



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:51 am BST

PDB ID : 1EFW
Title : Crystal structure of aspartyl-tRNA synthetase from *Thermus thermophilus* complexed to tRNA^{asp} from *Escherichia coli*
Authors : Briand, C.; Poterszman, A.; Eiler, S.; Webster, G.; Thierry, J.-C.; Moras, D.
Deposited on : 2000-02-10
Resolution : 3.00 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

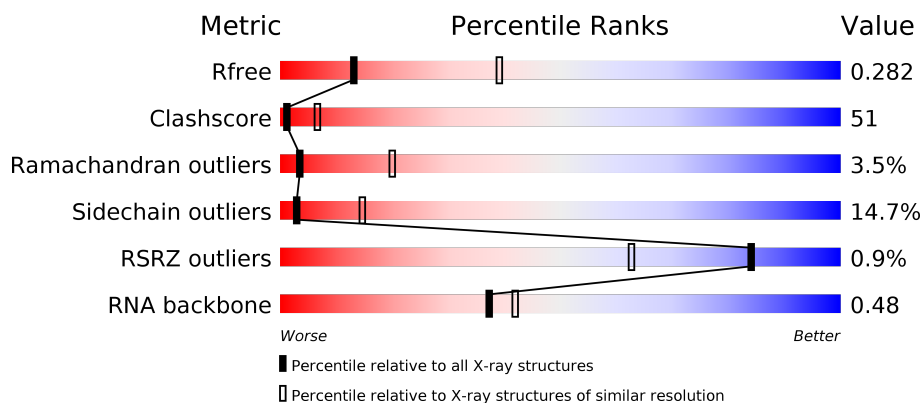
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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} | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |
| RNA backbone | 3102 | 1173 (3.30-2.70) |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | C | 73 | |
| 1 | D | 73 | |
| 2 | A | 580 | |
| 2 | B | 580 | |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12572 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 ASPARTYL-TRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 1 | C | 73 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1570 | 703 | 274 | 519 | 73 | 1 | | | |
| 1 | D | 73 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1570 | 703 | 274 | 519 | 73 | 1 | | | |

- Molecule 2 is a protein called ASPARTYL-TRNA SYNTHETASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | A | 580 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4668 | 2980 | 840 | 837 | 11 | | | |
| 2 | B | 580 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4668 | 2980 | 840 | 837 | 11 | | | |

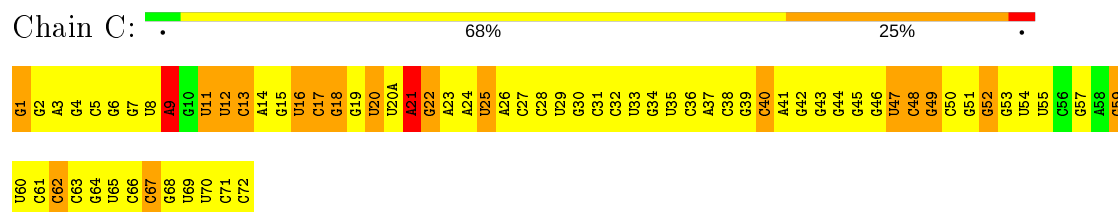
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | C | 12 | Total | O | 0 | 0 |
| | | | 12 | 12 | | |
| 3 | D | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |
| 3 | A | 43 | Total | O | 0 | 0 |
| | | | 43 | 43 | | |
| 3 | B | 31 | Total | O | 0 | 0 |
| | | | 31 | 31 | | |

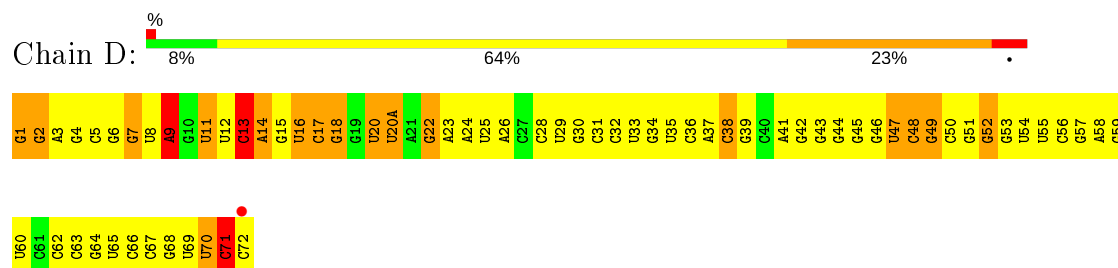
3 Residue-property plots

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.

