%) | 65 (28%) | 21 (9%) | 1 | 2 |
| 3 | C | 205/239 (86%) | 135 (66%) | 44 (22%) | 26 (13%) | 0 | 1 |
| 4 | D | 206/209 (99%) | 169 (82%) | 29 (14%) | 8 (4%) | 3 | 13 |
| 5 | E | 149/162 (92%) | 132 (89%) | 16 (11%) | 1 (1%) | 24 | 58 |
| 6 | F | 99/101 (98%) | 73 (74%) | 22 (22%) | 4 (4%) | 3 | 13 |
| 7 | G | 153/156 (98%) | 120 (78%) | 25 (16%) | 8 (5%) | 2 | 7 |
| 8 | H | 136/138 (99%) | 123 (90%) | 11 (8%) | 2 (2%) | 11 | 37 |
| 9 | I | 125/128 (98%) | 95 (76%) | 22 (18%) | 8 (6%) | 1 | 4 |
| 10 | J | 97/105 (92%) | 62 (64%) | 19 (20%) | 16 (16%) | 0 | 0 |
| 11 | K | 117/129 (91%) | 94 (80%) | 18 (15%) | 5 (4%) | 3 | 11 |
| 12 | L | 123/135 (91%) | 90 (73%) | 21 (17%) | 12 (10%) | 1 | 1 |
| 13 | M | 123/126 (98%) | 97 (79%) | 14 (11%) | 12 (10%) | 1 | 1 |
| 14 | N | 58/61 (95%) | 44 (76%) | 10 (17%) | 4 (7%) | 1 | 3 |
| 15 | O | 86/89 (97%) | 73 (85%) | 10 (12%) | 3 (4%) | 4 | 16 |
| 16 | P | 82/88 (93%) | 71 (87%) | 9 (11%) | 2 (2%) | 6 | 25 |
| 17 | Q | 102/105 (97%) | 88 (86%) | 12 (12%) | 2 (2%) | 8 | 30 |
| 18 | R | 71/88 (81%) | 55 (78%) | 13 (18%) | 3 (4%) | 3 | 12 |
| 19 | S | 79/93 (85%) | 60 (76%) | 13 (16%) | 6 (8%) | 1 | 3 |
| 20 | T | 97/106 (92%) | 73 (75%) | 15 (16%) | 9 (9%) | 1 | 1 |
| 21 | U | 23/27 (85%) | 16 (70%) | 6 (26%) | 1 (4%) | 3 | 11 |
| All | All | 2364/2541 (93%) | 1817 (77%) | 394 (17%) | 153 (6%) | 1 | 4 |

All (153) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 15 | VAL |
| 2 | B | 16 | HIS |
| 2 | B | 20 | GLU |
| 2 | B | 21 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 74 | LYS |
| 2 | B | 123 | ALA |
| 2 | B | 230 | VAL |
| 2 | B | 232 | PRO |
| 3 | C | 15 | THR |
| 3 | C | 16 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 26 | LYS |
| 3 | C | 61 | ALA |
| 3 | C | 101 | LEU |
| 3 | C | 154 | SER |
| 3 | C | 156 | ARG |
| 3 | C | 189 | ALA |
| 3 | C | 207 | VAL |
| 4 | D | 3 | ARG |
| 6 | F | 14 | LEU |
| 6 | F | 64 | GLN |
| 7 | G | 17 | VAL |
| 7 | G | 53 | LYS |
| 8 | H | 91 | ARG |
| 9 | I | 23 | ASN |
| 9 | I | 55 | ALA |
| 9 | I | 88 | TYR |
| 10 | J | 30 | SER |
| 10 | J | 32 | ALA |
| 10 | J | 34 | VAL |
| 11 | K | 12 | ARG |
| 12 | L | 27 | LEU |
| 12 | L | 28 | LYS |
| 12 | L | 47 | LYS |
| 12 | L | 48 | PRO |
| 13 | M | 23 | TYR |
| 13 | M | 24 | GLY |
| 13 | M | 67 | GLU |
| 13 | M | 86 | CYS |
| 17 | Q | 80 | GLY |
| 17 | Q | 81 | ARG |
| 18 | R | 87 | ARG |
| 19 | S | 6 | LYS |
| 19 | S | 81 | ARG |
| 20 | T | 11 | SER |
| 20 | T | 73 | HIS |
| 20 | T | 95 | ALA |
| 20 | T | 99 | LEU |
| 20 | T | 100 | ILE |
| 2 | B | 8 | LYS |
| 2 | B | 95 | GLN |
| 2 | B | 190 | THR |
| 2 | B | 207 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 224 | GLN |
| 3 | C | 47 | LEU |
| 3 | C | 54 | ARG |
| 3 | C | 100 | ALA |
| 3 | C | 146 | ALA |
| 3 | C | 188 | LEU |
| 4 | D | 171 | GLY |
| 6 | F | 70 | ASP |
| 7 | G | 7 | ALA |
| 7 | G | 81 | GLY |
| 7 | G | 155 | ARG |
| 8 | H | 83 | ILE |
| 9 | I | 41 | VAL |
| 10 | J | 39 | PRO |
| 10 | J | 57 | LYS |
| 12 | L | 29 | GLY |
| 12 | L | 91 | LYS |
| 12 | L | 128 | ALA |
| 13 | M | 59 | TYR |
| 13 | M | 68 | GLY |
| 13 | M | 85 | GLY |
| 14 | N | 15 | LYS |
| 14 | N | 23 | ARG |
| 15 | O | 85 | LEU |
| 16 | P | 10 | GLY |
| 16 | P | 83 | GLU |
| 19 | S | 9 | VAL |
| 19 | S | 30 | LEU |
| 20 | T | 74 | LYS |
| 20 | T | 94 | ALA |
| 20 | T | 102 | GLY |
| 2 | B | 18 | GLY |
| 3 | C | 55 | VAL |
| 3 | C | 81 | GLY |
| 3 | C | 96 | GLY |
| 3 | C | 168 | ALA |
| 4 | D | 4 | TYR |
| 4 | D | 35 | ARG |
| 4 | D | 39 | PRO |
| 7 | G | 83 | ALA |
| 9 | I | 38 | GLN |
| 9 | I | 119 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 61 | GLU |
| 12 | L | 41 | ARG |
| 12 | L | 116 | SER |
| 13 | M | 7 | VAL |
| 14 | N | 17 | LYS |
| 20 | T | 9 | ASN |
| 2 | B | 228 | GLY |
| 3 | C | 20 | SER |
| 3 | C | 98 | ASN |
| 3 | C | 108 | ASN |
| 4 | D | 88 | VAL |
| 6 | F | 32 | ASN |
| 9 | I | 24 | GLY |
| 10 | J | 40 | LEU |
| 10 | J | 72 | VAL |
| 11 | K | 50 | TYR |
| 11 | K | 117 | ASN |
| 13 | M | 60 | VAL |
| 14 | N | 22 | THR |
| 18 | R | 20 | ALA |
| 18 | R | 25 | THR |
| 19 | S | 8 | GLY |
| 21 | U | 25 | LYS |
| 2 | B | 11 | LEU |
| 3 | C | 4 | LYS |
| 3 | C | 167 | TRP |
| 4 | D | 58 | LEU |
| 7 | G | 37 | ASN |
| 9 | I | 58 | ARG |
| 10 | J | 23 | ILE |
| 10 | J | 73 | ASP |
| 10 | J | 77 | PRO |
| 10 | J | 86 | MET |
| 11 | K | 13 | GLN |
| 11 | K | 128 | ALA |
| 12 | L | 51 | ALA |
| 2 | B | 27 | LYS |
| 3 | C | 39 | ILE |
| 10 | J | 55 | LYS |
| 10 | J | 90 | LEU |
| 12 | L | 62 | SER |
| 13 | M | 4 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | M | 124 | PRO |
| 15 | O | 86 | GLY |
| 19 | S | 43 | GLU |
| 4 | D | 5 | ILE |
| 7 | G | 112 | PRO |
| 13 | M | 117 | VAL |
| 2 | B | 227 | GLY |
| 3 | C | 14 | ILE |
| 3 | C | 75 | VAL |
| 12 | L | 121 | GLY |
| 2 | B | 183 | PRO |
| 5 | E | 154 | GLY |
| 10 | J | 41 | PRO |
| 10 | J | 76 | ASN |
| 2 | B | 233 | SER |
| 15 | O | 3 | ILE |

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%) | 182 (90%) | 20 (10%) | 8 | 26 |
| 3 | C | 160/188 (85%) | 144 (90%) | 16 (10%) | 8 | 26 |
| 4 | D | 180/181 (99%) | 172 (96%) | 8 (4%) | 31 | 65 |
| 5 | E | 115/123 (94%) | 101 (88%) | 14 (12%) | 5 | 16 |
| 6 | F | 90/90 (100%) | 87 (97%) | 3 (3%) | 41 | 75 |
| 7 | G | 126/127 (99%) | 121 (96%) | 5 (4%) | 34 | 69 |
| 8 | H | 119/119 (100%) | 109 (92%) | 10 (8%) | 12 | 34 |
| 9 | I | 98/99 (99%) | 91 (93%) | 7 (7%) | 16 | 43 |
| 10 | J | 87/92 (95%) | 81 (93%) | 6 (7%) | 17 | 44 |
| 11 | K | 90/99 (91%) | 88 (98%) | 2 (2%) | 55 | 84 |