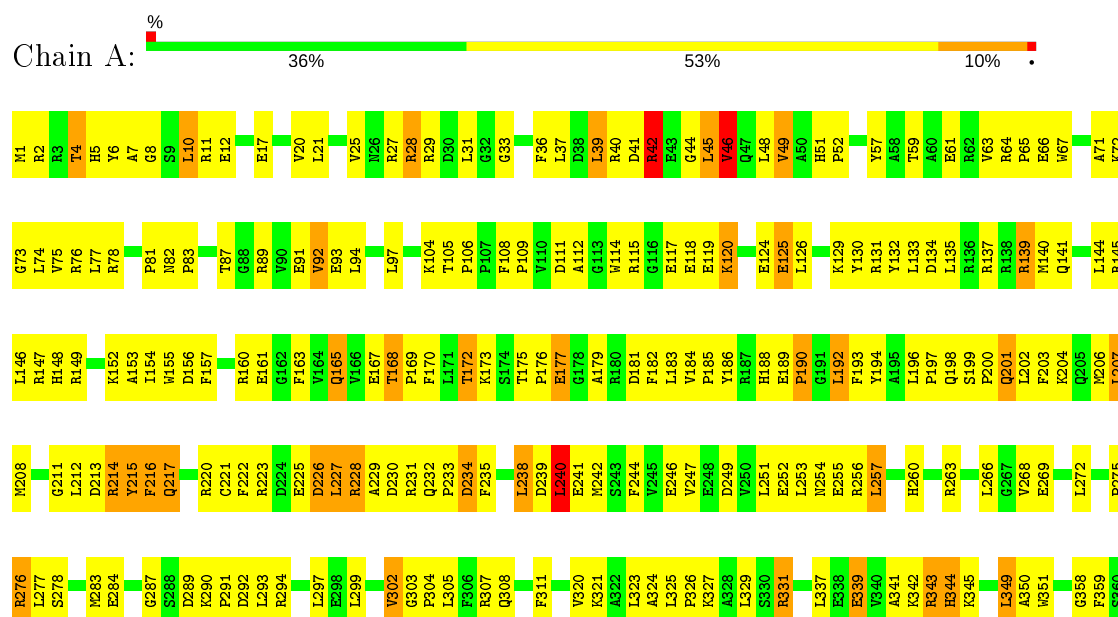
• Molecule 1: ASPARTYL-TRNA



• Molecule 1: ASPARTYL-TRNA



• Molecule 2: ASPARTYL-TRNA SYNTHETASE



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 63 | Depositor |
| Cell constants a, b, c, α , β , γ | 251.45Å 251.45Å 88.70Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 15.00 – 3.00 14.99 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 91.8 (15.00-3.00) 91.8 (14.99-3.00) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.87 (at 3.01Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.248 , 0.293 0.238 , 0.282 | Depositor DCC |
| R_{free} test set | 2969 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 43.3 | Xtriage |
| Anisotropy | 0.299 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 16.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | 0.035 for h,-h-k,-l | Xtriage |
| F_o, F_c correlation | 0.87 | EDS |
| Total number of atoms | 12572 | wwPDB-VP |
| Average B, all atoms (Å ²) | 40.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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: 5MU, G7M, H2U, 2MA, 4SU, QUO, PSU

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 | C | 0.98 | 6/1506 (0.4%) | 1.08 | 10/2343 (0.4%) |
| 1 | D | 0.74 | 1/1506 (0.1%) | 0.98 | 8/2343 (0.3%) |
| 2 | A | 0.55 | 2/4780 (0.0%) | 1.01 | 16/6467 (0.2%) |
| 2 | B | 0.59 | 6/4780 (0.1%) | 1.03 | 18/6467 (0.3%) |
| All | All | 0.65 | 15/12572 (0.1%) | 1.02 | 52/17620 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | C | 0 | 4 |
| 1 | D | 0 | 4 |
| All | All | 0 | 8 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2 | B | 580 | PRO | C-OXT | 15.85 | 1.53 | 1.23 |
| 1 | C | 1 | G | O3'-P | -15.47 | 1.42 | 1.61 |
| 1 | C | 59 | G | O3'-P | 12.60 | 1.76 | 1.61 |
| 2 | A | 495 | ARG | CZ-NH1 | 11.61 | 1.48 | 1.33 |
| 2 | A | 495 | ARG | CZ-NH2 | 10.79 | 1.47 | 1.33 |
| 2 | B | 580 | PRO | CA-C | 9.90 | 1.72 | 1.52 |
| 1 | C | 11 | U | O3'-P | -8.11 | 1.51 | 1.61 |
| 2 | B | 307 | ARG | NE-CZ | 7.48 | 1.42 | 1.33 |
| 2 | B | 580 | PRO | C-O | 6.65 | 1.36 | 1.23 |
| 1 | C | 62 | C | O3'-P | -6.63 | 1.53 | 1.61 |
| 2 | B | 307 | ARG | CD-NE | 6.39 | 1.57 | 1.46 |
| 1 | C | 12 | U | O3'-P | 6.21 | 1.68 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | C | 67 | C | O3'-P | 5.74 | 1.68 | 1.61 |
| 2 | B | 307 | ARG | CG-CD | 5.58 | 1.65 | 1.51 |
| 1 | D | 70 | U | O3'-P | -5.07 | 1.55 | 1.61 |