| 12 | L | 104/111 (94%) | 96 (92%) | 8 (8%) | 14 | 38 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 13 | M | 100/101 (99%) | 90 (90%) | 10 (10%) | 8 | 26 |
| 14 | N | 49/50 (98%) | 47 (96%) | 2 (4%) | 33 | 68 |
| 15 | O | 79/80 (99%) | 73 (92%) | 6 (8%) | 14 | 39 |
| 16 | P | 72/74 (97%) | 68 (94%) | 4 (6%) | 23 | 55 |
| 17 | Q | 96/97 (99%) | 90 (94%) | 6 (6%) | 20 | 50 |
| 18 | R | 64/77 (83%) | 60 (94%) | 4 (6%) | 20 | 50 |
| 19 | S | 71/80 (89%) | 68 (96%) | 3 (4%) | 32 | 67 |
| 20 | T | 76/82 (93%) | 68 (90%) | 8 (10%) | 7 | 23 |
| 21 | U | 19/22 (86%) | 17 (90%) | 2 (10%) | 7 | 23 |
| All | All | 1997/2112 (95%) | 1853 (93%) | 144 (7%) | 16 | 42 |

All (144) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 8 | LYS |
| 2 | B | 9 | GLU |
| 2 | B | 12 | GLU |
| 2 | B | 15 | VAL |
| 2 | B | 17 | PHE |
| 2 | B | 23 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 25 | ASN |
| 2 | B | 44 | LEU |
| 2 | B | 67 | THR |
| 2 | B | 82 | ARG |
| 2 | B | 92 | TYR |
| 2 | B | 98 | LEU |
| 2 | B | 140 | HIS |
| 2 | B | 157 | ARG |
| 2 | B | 178 | ARG |
| 2 | B | 204 | ASN |
| 2 | B | 221 | LEU |
| 2 | B | 232 | PRO |
| 2 | B | 236 | TYR |
| 3 | C | 5 | ILE |
| 3 | C | 23 | TYR |
| 3 | C | 26 | LYS |
| 3 | C | 36 | ASP |
| 3 | C | 37 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 52 | LEU |
| 3 | C | 56 | ASP |
| 3 | C | 82 | GLU |
| 3 | C | 102 | ASN |
| 3 | C | 107 | GLN |
| 3 | C | 143 | GLU |
| 3 | C | 167 | TRP |
| 3 | C | 188 | LEU |
| 3 | C | 191 | THR |
| 3 | C | 196 | LEU |
| 3 | C | 204 | LEU |
| 4 | D | 36 | ARG |
| 4 | D | 58 | LEU |
| 4 | D | 76 | ARG |
| 4 | D | 122 | ARG |
| 4 | D | 162 | LEU |
| 4 | D | 168 | ARG |
| 4 | D | 192 | GLU |
| 4 | D | 199 | ASN |
| 5 | E | 12 | LEU |
| 5 | E | 20 | GLN |
| 5 | E | 31 | LEU |
| 5 | E | 33 | VAL |
| 5 | E | 34 | VAL |
| 5 | E | 41 | VAL |
| 5 | E | 43 | LEU |
| 5 | E | 53 | LEU |
| 5 | E | 73 | ASN |
| 5 | E | 75 | THR |
| 5 | E | 79 | GLU |
| 5 | E | 80 | ILE |
| 5 | E | 147 | ASP |
| 5 | E | 150 | ARG |
| 6 | F | 43 | LEU |
| 6 | F | 47 | ARG |
| 6 | F | 63 | TYR |
| 7 | G | 8 | GLU |
| 7 | G | 38 | LEU |
| 7 | G | 114 | ARG |
| 7 | G | 126 | ASP |
| 7 | G | 140 | ASP |
| 8 | H | 21 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | H | 24 | THR |
| 8 | H | 26 | VAL |
| 8 | H | 39 | LEU |
| 8 | H | 63 | LEU |
| 8 | H | 85 | ARG |
| 8 | H | 91 | ARG |
| 8 | H | 112 | LEU |
| 8 | H | 119 | LEU |
| 8 | H | 133 | LEU |
| 9 | I | 23 | ASN |
| 9 | I | 60 | ASP |
| 9 | I | 79 | LEU |
| 9 | I | 102 | LEU |
| 9 | I | 114 | TYR |
| 9 | I | 121 | ARG |
| 9 | I | 127 | LYS |
| 10 | J | 3 | LYS |
| 10 | J | 29 | ARG |
| 10 | J | 57 | LYS |
| 10 | J | 71 | LEU |
| 10 | J | 73 | ASP |
| 10 | J | 83 | GLU |
| 11 | K | 11 | LYS |
| 11 | K | 92 | GLU |
| 12 | L | 33 | ARG |
| 12 | L | 48 | PRO |
| 12 | L | 53 | ARG |
| 12 | L | 59 | ARG |
| 12 | L | 73 | GLU |
| 12 | L | 93 | LEU |
| 12 | L | 113 | ARG |
| 12 | L | 126 | LYS |
| 13 | M | 9 | ILE |
| 13 | M | 11 | ARG |
| 13 | M | 16 | ASP |
| 13 | M | 40 | ASN |
| 13 | M | 70 | LEU |
| 13 | M | 102 | ARG |
| 13 | M | 108 | ARG |
| 13 | M | 110 | ARG |
| 13 | M | 115 | LYS |
| 13 | M | 125 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | N | 41 | ARG |
| 14 | N | 44 | LEU |
| 15 | O | 5 | LYS |
| 15 | O | 10 | LYS |
| 15 | O | 31 | LEU |
| 15 | O | 34 | LEU |
| 15 | O | 64 | ARG |
| 15 | O | 81 | LEU |
| 16 | P | 2 | VAL |
| 16 | P | 43 | LYS |
| 16 | P | 55 | ARG |
| 16 | P | 61 | SER |
| 17 | Q | 9 | VAL |
| 17 | Q | 38 | ARG |
| 17 | Q | 52 | LYS |
| 17 | Q | 59 | ILE |
| 17 | Q | 68 | ARG |
| 17 | Q | 74 | LEU |
| 18 | R | 36 | ASN |
| 18 | R | 54 | ARG |
| 18 | R | 84 | LYS |
| 18 | R | 87 | ARG |
| 19 | S | 7 | LYS |
| 19 | S | 12 | ASP |
| 19 | S | 15 | LEU |
| 20 | T | 10 | LEU |
| 20 | T | 24 | LEU |
| 20 | T | 42 | GLN |
| 20 | T | 45 | GLN |
| 20 | T | 57 | ARG |
| 20 | T | 73 | HIS |
| 20 | T | 75 | ASN |
| 20 | T | 84 | LEU |
| 21 | U | 6 | ARG |
| 21 | U | 15 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 25 | ASN |
| 2 | B | 204 | ASN |
| 3 | C | 3 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 31 | HIS |
| 3 | C | 63 | ASN |
| 3 | C | 102 | ASN |
| 3 | C | 107 | GLN |
| 3 | C | 110 | ASN |
| 4 | D | 42 | GLN |
| 4 | D | 62 | GLN |
| 4 | D | 123 | HIS |
| 4 | D | 161 | ASN |
| 4 | D | 199 | ASN |
| 5 | E | 20 | GLN |
| 5 | E | 73 | ASN |
| 5 | E | 78 | HIS |
| 6 | F | 13 | ASN |
| 6 | F | 18 | GLN |
| 6 | F | 27 | GLN |
| 6 | F | 32 | ASN |
| 6 | F | 57 | GLN |
| 6 | F | 94 | GLN |
| 6 | F | 100 | ASN |
| 7 | G | 37 | ASN |
| 7 | G | 68 | ASN |
| 7 | G | 96 | GLN |
| 9 | I | 23 | ASN |
| 9 | I | 31 | GLN |
| 9 | I | 73 | GLN |
| 9 | I | 89 | ASN |
| 10 | J | 78 | ASN |
| 10 | J | 84 | GLN |
| 11 | K | 38 | ASN |
| 11 | K | 93 | GLN |
| 11 | K | 117 | ASN |
| 12 | L | 49 | ASN |
| 12 | L | 75 | HIS |
| 13 | M | 12 | ASN |
| 13 | M | 40 | ASN |
| 13 | M | 62 | ASN |
| 14 | N | 52 | GLN |
| 15 | O | 13 | GLN |
| 15 | O | 37 | ASN |
| 15 | O | 46 | HIS |
| 16 | P | 16 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 65 | GLN |
| 16 | P | 76 | GLN |
| 17 | Q | 16 | GLN |
| 17 | Q | 96 | GLN |
| 19 | S | 23 | ASN |
| 19 | S | 56 | GLN |
| 20 | T | 45 | GLN |
| 20 | T | 73 | HIS |
| 20 | T | 90 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1511/1522 (99%) | 202 (13%) | 68 (4%) |
| 22 | X | 3/6 (50%) | 1 (33%) | 0 |
| 23 | Y | 6/17 (35%) | 2 (33%) | 0 |
| All | All | 1520/1545 (98%) | 205 (13%) | 68 (4%) |