All (52) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | B | 307 | ARG | NE-CZ-NH1 | 35.08 | 137.84 | 120.30 |
| 2 | A | 495 | ARG | NE-CZ-NH2 | -31.89 | 104.36 | 120.30 |
| 2 | A | 495 | ARG | NH1-CZ-NH2 | 19.00 | 140.31 | 119.40 |
| 2 | B | 307 | ARG | NE-CZ-NH2 | -17.90 | 111.35 | 120.30 |
| 2 | B | 307 | ARG | CG-CD-NE | 17.16 | 147.83 | 111.80 |
| 2 | B | 307 | ARG | CD-NE-CZ | 13.53 | 142.55 | 123.60 |
| 2 | A | 495 | ARG | NE-CZ-NH1 | -10.91 | 114.84 | 120.30 |
| 2 | B | 307 | ARG | NH1-CZ-NH2 | -9.35 | 109.11 | 119.40 |
| 1 | D | 70 | U | N1-C1'-C2' | -8.57 | 102.57 | 112.00 |
| 2 | B | 307 | ARG | CB-CG-CD | 8.52 | 133.75 | 111.60 |
| 2 | B | 307 | ARG | CA-CB-CG | -8.48 | 94.74 | 113.40 |
| 2 | A | 344 | HIS | N-CA-C | -8.41 | 88.28 | 111.00 |
| 1 | C | 59 | G | O3'-P-O5' | 8.35 | 119.86 | 104.00 |
| 2 | A | 240 | LEU | CA-CB-CG | 7.31 | 132.12 | 115.30 |
| 2 | A | 431 | TRP | N-CA-C | 7.31 | 130.74 | 111.00 |
| 1 | D | 13 | C | O4'-C1'-N1 | 7.12 | 113.89 | 108.20 |
| 1 | D | 1 | G | P-O3'-C3' | -7.04 | 111.25 | 119.70 |
| 1 | C | 22 | G | O3'-P-O5' | 6.92 | 117.15 | 104.00 |
| 2 | A | 432 | ASP | N-CA-C | 6.88 | 129.59 | 111.00 |
| 1 | C | 21 | A | P-O3'-C3' | 6.67 | 127.70 | 119.70 |
| 2 | A | 435 | GLU | N-CA-C | -6.42 | 93.68 | 111.00 |
| 2 | B | 417 | GLY | N-CA-C | 6.41 | 129.13 | 113.10 |
| 2 | A | 512 | LEU | CA-CB-CG | 6.24 | 129.65 | 115.30 |
| 1 | D | 14 | A | O4'-C1'-N9 | 6.13 | 113.11 | 108.20 |
| 2 | B | 240 | LEU | CA-CB-CG | 6.06 | 129.23 | 115.30 |
| 2 | B | 434 | GLU | N-CA-C | -5.92 | 95.02 | 111.00 |
| 1 | C | 22 | G | P-O5'-C5' | -5.90 | 111.46 | 120.90 |
| 2 | B | 42 | ARG | NE-CZ-NH2 | -5.83 | 117.38 | 120.30 |
| 2 | B | 344 | HIS | N-CA-C | -5.81 | 95.31 | 111.00 |
| 2 | B | 345 | LYS | N-CA-C | 5.81 | 126.68 | 111.00 |
| 1 | C | 52 | G | N9-C1'-C2' | -5.68 | 105.75 | 112.00 |
| 1 | C | 9 | A | C5'-C4'-C3' | -5.68 | 106.91 | 116.00 |
| 2 | A | 238 | LEU | N-CA-C | -5.67 | 95.69 | 111.00 |
| 1 | D | 71 | C | O4'-C1'-N1 | -5.66 | 103.67 | 108.20 |
| 2 | B | 218 | ILE | N-CA-C | -5.66 | 95.72 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | A | 46 | VAL | CB-CA-C | -5.63 | 100.70 | 111.40 |
| 2 | A | 436 | GLU | N-CA-C | 5.60 | 126.11 | 111.00 |
| 1 | C | 12 | U | N1-C1'-C2' | -5.58 | 105.86 | 112.00 |
| 1 | D | 2 | G | P-O5'-C5' | -5.58 | 111.97 | 120.90 |
| 1 | C | 60 | U | OP1-P-OP2 | -5.50 | 111.35 | 119.60 |
| 2 | B | 212 | LEU | CA-CB-CG | -5.44 | 102.78 | 115.30 |
| 2 | A | 431 | TRP | C-N-CA | -5.43 | 108.12 | 121.70 |
| 2 | A | 46 | VAL | N-CA-C | -5.38 | 96.48 | 111.00 |
| 2 | B | 238 | LEU | N-CA-C | -5.36 | 96.54 | 111.00 |
| 1 | C | 60 | U | O5'-P-OP2 | 5.30 | 117.06 | 110.70 |
| 2 | B | 528 | GLY | N-CA-C | -5.20 | 100.10 | 113.10 |
| 2 | A | 532 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 2 | A | 45 | LEU | CA-CB-CG | 5.16 | 127.16 | 115.30 |
| 1 | D | 52 | G | N9-C1'-C2' | -5.14 | 106.34 | 112.00 |
| 1 | D | 41 | A | N9-C1'-C2' | -5.08 | 106.41 | 112.00 |
| 2 | B | 570 | LEU | CA-CB-CG | 5.04 | 126.88 | 115.30 |
| 1 | C | 13 | C | OP1-P-OP2 | -5.02 | 112.08 | 119.60 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | C | 21 | A | Sidechain |
| 1 | C | 25 | U | Sidechain |
| 1 | C | 40 | C | Sidechain |
| 1 | C | 9 | A | Sidechain |
| 1 | D | 11 | U | Sidechain |
| 1 | D | 42 | G | Sidechain |
| 1 | D | 7 | G | Sidechain |
| 1 | D | 9 | A | 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 | C | 1570 | 0 | 807 | 111 | 0 |
| 1 | D | 1570 | 0 | 805 | 132 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | A | 4668 | 0 | 4679 | 469 | 0 |
| 2 | B | 4668 | 0 | 4679 | 548 | 0 |
| 3 | A | 43 | 0 | 0 | 3 | 0 |
| 3 | B | 31 | 0 | 0 | 7 | 0 |
| 3 | C | 12 | 0 | 0 | 1 | 0 |
| 3 | D | 10 | 0 | 0 | 0 | 0 |
| All | All | 12572 | 0 | 10970 | 1183 | 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 51.

All (1183) 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:D:2:G:H1 | 1:D:71:C:N4 | 1.40 | 1.20 |
| 2:B:27:ARG:HH21 | 2:B:29:ARG:NH1 | 1.42 | 1.17 |
| 1:D:37:2MA:H5'' | 2:B:27:ARG:HH12 | 1.01 | 1.11 |
| 1:D:68:G:H2' | 1:D:69:U:C6 | 1.88 | 1.08 |
| 1:D:34:QUO:H4' | 1:D:35:U:H5' | 1.35 | 1.08 |
| 2:B:408:ALA:HA | 2:B:413:LEU:HD13 | 1.35 | 1.07 |
| 2:B:10:LEU:H | 2:B:10:LEU:HD12 | 1.18 | 1.07 |
| 2:B:28:ARG:HH11 | 2:B:28:ARG:HG2 | 1.14 | 1.07 |
| 2:A:168:THR:HB | 2:A:217:GLN:HE22 | 1.16 | 1.07 |
| 1:D:48:C:H4' | 1:D:49:G:OP2 | 1.54 | 1.06 |
| 1:D:1:G:H2' | 1:D:2:G:O4' | 1.55 | 1.04 |
| 2:A:479:GLY:O | 2:A:525:ILE:HG13 | 1.60 | 1.02 |
| 2:B:331:ARG:HA | 2:B:331:ARG:HE | 1.21 | 1.01 |
| 2:B:546:ILE:O | 2:B:549:PRO:HD3 | 1.57 | 1.01 |
| 2:B:227:LEU:HD22 | 2:B:227:LEU:H | 1.23 | 1.00 |
| 2:B:323:LEU:HB2 | 2:B:400:LEU:HD11 | 1.42 | 1.00 |
| 1:C:17:C:H4' | 1:C:18:G:OP2 | 1.60 | 1.00 |
| 2:B:329:LEU:HD12 | 2:B:385:THR:HG21 | 1.43 | 1.00 |
| 1:C:61:C:O2' | 1:C:62:C:H5' | 1.61 | 1.00 |
| 2:B:127:ARG:NH2 | 2:B:137:ARG:HH22 | 1.58 | 1.00 |
| 2:B:349:LEU:HD12 | 2:B:350:ALA:H | 1.24 | 1.00 |
| 2:A:226:ASP:HB2 | 2:A:228:ARG:HG2 | 1.44 | 0.99 |
| 2:B:27:ARG:NH2 | 2:B:29:ARG:HH11 | 1.61 | 0.99 |
| 2:A:299:LEU:HD22 | 2:A:400:LEU:HD13 | 1.40 | 0.98 |
| 1:D:68:G:H2' | 1:D:69:U:H6 | 1.23 | 0.98 |
| 2:A:421:LEU:CD2 | 2:A:471:VAL:HG22 | 1.94 | 0.97 |
| 2:B:263:ARG:HD3 | 2:B:269:GLU:OE1 | 1.64 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:227:LEU:HA | 2:A:231:ARG:HB2 | 1.48 | 0.95 |
| 1:D:3:A:H2' | 1:D:4:G:C8 | 2.01 | 0.95 |
| 2:B:475:VAL:HG21 | 2:B:535:LEU:HD11 | 1.50 | 0.94 |
| 2:B:27:ARG:HH11 | 2:B:115:ARG:NE | 1.65 | 0.93 |
| 2:B:27:ARG:CD | 2:B:115:ARG:HE | 1.81 | 0.93 |
| 2:A:254:ASN:HD21 | 2:A:525:ILE:HG21 | 1.33 | 0.93 |
| 1:D:37:2MA:H5'' | 2:B:27:ARG:NH1 | 1.82 | 0.93 |
| 2:B:147:ARG:HG3 | 2:B:533:LEU:CD1 | 1.98 | 0.93 |
| 2:A:231:ARG:HG3 | 2:A:231:ARG:HH11 | 1.34 | 0.93 |
| 2:A:331:ARG:HE | 2:A:331:ARG:H | 1.09 | 0.92 |
| 2:B:172:THR:HG22 | 2:B:195:ALA:O | 1.69 | 0.92 |
| 2:A:421:LEU:HD21 | 2:A:471:VAL:HG22 | 1.50 | 0.91 |
| 2:B:202:LEU:HD21 | 2:B:445:PHE:HE1 | 1.33 | 0.91 |
| 2:A:147:ARG:HD2 | 2:A:533:LEU:CD1 | 2.02 | 0.90 |
| 2:B:166:VAL:HG11 | 2:B:207:LEU:HD21 | 1.53 | 0.89 |