All (205) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 31 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 51 | A |
| 1 | A | 61 | G |
| 1 | A | 101 | A |
| 1 | A | 116 | A |
| 1 | A | 120 | A |
| 1 | A | 121 | C |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 163 | C |
| 1 | A | 182 | U |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 202 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 204 | U |
| 1 | A | 216 | G |
| 1 | A | 244 | U |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 289 | G |
| 1 | A | 321 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 332 | G |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 366 | C |
| 1 | A | 367 | U |
| 1 | A | 373 | A |
| 1 | A | 390 | C |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 410 | G |
| 1 | A | 411 | A |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 414 | A |
| 1 | A | 421 | U |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 430 | A |
| 1 | A | 433 | C |
| 1 | A | 434 | U |
| 1 | A | 439 | A |
| 1 | A | 442 | C |
| 1 | A | 452 | A |
| 1 | A | 461 | C |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 497 | A |
| 1 | A | 498 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |
| 1 | A | 527 | G |
| 1 | A | 531 | U |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 534 | U |
| 1 | A | 547 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 562 | C |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 575 | G |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 630 | G |
| 1 | A | 653 | A |
| 1 | A | 665 | A |
| 1 | A | 688 | G |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 723 | U |
| 1 | A | 731 | G |
| 1 | A | 749 | C |
| 1 | A | 755 | G |
| 1 | A | 777 | A |
| 1 | A | 781 | A |
| 1 | A | 782 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 813 | U |
| 1 | A | 817 | C |
| 1 | A | 819 | A |
| 1 | A | 821 | G |
| 1 | A | 828 | A |
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 848 | C |
| 1 | A | 902 | G |
| 1 | A | 914 | A |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 960 | U |
| 1 | A | 961 | U |
| 1 | A | 966 | G |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 978 | A |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 994 | A |
| 1 | A | 1004 | A |
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1027 | C |
| 1 | A | 1050 | G |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1068 | G |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1101 | A |
| 1 | A | 1117 | G |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1127 | G |
| 1 | A | 1128 | C |
| 1 | A | 1129 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1145 | C |
| 1 | A | 1152 | A |
| 1 | A | 1159 | U |
| 1 | A | 1161 | C |
| 1 | A | 1176 | A |
| 1 | A | 1180 | A |
| 1 | A | 1183 | A |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1214 | C |
| 1 | A | 1227 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1282 | C |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1320 | C |
| 1 | A | 1331 | G |
| 1 | A | 1338 | G |
| 1 | A | 1346 | A |
| 1 | A | 1348 | U |
| 1 | A | 1362 | C |
| 1 | A | 1379 | G |
| 1 | A | 1398 | A |
| 1 | A | 1442 | G |
| 1 | A | 1446 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1452 | C |
| 1 | A | 1492 | A |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1517 | G |
| 1 | A | 1520 | G |
| 1 | A | 1528 | U |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1533 | C |
| 22 | X | 2 | U |
| 23 | Y | 35 | A |
| 23 | Y | 39 | C |

All (68) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 7 | G |
| 1 | A | 30 | U |
| 1 | A | 60 | A |
| 1 | A | 115 | G |
| 1 | A | 119 | A |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 243 | A |
| 1 | A | 250 | A |
| 1 | A | 266 | G |
| 1 | A | 328 | C |
| 1 | A | 344 | A |
| 1 | A | 351 | G |
| 1 | A | 353 | A |
| 1 | A | 366 | C |
| 1 | A | 372 | C |
| 1 | A | 410 | G |
| 1 | A | 412 | A |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 433 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 438 | G |
| 1 | A | 484 | G |
| 1 | A | 496 | A |
| 1 | A | 497 | A |
| 1 | A | 509 | A |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 575 | G |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 748 | C |
| 1 | A | 793 | U |
| 1 | A | 812 | C |
| 1 | A | 913 | A |
| 1 | A | 960 | U |
| 1 | A | 965 | A |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 1049 | U |
| 1 | A | 1063 | C |
| 1 | A | 1065 | U |
| 1 | A | 1067 | A |
| 1 | A | 1127 | G |
| 1 | A | 1129 | C |
| 1 | A | 1160 | G |
| 1 | A | 1175 | G |
| 1 | A | 1182 | G |
| 1 | A | 1191 | A |
| 1 | A | 1201 | A |
| 1 | A | 1211 | U |
| 1 | A | 1225 | A |
| 1 | A | 1281 | U |
| 1 | A | 1285 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1347 | G |
| 1 | A | 1397 | C |
| 1 | A | 1443 | G |
| 1 | A | 1451 | A |
| 1 | A | 1498 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1528 | U |
| 1 | A | 1532 | U |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 290 ligands modelled in this entry, 289 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 | $\# Z > 2$ |
| 24 | PAR | A | 1601 | - | 44,45,45 | 1.33 | 6 (13%) | 62,67,67 | 1.31 | 6 (9%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 24 | PAR | A | 1601 | - | - | 0/18/94/94 | 0/4/4/4 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 24 | A | 1601 | PAR | O51-C11 | 2.17 | 1.47 | 1.41 |
| 24 | A | 1601 | PAR | C14-C24 | 2.36 | 1.57 | 1.52 |
| 24 | A | 1601 | PAR | C11-C21 | 2.54 | 1.57 | 1.52 |
| 24 | A | 1601 | PAR | C31-C21 | 2.56 | 1.56 | 1.53 |
| 24 | A | 1601 | PAR | C52-C42 | 2.59 | 1.57 | 1.52 |
| 24 | A | 1601 | PAR | O54-C14 | 2.79 | 1.49 | 1.41 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24 | A | 1601 | PAR | O52-C13-O43 | -2.70 | 108.50 | 111.43 |
| 24 | A | 1601 | PAR | C22-C32-C42 | 2.12 | 114.96 | 109.54 |
| 24 | A | 1601 | PAR | O52-C13-C23 | 3.36 | 114.92 | 107.96 |
| 24 | A | 1601 | PAR | C14-O54-C54 | 3.60 | 120.80 | 113.71 |
| 24 | A | 1601 | PAR | O54-C54-C64 | 3.76 | 113.13 | 106.01 |
| 24 | A | 1601 | PAR | O33-C14-C24 | 4.63 | 116.49 | 108.24 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24 | A | 1601 | PAR | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | A | 11 |
| 23 | Y | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 1064:G | O3' | 1065:U | P | 1.98 |
| 1 | Y | 35:A | O3' | 36:A | P | 1.36 |
| 1 | A | 1160:G | O3' | 1161:C | P | 1.32 |
| 1 | A | 1541:U | O3' | 1542:U | P | 1.30 |
| 1 | A | 1156:G | O3' | 1157:A | P | 1.09 |
| 1 | A | 1532:U | O3' | 1533:C | P | 1.04 |
| 1 | A | 1144:G | O3' | 1145:C | P | 1.00 |
| 1 | A | 1191:A | O3' | 1192:C | P | 0.96 |
| 1 | A | 1192:C | O3' | 1193:G | P | 0.95 |
| 1 | A | 1175:G | O3' | 1176:A | P | 0.86 |
| 1 | A | 1063:C | O3' | 1064:G | P | 0.73 |
| 1 | A | 1179:A | O3' | 1180:A | P | 0.67 |

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, 95th 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 ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-----|-----|-----------------------|-------|
| 1 | A | 1513/1522 (99%) | 0.26 | 55 (3%) | 42 | 37 | 44, 78, 143, 201 | 0 |
| 2 | B | 235/256 (91%) | 0.31 | 9 (3%) | 40 | 35 | 67, 107, 151, 161 | 0 |
| 3 | C | 207/239 (86%) | 0.39 | 15 (7%) | 15 | 11 | 75, 100, 145, 149 | 0 |
| 4 | D | 208/209 (99%) | 0.23 | 13 (6%) | 20 | 15 | 62, 87, 111, 119 | 0 |
| 5 | E | 151/162 (93%) | -0.08 | 1 (0%) | 87 | 87 | 55, 70, 97, 114 | 0 |
| 6 | F | 101/101 (100%) | 0.08 | 4 (3%) | 38 | 33 | 73, 105, 120, 124 | 0 |
| 7 | G | 155/156 (99%) | 0.16 | 4 (2%) | 56 | 52 | 72, 98, 130, 148 | 0 |
| 8 | H | 138/138 (100%) | -0.10 | 0 | 100 | 100 | 51, 69, 83, 94 | 0 |
| 9 | I | 127/128 (99%) | 0.53 | 10 (7%) | 12 | 9 | 66, 110, 126, 132 | 0 |
| 10 | J | 99/105 (94%) | 1.24 | 19 (19%) | 1 | 1 | 72, 138, 174, 177 | 0 |
| 11 | K | 119/129 (92%) | 0.18 | 2 (1%) | 70 | 69 | 54, 81, 109, 134 | 0 |
| 12 | L | 125/135 (92%) | 0.16 | 0 | 100 | 100 | 43, 83, 104, 127 | 0 |
| 13 | M | 125/126 (99%) | 1.09 | 16 (12%) | 3 | 3 | 76, 97, 145, 188 | 0 |
| 14 | N | 60/61 (98%) | 0.42 | 3 (5%) | 29 | 24 | 78, 98, 125, 131 | 0 |
| 15 | O | 88/89 (98%) | 0.17 | 4 (4%) | 33 | 29 | 64, 83, 113, 137 | 0 |
| 16 | P | 84/88 (95%) | 0.02 | 0 | 100 | 100 | 56, 70, 84, 108 | 0 |
| 17 | Q | 104/105 (99%) | 0.25 | 5 (4%) | 30 | 26 | 52, 71, 113, 156 | 0 |
| 18 | R | 73/88 (82%) | 0.35 | 5 (6%) | 17 | 13 | 76, 90, 136, 161 | 0 |
| 19 | S | 81/93 (87%) | 0.42 | 8 (9%) | 7 | 5 | 83, 121, 144, 149 | 0 |
| 20 | T | 99/106 (93%) | 0.24 | 4 (4%) | 38 | 33 | 57, 75, 105, 112 | 0 |
| 21 | U | 25/27 (92%) | 0.53 | 1 (4%) | 38 | 33 | 74, 86, 116, 120 | 0 |
| 22 | X | 4/6 (66%) | 1.42 | 1 (25%) | 0 | 0 | 77, 107, 116, 120 | 0 |
| 23 | Y | 6/17 (35%) | 2.09 | 2 (33%) | 0 | 0 | 101, 142, 154, 161 | 0 |
| All | All | 3927/4086 (96%) | 0.29 | 181 (4%) | 32 | 28 | 43, 86, 142, 201 | 0 |

All (181) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 13 | M | 121 | LYS | 17.5 |
| 13 | M | 124 | PRO | 15.4 |
| 13 | M | 125 | ARG | 14.9 |
| 1 | A | 1534 | A | 12.1 |
| 13 | M | 120 | LYS | 12.1 |
| 13 | M | 126 | LYS | 11.2 |
| 13 | M | 123 | ALA | 11.1 |
| 19 | S | 3 | ARG | 8.8 |
| 17 | Q | 105 | ALA | 8.7 |
| 10 | J | 70 | ARG | 8.6 |
| 1 | A | 1129 | C | 8.6 |
| 23 | Y | 33 | U | 8.4 |
| 1 | A | 1540 | U | 8.2 |
| 1 | A | 1541 | U | 7.0 |
| 18 | R | 17 | SER | 6.9 |
| 2 | B | 16 | HIS | 6.9 |
| 17 | Q | 104 | LYS | 6.8 |
| 11 | K | 129 | SER | 6.5 |
| 10 | J | 17 | ASP | 6.4 |
| 10 | J | 10 | GLY | 6.4 |
| 13 | M | 7 | VAL | 5.6 |
| 1 | A | 1539 | C | 5.5 |
| 7 | G | 5 | ARG | 5.4 |
| 13 | M | 122 | LYS | 5.3 |
| 10 | J | 24 | VAL | 5.3 |
| 1 | A | 1004 | A | 5.3 |
| 13 | M | 118 | ALA | 5.3 |
| 18 | R | 16 | PRO | 5.2 |
| 1 | A | 1034 | G | 5.2 |
| 4 | D | 32 | ALA | 5.2 |
| 17 | Q | 102 | GLY | 5.1 |
| 1 | A | 1027 | C | 5.0 |
| 1 | A | 1024 | G | 5.0 |
| 3 | C | 76 | VAL | 4.7 |
| 4 | D | 35 | ARG | 4.7 |
| 10 | J | 71 | LEU | 4.6 |
| 10 | J | 90 | LEU | 4.5 |
| 7 | G | 156 | TRP | 4.5 |
| 1 | A | 1002 | G | 4.5 |
| 1 | A | 1003(A) | G | 4.3 |
| 3 | C | 68 | VAL | 4.3 |
| 4 | D | 36 | ARG | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | A | 1006 | C | 4.3 |
| 11 | K | 128 | ALA | 4.3 |
| 15 | O | 23 | GLY | 4.3 |
| 17 | Q | 103 | GLY | 4.3 |
| 10 | J | 36 | GLY | 4.2 |
| 1 | A | 1036 | G | 4.2 |
| 1 | A | 1533 | C | 4.1 |
| 9 | I | 19 | LEU | 4.1 |
| 1 | A | 1003 | G | 4.0 |
| 14 | N | 6 | LEU | 4.0 |
| 1 | A | 1025 | U | 3.9 |
| 10 | J | 72 | VAL | 3.9 |
| 2 | B | 136 | VAL | 3.9 |
| 1 | A | 1033 | G | 3.9 |
| 13 | M | 117 | VAL | 3.8 |
| 7 | G | 155 | ARG | 3.7 |
| 22 | X | 4 | A | 3.7 |
| 15 | O | 89 | GLY | 3.7 |
| 21 | U | 24 | ARG | 3.6 |
| 1 | A | 1026 | G | 3.6 |
| 19 | S | 49 | ILE | 3.6 |
| 1 | A | 1143 | G | 3.5 |
| 1 | A | 1144 | G | 3.5 |
| 1 | A | 1031 | G | 3.5 |
| 1 | A | 1131 | G | 3.5 |
| 9 | I | 66 | ARG | 3.5 |
| 3 | C | 77 | ILE | 3.5 |
| 1 | A | 1030(A) | G | 3.5 |
| 1 | A | 1001 | A | 3.5 |
| 1 | A | 1035 | A | 3.5 |
| 10 | J | 8 | LEU | 3.4 |
| 10 | J | 16 | LEU | 3.4 |
| 1 | A | 1032 | G | 3.4 |
| 14 | N | 3 | ARG | 3.4 |
| 2 | B | 19 | HIS | 3.3 |
| 1 | A | 1132 | C | 3.2 |
| 15 | O | 22 | THR | 3.2 |
| 1 | A | 412 | A | 3.2 |
| 13 | M | 119 | GLY | 3.2 |
| 10 | J | 7 | LYS | 3.2 |
| 3 | C | 78 | GLY | 3.1 |
| 1 | A | 1130 | A | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 4 | D | 25 | ARG | 3.1 |
| 9 | I | 15 | ALA | 3.1 |
| 1 | A | 1038 | C | 3.1 |
| 13 | M | 8 | GLU | 3.1 |
| 1 | A | 1260 | C | 3.1 |
| 19 | S | 28 | LYS | 3.1 |
| 1 | A | 1030(D) | A | 3.0 |
| 1 | A | 160 | A | 3.0 |
| 20 | T | 104 | LEU | 2.9 |
| 2 | B | 40 | HIS | 2.9 |
| 10 | J | 37 | PRO | 2.9 |
| 4 | D | 156 | GLU | 2.9 |
| 10 | J | 34 | VAL | 2.9 |
| 1 | A | 1023 | G | 2.9 |
| 9 | I | 102 | LEU | 2.9 |
| 18 | R | 18 | ARG | 2.8 |
| 13 | M | 11 | ARG | 2.8 |
| 1 | A | 1128 | C | 2.8 |
| 14 | N | 2 | ALA | 2.8 |
| 10 | J | 75 | ILE | 2.8 |
| 1 | A | 1030(B) | C | 2.8 |
| 1 | A | 1037 | C | 2.8 |
| 10 | J | 43 | ARG | 2.7 |
| 3 | C | 196 | LEU | 2.7 |
| 17 | Q | 101 | ARG | 2.7 |
| 2 | B | 206 | ASP | 2.7 |
| 19 | S | 27 | GLU | 2.7 |
| 1 | A | 1420 | C | 2.7 |
| 3 | C | 60 | ALA | 2.7 |
| 1 | A | 202 | U | 2.6 |
| 2 | B | 133 | LYS | 2.6 |
| 3 | C | 65 | ALA | 2.6 |
| 1 | A | 1005 | A | 2.6 |
| 3 | C | 103 | VAL | 2.6 |
| 1 | A | 1139 | G | 2.6 |
| 10 | J | 69 | ASN | 2.6 |
| 10 | J | 98 | ILE | 2.6 |
| 1 | A | 1029 | C | 2.6 |
| 13 | M | 116 | THR | 2.5 |
| 1 | A | 993 | G | 2.5 |
| 1 | A | 1138 | G | 2.5 |
| 13 | M | 13 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 20 | T | 101 | GLY | 2.5 |
| 9 | I | 92 | TYR | 2.5 |
| 9 | I | 101 | PHE | 2.5 |
| 10 | J | 87 | THR | 2.5 |
| 9 | I | 70 | LYS | 2.5 |
| 1 | A | 1030 | C | 2.5 |
| 20 | T | 9 | ASN | 2.5 |
| 5 | E | 119 | LEU | 2.4 |
| 19 | S | 2 | PRO | 2.4 |
| 1 | A | 1419 | G | 2.4 |
| 3 | C | 81 | GLY | 2.4 |
| 7 | G | 4 | ARG | 2.4 |
| 4 | D | 42 | GLN | 2.4 |
| 1 | A | 1019 | C | 2.4 |
| 4 | D | 49 | ARG | 2.4 |
| 3 | C | 69 | HIS | 2.3 |
| 10 | J | 33 | GLN | 2.3 |
| 9 | I | 96 | LEU | 2.3 |
| 3 | C | 188 | LEU | 2.3 |
| 6 | F | 61 | LEU | 2.3 |
| 4 | D | 20 | TYR | 2.3 |
| 3 | C | 67 | THR | 2.3 |
| 19 | S | 29 | ARG | 2.3 |
| 9 | I | 65 | VAL | 2.3 |
| 4 | D | 31 | CYS | 2.3 |
| 1 | A | 1028 | C | 2.3 |
| 1 | A | 1478 | C | 2.3 |
| 20 | T | 103 | GLY | 2.3 |
| 3 | C | 66 | VAL | 2.2 |
| 18 | R | 19 | LYS | 2.2 |
| 19 | S | 71 | LEU | 2.2 |
| 1 | A | 723 | U | 2.2 |
| 4 | D | 23 | GLY | 2.2 |
| 2 | B | 208 | ILE | 2.2 |
| 4 | D | 29 | PRO | 2.2 |
| 2 | B | 38 | GLY | 2.2 |
| 6 | F | 14 | LEU | 2.2 |
| 2 | B | 125 | PRO | 2.2 |
| 1 | A | 161 | A | 2.1 |
| 6 | F | 36 | ARG | 2.1 |
| 15 | O | 12 | ILE | 2.1 |
| 4 | D | 33 | MET | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | M | 104 | ARG | 2.1 |
| 19 | S | 34 | TRP | 2.1 |
| 1 | A | 1418 | A | 2.1 |
| 1 | A | 159 | G | 2.1 |
| 6 | F | 65 | VAL | 2.1 |
| 1 | A | 1135 | U | 2.0 |
| 4 | D | 157 | LEU | 2.0 |
| 1 | A | 1009 | G | 2.0 |
| 23 | Y | 39 | C | 2.0 |
| 3 | C | 104 | GLN | 2.0 |
| 9 | I | 36 | TYR | 2.0 |
| 3 | C | 201 | TYR | 2.0 |
| 18 | R | 31 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95th 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(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 26 | K | A | 1837 | 1/1 | -0.00 | 0.31 | 168,168,168,168 | 0 |
| 25 | MG | A | 1656 | 1/1 | 0.04 | 0.39 | 142,142,142,142 | 0 |
| 25 | MG | A | 1625 | 1/1 | 0.10 | 0.83 | 119,119,119,119 | 0 |
| 25 | MG | A | 1692 | 1/1 | 0.11 | 1.53 | 126,126,126,126 | 0 |
| 25 | MG | A | 1632 | 1/1 | 0.16 | 0.92 | 186,186,186,186 | 0 |
| 25 | MG | A | 1672 | 1/1 | 0.17 | 0.21 | 159,159,159,159 | 0 |
| 25 | MG | A | 1728 | 1/1 | 0.18 | 1.65 | 125,125,125,125 | 0 |
| 26 | K | A | 1853 | 1/1 | 0.18 | 0.44 | 132,132,132,132 | 0 |
| 26 | K | A | 1835 | 1/1 | 0.22 | 0.66 | 138,138,138,138 | 0 |
| 25 | MG | A | 1720 | 1/1 | 0.22 | 0.30 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1668 | 1/1 | 0.23 | 1.28 | 153,153,153,153 | 0 |
| 25 | MG | A | 1663 | 1/1 | 0.24 | 1.38 | 115,115,115,115 | 0 |
| 25 | MG | A | 1675 | 1/1 | 0.27 | 0.66 | 114,114,114,114 | 0 |
| 25 | MG | A | 1697 | 1/1 | 0.27 | 0.46 | 139,139,139,139 | 0 |
| 25 | MG | A | 1612 | 1/1 | 0.28 | 0.67 | 88,88,88,88 | 0 |
| 26 | K | A | 1819 | 1/1 | 0.29 | 1.21 | 156,156,156,156 | 0 |
| 26 | K | A | 1833 | 1/1 | 0.32 | 1.44 | 159,159,159,159 | 0 |
| 26 | K | A | 1815 | 1/1 | 0.34 | 1.45 | 200,200,200,200 | 0 |
| 26 | K | A | 1857 | 1/1 | 0.35 | 0.82 | 151,151,151,151 | 0 |
| 25 | MG | A | 1713 | 1/1 | 0.36 | 0.75 | 114,114,114,114 | 0 |
| 25 | MG | A | 1774 | 1/1 | 0.36 | 0.98 | 118,118,118,118 | 0 |
| 26 | K | A | 1836 | 1/1 | 0.37 | 0.37 | 155,155,155,155 | 0 |
| 26 | K | A | 1854 | 1/1 | 0.38 | 0.36 | 157,157,157,157 | 0 |
| 25 | MG | A | 1718 | 1/1 | 0.38 | 0.51 | 115,115,115,115 | 0 |
| 26 | K | A | 1813 | 1/1 | 0.39 | 0.23 | 140,140,140,140 | 0 |
| 25 | MG | A | 1676 | 1/1 | 0.39 | 0.53 | 130,130,130,130 | 0 |
| 26 | K | A | 1808 | 1/1 | 0.39 | 0.46 | 150,150,150,150 | 0 |
| 26 | K | A | 1832 | 1/1 | 0.39 | 0.52 | 108,108,108,108 | 0 |
| 25 | MG | A | 1671 | 1/1 | 0.39 | 1.56 | 126,126,126,126 | 0 |
| 25 | MG | A | 1698 | 1/1 | 0.40 | 0.70 | 117,117,117,117 | 0 |
| 25 | MG | A | 1683 | 1/1 | 0.41 | 1.50 | 123,123,123,123 | 0 |
| 25 | MG | A | 1659 | 1/1 | 0.41 | 0.77 | 128,128,128,128 | 0 |
| 26 | K | M | 202 | 1/1 | 0.42 | 0.42 | 111,111,111,111 | 0 |
| 25 | MG | A | 1724 | 1/1 | 0.43 | 0.99 | 119,119,119,119 | 0 |
| 25 | MG | A | 1677 | 1/1 | 0.44 | 0.75 | 132,132,132,132 | 0 |
| 25 | MG | A | 1680 | 1/1 | 0.46 | 0.25 | 101,101,101,101 | 0 |
| 26 | K | P | 102 | 1/1 | 0.46 | 0.59 | 161,161,161,161 | 0 |
| 25 | MG | A | 1736 | 1/1 | 0.48 | 1.07 | 66,66,66,66 | 0 |
| 26 | K | A | 1834 | 1/1 | 0.48 | 0.94 | 152,152,152,152 | 0 |
| 25 | MG | A | 1651 | 1/1 | 0.48 | 1.45 | 109,109,109,109 | 0 |
| 25 | MG | A | 1626 | 1/1 | 0.48 | 1.98 | 130,130,130,130 | 0 |
| 25 | MG | A | 1702 | 1/1 | 0.48 | 0.81 | 110,110,110,110 | 0 |
| 25 | MG | A | 1716 | 1/1 | 0.50 | 0.52 | 112,112,112,112 | 0 |
| 25 | MG | A | 1695 | 1/1 | 0.50 | 0.58 | 107,107,107,107 | 0 |
| 26 | K | A | 1847 | 1/1 | 0.50 | 0.41 | 145,145,145,145 | 0 |
| 25 | MG | A | 1778 | 1/1 | 0.51 | 0.22 | 96,96,96,96 | 0 |
| 25 | MG | A | 1722 | 1/1 | 0.52 | 0.96 | 123,123,123,123 | 0 |
| 25 | MG | A | 1800 | 1/1 | 0.52 | 0.31 | 131,131,131,131 | 0 |
| 25 | MG | A | 1673 | 1/1 | 0.53 | 0.55 | 114,114,114,114 | 0 |
| 25 | MG | A | 1717 | 1/1 | 0.53 | 0.14 | 107,107,107,107 | 0 |
| 26 | K | A | 1816 | 1/1 | 0.54 | 0.23 | 157,157,157,157 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1647 | 1/1 | 0.54 | 0.84 | 104,104,104,104 | 0 |
| 26 | K | A | 1831 | 1/1 | 0.54 | 0.39 | 140,140,140,140 | 0 |
| 25 | MG | A | 1782 | 1/1 | 0.54 | 0.18 | 143,143,143,143 | 0 |
| 26 | K | A | 1825 | 1/1 | 0.54 | 0.71 | 146,146,146,146 | 0 |
| 25 | MG | A | 1610 | 1/1 | 0.55 | 4.56 | 181,181,181,181 | 0 |
| 25 | MG | A | 1733 | 1/1 | 0.56 | 0.49 | 104,104,104,104 | 0 |
| 26 | K | A | 1812 | 1/1 | 0.57 | 0.19 | 129,129,129,129 | 0 |
| 25 | MG | A | 1634 | 1/1 | 0.57 | 0.39 | 125,125,125,125 | 0 |
| 26 | K | A | 1858 | 1/1 | 0.57 | 0.84 | 121,121,121,121 | 0 |
| 25 | MG | A | 1788 | 1/1 | 0.57 | 1.04 | 125,125,125,125 | 0 |
| 25 | MG | A | 1667 | 1/1 | 0.58 | 0.33 | 98,98,98,98 | 0 |
| 26 | K | A | 1838 | 1/1 | 0.58 | 0.39 | 120,120,120,120 | 0 |
| 26 | K | A | 1855 | 1/1 | 0.59 | 0.91 | 161,161,161,161 | 0 |
| 26 | K | R | 102 | 1/1 | 0.59 | 0.53 | 173,173,173,173 | 0 |
| 26 | K | A | 1845 | 1/1 | 0.59 | 0.69 | 149,149,149,149 | 0 |
| 25 | MG | A | 1757 | 1/1 | 0.59 | 1.13 | 152,152,152,152 | 0 |
| 25 | MG | A | 1657 | 1/1 | 0.60 | 0.87 | 88,88,88,88 | 0 |
| 25 | MG | A | 1791 | 1/1 | 0.60 | 0.17 | 200,200,200,200 | 0 |
| 25 | MG | A | 1777 | 1/1 | 0.60 | 0.13 | 104,104,104,104 | 0 |
| 26 | K | A | 1863 | 1/1 | 0.60 | 0.65 | 116,116,116,116 | 0 |
| 25 | MG | A | 1655 | 1/1 | 0.61 | 0.79 | 141,141,141,141 | 0 |
| 25 | MG | A | 1624 | 1/1 | 0.61 | 0.40 | 105,105,105,105 | 0 |
| 26 | K | E | 203 | 1/1 | 0.62 | 0.57 | 132,132,132,132 | 0 |
| 26 | K | A | 1828 | 1/1 | 0.62 | 1.37 | 167,167,167,167 | 0 |
| 25 | MG | A | 1607 | 1/1 | 0.62 | 1.17 | 117,117,117,117 | 0 |
| 25 | MG | A | 1729 | 1/1 | 0.63 | 0.17 | 84,84,84,84 | 0 |
| 25 | MG | A | 1687 | 1/1 | 0.63 | 0.31 | 97,97,97,97 | 0 |
| 25 | MG | A | 1638 | 1/1 | 0.63 | 0.43 | 124,124,124,124 | 0 |
| 26 | K | A | 1830 | 1/1 | 0.63 | 0.24 | 146,146,146,146 | 0 |
| 25 | MG | A | 1739 | 1/1 | 0.63 | 0.73 | 99,99,99,99 | 0 |
| 25 | MG | A | 1641 | 1/1 | 0.63 | 1.09 | 104,104,104,104 | 0 |
| 25 | MG | A | 1714 | 1/1 | 0.64 | 2.62 | 171,171,171,171 | 0 |
| 25 | MG | A | 1754 | 1/1 | 0.64 | 0.27 | 88,88,88,88 | 0 |
| 25 | MG | N | 102 | 1/1 | 0.64 | 0.80 | 95,95,95,95 | 0 |
| 25 | MG | A | 1753 | 1/1 | 0.64 | 1.06 | 102,102,102,102 | 0 |
| 26 | K | A | 1848 | 1/1 | 0.64 | 0.95 | 150,150,150,150 | 0 |
| 26 | K | A | 1842 | 1/1 | 0.64 | 0.59 | 168,168,168,168 | 0 |
| 26 | K | A | 1865 | 1/1 | 0.64 | 0.35 | 113,113,113,113 | 0 |
| 26 | K | A | 1852 | 1/1 | 0.65 | 0.42 | 155,155,155,155 | 0 |
| 26 | K | S | 101 | 1/1 | 0.65 | 0.13 | 164,164,164,164 | 0 |
| 25 | MG | A | 1629 | 1/1 | 0.65 | 0.74 | 89,89,89,89 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 26 | K | A | 1840 | 1/1 | 0.65 | 0.36 | 145,145,145,145 | 0 |
| 25 | MG | A | 1631 | 1/1 | 0.65 | 1.40 | 122,122,122,122 | 0 |
| 25 | MG | E | 201 | 1/1 | 0.65 | 0.90 | 127,127,127,127 | 0 |
| 25 | MG | A | 1704 | 1/1 | 0.66 | 0.37 | 71,71,71,71 | 0 |
| 25 | MG | A | 1653 | 1/1 | 0.66 | 1.08 | 65,65,65,65 | 0 |
| 25 | MG | A | 1684 | 1/1 | 0.66 | 0.69 | 85,85,85,85 | 0 |
| 25 | MG | A | 1618 | 1/1 | 0.66 | 0.52 | 81,81,81,81 | 0 |
| 26 | K | A | 1824 | 1/1 | 0.67 | 0.42 | 117,117,117,117 | 0 |
| 25 | MG | A | 1621 | 1/1 | 0.67 | 0.61 | 51,51,51,51 | 0 |
| 26 | K | A | 1826 | 1/1 | 0.67 | 0.35 | 130,130,130,130 | 0 |
| 26 | K | I | 203 | 1/1 | 0.68 | 0.99 | 78,78,78,78 | 0 |
| 25 | MG | A | 1640 | 1/1 | 0.68 | 1.56 | 131,131,131,131 | 0 |
| 25 | MG | A | 1747 | 1/1 | 0.68 | 0.51 | 102,102,102,102 | 0 |
| 25 | MG | A | 1690 | 1/1 | 0.68 | 2.07 | 149,149,149,149 | 0 |
| 27 | ZN | D | 301 | 1/1 | 0.68 | 0.75 | 174,174,174,174 | 0 |
| 25 | MG | Q | 201 | 1/1 | 0.68 | 0.21 | 117,117,117,117 | 0 |
| 25 | MG | A | 1623 | 1/1 | 0.68 | 0.86 | 113,113,113,113 | 0 |
| 25 | MG | A | 1664 | 1/1 | 0.68 | 0.92 | 141,141,141,141 | 0 |
| 26 | K | D | 302 | 1/1 | 0.69 | 0.53 | 123,123,123,123 | 0 |
| 25 | MG | A | 1666 | 1/1 | 0.70 | 1.18 | 125,125,125,125 | 0 |
| 25 | MG | A | 1784 | 1/1 | 0.70 | 0.24 | 92,92,92,92 | 0 |
| 25 | MG | A | 1645 | 1/1 | 0.70 | 0.51 | 138,138,138,138 | 0 |
| 26 | K | A | 1841 | 1/1 | 0.71 | 0.21 | 111,111,111,111 | 0 |
| 25 | MG | A | 1614 | 1/1 | 0.71 | 0.34 | 84,84,84,84 | 0 |
| 25 | MG | A | 1633 | 1/1 | 0.71 | 0.42 | 119,119,119,119 | 0 |
| 26 | K | A | 1809 | 1/1 | 0.71 | 0.30 | 129,129,129,129 | 0 |
| 26 | K | A | 1839 | 1/1 | 0.72 | 0.86 | 94,94,94,94 | 0 |
| 25 | MG | A | 1652 | 1/1 | 0.72 | 0.34 | 74,74,74,74 | 0 |
| 25 | MG | A | 1734 | 1/1 | 0.73 | 0.38 | 87,87,87,87 | 0 |
| 25 | MG | A | 1737 | 1/1 | 0.73 | 0.20 | 75,75,75,75 | 0 |
| 25 | MG | A | 1620 | 1/1 | 0.73 | 0.67 | 85,85,85,85 | 0 |
| 26 | K | A | 1861 | 1/1 | 0.73 | 0.16 | 129,129,129,129 | 0 |
| 25 | MG | A | 1710 | 1/1 | 0.73 | 1.87 | 130,130,130,130 | 0 |
| 25 | MG | A | 1681 | 1/1 | 0.73 | 0.25 | 95,95,95,95 | 0 |
| 26 | K | A | 1817 | 1/1 | 0.74 | 1.43 | 188,188,188,188 | 0 |
| 25 | MG | A | 1727 | 1/1 | 0.74 | 0.33 | 88,88,88,88 | 0 |
| 25 | MG | A | 1635 | 1/1 | 0.75 | 2.33 | 134,134,134,134 | 0 |
| 25 | MG | A | 1797 | 1/1 | 0.75 | 0.32 | 80,80,80,80 | 0 |
| 25 | MG | A | 1627 | 1/1 | 0.75 | 0.27 | 148,148,148,148 | 0 |
| 25 | MG | A | 1619 | 1/1 | 0.76 | 0.17 | 92,92,92,92 | 0 |
| 26 | K | A | 1862 | 1/1 | 0.76 | 0.60 | 88,88,88,88 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 26 | K | A | 1843 | 1/1 | 0.76 | 0.32 | 146,146,146,146 | 0 |
| 26 | K | A | 1805 | 1/1 | 0.76 | 0.40 | 106,106,106,106 | 0 |
| 26 | K | A | 1811 | 1/1 | 0.77 | 0.14 | 106,106,106,106 | 0 |
| 25 | MG | A | 1686 | 1/1 | 0.77 | 1.06 | 124,124,124,124 | 0 |
| 25 | MG | A | 1719 | 1/1 | 0.77 | 0.22 | 75,75,75,75 | 0 |
| 26 | K | A | 1827 | 1/1 | 0.77 | 0.29 | 108,108,108,108 | 0 |
| 25 | MG | A | 1678 | 1/1 | 0.77 | 2.13 | 137,137,137,137 | 0 |
| 25 | MG | A | 1751 | 1/1 | 0.78 | 0.51 | 116,116,116,116 | 0 |
| 25 | MG | A | 1689 | 1/1 | 0.78 | 1.18 | 133,133,133,133 | 0 |
| 26 | K | A | 1821 | 1/1 | 0.78 | 0.25 | 128,128,128,128 | 0 |
| 25 | MG | A | 1615 | 1/1 | 0.79 | 1.18 | 169,169,169,169 | 0 |
| 25 | MG | A | 1643 | 1/1 | 0.79 | 0.57 | 118,118,118,118 | 0 |
| 25 | MG | A | 1688 | 1/1 | 0.79 | 0.50 | 114,114,114,114 | 0 |
| 25 | MG | A | 1628 | 1/1 | 0.80 | 1.35 | 94,94,94,94 | 0 |
| 25 | MG | A | 1798 | 1/1 | 0.80 | 0.84 | 136,136,136,136 | 0 |
| 26 | K | A | 1849 | 1/1 | 0.81 | 1.01 | 94,94,94,94 | 0 |
| 25 | MG | A | 1703 | 1/1 | 0.81 | 0.25 | 80,80,80,80 | 0 |
| 25 | MG | A | 1750 | 1/1 | 0.81 | 0.62 | 104,104,104,104 | 0 |
| 25 | MG | A | 1699 | 1/1 | 0.81 | 0.20 | 52,52,52,52 | 0 |
| 25 | MG | A | 1658 | 1/1 | 0.81 | 0.79 | 98,98,98,98 | 0 |
| 25 | MG | A | 1795 | 1/1 | 0.81 | 0.71 | 90,90,90,90 | 0 |
| 25 | MG | A | 1630 | 1/1 | 0.82 | 1.49 | 117,117,117,117 | 0 |
| 25 | MG | A | 1743 | 1/1 | 0.82 | 0.40 | 94,94,94,94 | 0 |
| 25 | MG | A | 1726 | 1/1 | 0.82 | 3.81 | 135,135,135,135 | 0 |
| 25 | MG | A | 1660 | 1/1 | 0.83 | 0.95 | 105,105,105,105 | 0 |
| 25 | MG | A | 1602 | 1/1 | 0.83 | 0.12 | 148,148,148,148 | 0 |
| 25 | MG | A | 1730 | 1/1 | 0.83 | 0.63 | 104,104,104,104 | 0 |
| 26 | K | A | 1829 | 1/1 | 0.83 | 0.17 | 119,119,119,119 | 0 |
| 25 | MG | A | 1617 | 1/1 | 0.83 | 0.13 | 68,68,68,68 | 0 |
| 25 | MG | A | 1755 | 1/1 | 0.84 | 0.85 | 48,48,48,48 | 0 |
| 25 | MG | A | 1783 | 1/1 | 0.84 | 0.33 | 76,76,76,76 | 0 |
| 25 | MG | A | 1735 | 1/1 | 0.84 | 0.91 | 99,99,99,99 | 0 |
| 25 | MG | A | 1709 | 1/1 | 0.84 | 0.93 | 124,124,124,124 | 0 |
| 25 | MG | A | 1609 | 1/1 | 0.84 | 0.43 | 67,67,67,67 | 0 |
| 25 | MG | M | 201 | 1/1 | 0.84 | 0.24 | 80,80,80,80 | 0 |
| 25 | MG | A | 1738 | 1/1 | 0.84 | 0.70 | 100,100,100,100 | 0 |
| 26 | K | A | 1818 | 1/1 | 0.84 | 0.34 | 125,125,125,125 | 0 |
| 25 | MG | R | 101 | 1/1 | 0.85 | 0.45 | 142,142,142,142 | 0 |
| 25 | MG | A | 1748 | 1/1 | 0.85 | 0.91 | 109,109,109,109 | 0 |
| 25 | MG | A | 1604 | 1/1 | 0.85 | 0.29 | 47,47,47,47 | 0 |
| 25 | MG | A | 1760 | 1/1 | 0.85 | 0.10 | 61,61,61,61 | 0 |
| 25 | MG | A | 1802 | 1/1 | 0.85 | 0.74 | 95,95,95,95 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1622 | 1/1 | 0.85 | 0.43 | 65,65,65,65 | 0 |
| 25 | MG | A | 1661 | 1/1 | 0.85 | 0.94 | 92,92,92,92 | 0 |
| 25 | MG | A | 1611 | 1/1 | 0.86 | 0.34 | 111,111,111,111 | 0 |
| 25 | MG | A | 1758 | 1/1 | 0.86 | 0.81 | 154,154,154,154 | 0 |
| 25 | MG | A | 1781 | 1/1 | 0.86 | 1.14 | 86,86,86,86 | 0 |
| 25 | MG | B | 301 | 1/1 | 0.86 | 0.09 | 83,83,83,83 | 0 |
| 26 | K | A | 1850 | 1/1 | 0.86 | 0.69 | 84,84,84,84 | 0 |
| 25 | MG | A | 1670 | 1/1 | 0.86 | 1.72 | 99,99,99,99 | 0 |
| 25 | MG | A | 1636 | 1/1 | 0.87 | 0.36 | 96,96,96,96 | 0 |
| 25 | MG | A | 1715 | 1/1 | 0.87 | 1.14 | 132,132,132,132 | 0 |
| 26 | K | A | 1859 | 1/1 | 0.87 | 0.19 | 151,151,151,151 | 0 |
| 25 | MG | A | 1731 | 1/1 | 0.87 | 0.66 | 106,106,106,106 | 0 |
| 25 | MG | A | 1679 | 1/1 | 0.87 | 0.58 | 28,28,28,28 | 0 |
| 26 | K | A | 1810 | 1/1 | 0.87 | 0.52 | 120,120,120,120 | 0 |
| 25 | MG | A | 1650 | 1/1 | 0.87 | 0.26 | 96,96,96,96 | 0 |
| 25 | MG | A | 1867 | 1/1 | 0.87 | 0.10 | 68,68,68,68 | 0 |
| 25 | MG | A | 1665 | 1/1 | 0.87 | 1.15 | 130,130,130,130 | 0 |
| 25 | MG | A | 1752 | 1/1 | 0.87 | 0.90 | 120,120,120,120 | 0 |
| 25 | MG | A | 1685 | 1/1 | 0.88 | 0.49 | 124,124,124,124 | 0 |
| 25 | MG | A | 1648 | 1/1 | 0.88 | 1.65 | 130,130,130,130 | 0 |
| 26 | K | T | 201 | 1/1 | 0.88 | 0.58 | 98,98,98,98 | 0 |
| 26 | K | A | 1851 | 1/1 | 0.88 | 0.38 | 81,81,81,81 | 0 |
| 26 | K | K | 202 | 1/1 | 0.88 | 0.17 | 72,72,72,72 | 0 |
| 25 | MG | A | 1732 | 1/1 | 0.88 | 0.64 | 96,96,96,96 | 0 |
| 25 | MG | A | 1707 | 1/1 | 0.88 | 0.82 | 90,90,90,90 | 0 |
| 26 | K | A | 1844 | 1/1 | 0.88 | 0.49 | 136,136,136,136 | 0 |
| 25 | MG | A | 1649 | 1/1 | 0.88 | 0.34 | 89,89,89,89 | 0 |
| 25 | MG | A | 1616 | 1/1 | 0.88 | 0.17 | 69,69,69,69 | 0 |
| 25 | MG | A | 1613 | 1/1 | 0.88 | 0.27 | 62,62,62,62 | 0 |
| 25 | MG | A | 1700 | 1/1 | 0.89 | 0.59 | 88,88,88,88 | 0 |
| 26 | K | E | 202 | 1/1 | 0.89 | 0.44 | 85,85,85,85 | 0 |
| 25 | MG | A | 1669 | 1/1 | 0.89 | 0.61 | 104,104,104,104 | 0 |
| 25 | MG | A | 1794 | 1/1 | 0.89 | 0.16 | 68,68,68,68 | 0 |
| 26 | K | A | 1864 | 1/1 | 0.89 | 1.13 | 117,117,117,117 | 0 |
| 25 | MG | A | 1756 | 1/1 | 0.89 | 0.85 | 69,69,69,69 | 0 |
| 25 | MG | A | 1712 | 1/1 | 0.89 | 1.12 | 113,113,113,113 | 0 |
| 25 | MG | A | 1696 | 1/1 | 0.90 | 0.67 | 103,103,103,103 | 0 |
| 25 | MG | K | 201 | 1/1 | 0.90 | 0.50 | 100,100,100,100 | 0 |
| 25 | MG | A | 1801 | 1/1 | 0.90 | 0.63 | 80,80,80,80 | 0 |
| 25 | MG | A | 1780 | 1/1 | 0.90 | 0.82 | 65,65,65,65 | 0 |
| 26 | K | A | 1823 | 1/1 | 0.90 | 0.64 | 98,98,98,98 | 0 |
| 25 | MG | A | 1799 | 1/1 | 0.90 | 0.34 | 81,81,81,81 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1766 | 1/1 | 0.90 | 0.16 | 71,71,71,71 | 0 |
| 25 | MG | A | 1742 | 1/1 | 0.90 | 0.18 | 54,54,54,54 | 0 |
| 25 | MG | A | 1711 | 1/1 | 0.90 | 1.23 | 139,139,139,139 | 0 |
| 25 | MG | A | 1740 | 1/1 | 0.90 | 0.47 | 76,76,76,76 | 0 |
| 25 | MG | A | 1772 | 1/1 | 0.90 | 0.92 | 66,66,66,66 | 0 |
| 25 | MG | A | 1723 | 1/1 | 0.90 | 0.25 | 79,79,79,79 | 0 |
| 25 | MG | A | 1603 | 1/1 | 0.91 | 1.89 | 152,152,152,152 | 0 |
| 25 | MG | A | 1693 | 1/1 | 0.91 | 0.38 | 70,70,70,70 | 0 |
| 25 | MG | A | 1763 | 1/1 | 0.91 | 0.28 | 94,94,94,94 | 0 |
| 25 | MG | A | 1606 | 1/1 | 0.91 | 0.07 | 82,82,82,82 | 0 |
| 26 | K | A | 1846 | 1/1 | 0.91 | 0.82 | 94,94,94,94 | 0 |
| 25 | MG | A | 1749 | 1/1 | 0.91 | 0.68 | 76,76,76,76 | 0 |
| 26 | K | A | 1866 | 1/1 | 0.92 | 0.11 | 122,122,122,122 | 0 |
| 25 | MG | A | 1708 | 1/1 | 0.92 | 0.33 | 73,73,73,73 | 0 |
| 25 | MG | A | 1608 | 1/1 | 0.92 | 1.08 | 95,95,95,95 | 0 |
| 25 | MG | A | 1785 | 1/1 | 0.92 | 0.81 | 66,66,66,66 | 0 |
| 25 | MG | A | 1682 | 1/1 | 0.92 | 0.44 | 96,96,96,96 | 0 |
| 25 | MG | A | 1654 | 1/1 | 0.92 | 1.25 | 119,119,119,119 | 0 |
| 25 | MG | A | 1701 | 1/1 | 0.92 | 0.60 | 74,74,74,74 | 0 |
| 25 | MG | A | 1639 | 1/1 | 0.92 | 0.29 | 100,100,100,100 | 0 |
| 26 | K | A | 1814 | 1/1 | 0.92 | 0.32 | 142,142,142,142 | 0 |
| 25 | MG | A | 1694 | 1/1 | 0.93 | 0.38 | 75,75,75,75 | 0 |
| 26 | K | A | 1856 | 1/1 | 0.93 | 0.74 | 184,184,184,184 | 0 |
| 25 | MG | A | 1759 | 1/1 | 0.93 | 0.07 | 112,112,112,112 | 0 |
| 25 | MG | A | 1746 | 1/1 | 0.93 | 0.49 | 99,99,99,99 | 0 |
| 25 | MG | A | 1691 | 1/1 | 0.93 | 0.50 | 104,104,104,104 | 0 |
| 26 | K | A | 1820 | 1/1 | 0.93 | 0.16 | 136,136,136,136 | 0 |
| 26 | K | A | 1806 | 1/1 | 0.93 | 0.16 | 101,101,101,101 | 0 |
| 25 | MG | A | 1787 | 1/1 | 0.93 | 0.39 | 96,96,96,96 | 0 |
| 25 | MG | A | 1744 | 1/1 | 0.93 | 0.69 | 101,101,101,101 | 0 |
| 26 | K | A | 1822 | 1/1 | 0.93 | 0.21 | 128,128,128,128 | 0 |
| 25 | MG | A | 1646 | 1/1 | 0.93 | 0.82 | 107,107,107,107 | 0 |
| 26 | K | A | 1807 | 1/1 | 0.93 | 0.39 | 127,127,127,127 | 0 |
| 25 | MG | A | 1725 | 1/1 | 0.94 | 0.82 | 132,132,132,132 | 0 |
| 25 | MG | A | 1605 | 1/1 | 0.94 | 1.30 | 110,110,110,110 | 0 |
| 25 | MG | I | 202 | 1/1 | 0.94 | 0.36 | 73,73,73,73 | 0 |
| 24 | PAR | A | 1601 | 42/42 | 0.94 | 0.23 | 66,72,84,88 | 0 |
| 25 | MG | A | 1790 | 1/1 | 0.94 | 0.58 | 56,56,56,56 | 0 |
| 25 | MG | A | 1796 | 1/1 | 0.94 | 0.12 | 68,68,68,68 | 0 |
| 25 | MG | A | 1705 | 1/1 | 0.94 | 1.09 | 106,106,106,106 | 0 |
| 25 | MG | A | 1662 | 1/1 | 0.94 | 2.45 | 111,111,111,111 | 0 |
| 25 | MG | A | 1776 | 1/1 | 0.94 | 0.34 | 91,91,91,91 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1769 | 1/1 | 0.94 | 0.54 | 58,58,58,58 | 0 |
| 25 | MG | A | 1768 | 1/1 | 0.94 | 0.12 | 124,124,124,124 | 0 |
| 25 | MG | A | 1745 | 1/1 | 0.94 | 0.44 | 80,80,80,80 | 0 |
| 25 | MG | A | 1741 | 1/1 | 0.95 | 0.58 | 73,73,73,73 | 0 |
| 25 | MG | A | 1706 | 1/1 | 0.95 | 0.21 | 65,65,65,65 | 0 |
| 25 | MG | Q | 202 | 1/1 | 0.95 | 0.20 | 71,71,71,71 | 0 |
| 25 | MG | A | 1771 | 1/1 | 0.95 | 0.48 | 60,60,60,60 | 0 |
| 25 | MG | A | 1642 | 1/1 | 0.95 | 0.91 | 113,113,113,113 | 0 |
| 25 | MG | A | 1637 | 1/1 | 0.95 | 0.68 | 98,98,98,98 | 0 |
| 25 | MG | A | 1674 | 1/1 | 0.95 | 0.14 | 86,86,86,86 | 0 |
| 25 | MG | A | 1789 | 1/1 | 0.96 | 0.10 | 58,58,58,58 | 0 |
| 25 | MG | A | 1721 | 1/1 | 0.96 | 1.31 | 106,106,106,106 | 0 |
| 26 | K | A | 1860 | 1/1 | 0.96 | 0.22 | 143,143,143,143 | 0 |
| 25 | MG | A | 1786 | 1/1 | 0.96 | 0.11 | 123,123,123,123 | 0 |
| 26 | K | A | 1804 | 1/1 | 0.96 | 0.07 | 81,81,81,81 | 0 |
| 25 | MG | A | 1793 | 1/1 | 0.96 | 0.54 | 69,69,69,69 | 0 |
| 25 | MG | A | 1803 | 1/1 | 0.97 | 0.09 | 106,106,106,106 | 0 |
| 25 | MG | A | 1773 | 1/1 | 0.97 | 0.18 | 63,63,63,63 | 0 |
| 25 | MG | A | 1644 | 1/1 | 0.97 | 0.95 | 109,109,109,109 | 0 |
| 25 | MG | A | 1792 | 1/1 | 0.97 | 0.28 | 44,44,44,44 | 0 |
| 25 | MG | A | 1762 | 1/1 | 0.97 | 0.26 | 111,111,111,111 | 0 |
| 25 | MG | A | 1765 | 1/1 | 0.98 | 0.18 | 111,111,111,111 | 0 |
| 25 | MG | A | 1767 | 1/1 | 0.98 | 0.13 | 67,67,67,67 | 0 |
| 25 | MG | A | 1775 | 1/1 | 0.98 | 0.41 | 102,102,102,102 | 0 |
| 25 | MG | A | 1770 | 1/1 | 0.98 | 0.20 | 118,118,118,118 | 0 |
| 25 | MG | I | 201 | 1/1 | 0.98 | 0.29 | 145,145,145,145 | 0 |
| 25 | MG | P | 101 | 1/1 | 0.98 | 0.31 | 108,108,108,108 | 0 |
| 25 | MG | A | 1761 | 1/1 | 0.98 | 0.34 | 174,174,174,174 | 0 |
| 25 | MG | A | 1779 | 1/1 | 0.99 | 0.07 | 103,103,103,103 | 0 |
| 25 | MG | A | 1764 | 1/1 | 0.99 | 0.10 | 131,131,131,131 | 0 |
| 27 | ZN | N | 101 | 1/1 | 0.99 | 0.27 | 102,102,102,102 | 0 |

6.5 Other polymers

There are no such residues in this entry.