| 2:B:146:LEU:HD12 | 2:B:149:ARG:NH1 | 1.87 | 0.88 |
| 1:C:34:QUO:H4' | 1:C:35:U:H5' | 1.55 | 0.88 |
| 2:A:42:ARG:HD3 | 2:A:145:ARG:NH2 | 1.89 | 0.88 |
| 2:A:78:ARG:HG3 | 2:A:91:GLU:HG2 | 1.54 | 0.87 |
| 2:B:349:LEU:HD11 | 2:B:387:LEU:HB3 | 1.56 | 0.87 |
| 2:B:120:LYS:HD2 | 2:B:120:LYS:H | 1.40 | 0.86 |
| 1:C:22:G:O2' | 1:C:23:A:H5' | 1.75 | 0.86 |
| 1:D:37:2MA:C5' | 2:B:27:ARG:HH12 | 1.86 | 0.86 |
| 2:B:281:GLU:HG3 | 2:B:285:ARG:HD3 | 1.57 | 0.86 |
| 1:D:1:G:C2' | 1:D:2:G:H5' | 2.05 | 0.86 |
| 2:B:290:LYS:O | 2:B:474:GLY:HA2 | 1.75 | 0.85 |
| 2:B:28:ARG:NH1 | 2:B:28:ARG:HG2 | 1.90 | 0.85 |
| 2:A:431:TRP:HH2 | 2:A:436:GLU:HB3 | 1.39 | 0.84 |
| 2:B:27:ARG:NH2 | 2:B:29:ARG:NH1 | 2.23 | 0.83 |
| 1:D:3:A:H2' | 1:D:4:G:H8 | 1.44 | 0.83 |
| 1:D:8:4SU:H5'' | 1:D:49:G:OP2 | 1.77 | 0.83 |
| 2:A:192:LEU:HD22 | 2:B:562:PRO:HG2 | 1.59 | 0.83 |
| 2:A:170:PHE:O | 2:A:197:PRO:HD3 | 1.78 | 0.83 |
| 2:B:201:GLN:O | 2:B:204:LYS:HG2 | 1.78 | 0.83 |
| 2:B:28:ARG:HH11 | 2:B:28:ARG:CG | 1.90 | 0.82 |
| 2:A:220:ARG:HG2 | 2:B:170:PHE:CD1 | 2.15 | 0.82 |
| 2:A:546:ILE:O | 2:A:549:PRO:HD3 | 1.80 | 0.82 |
| 2:B:127:ARG:NH2 | 2:B:137:ARG:NH2 | 2.27 | 0.82 |
| 2:B:226:ASP:OD1 | 2:B:228:ARG:HG2 | 1.80 | 0.81 |
| 2:A:213:ASP:CG | 2:B:3:ARG:HH22 | 1.83 | 0.81 |
| 2:A:277:LEU:HD12 | 2:A:421:LEU:HD12 | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:2:G:H2' | 1:C:3:A:C8 | 2.16 | 0.81 |
| 2:A:203:PHE:O | 2:A:207:LEU:HD22 | 1.81 | 0.80 |
| 2:B:307:ARG:HD3 | 2:B:315:GLN:HA | 1.62 | 0.80 |
| 2:B:456:LEU:HD23 | 2:B:492:ARG:HD2 | 1.64 | 0.80 |
| 2:B:147:ARG:HG3 | 2:B:533:LEU:HD13 | 1.61 | 0.80 |
| 2:B:537:THR:HG23 | 2:B:539:SER:OG | 1.81 | 0.80 |
| 2:A:168:THR:HG23 | 2:A:169:PRO:HD2 | 1.64 | 0.80 |
| 2:B:146:LEU:HD12 | 2:B:149:ARG:HH12 | 1.46 | 0.80 |
| 2:B:323:LEU:HB2 | 2:B:400:LEU:CD1 | 2.12 | 0.79 |
| 2:B:411:LEU:HB2 | 2:B:413:LEU:CD1 | 2.13 | 0.79 |
| 2:A:201:GLN:O | 2:A:204:LYS:HG2 | 1.83 | 0.79 |
| 2:A:537:THR:CG2 | 2:A:539:SER:H | 1.95 | 0.79 |
| 2:B:127:ARG:HH21 | 2:B:137:ARG:NH2 | 1.81 | 0.79 |
| 2:B:202:LEU:HD21 | 2:B:445:PHE:CE1 | 2.18 | 0.79 |
| 1:D:2:G:H1 | 1:D:71:C:H42 | 0.81 | 0.79 |
| 2:A:10:LEU:HD23 | 2:A:46:VAL:HG11 | 1.65 | 0.78 |
| 2:A:537:THR:HG22 | 2:A:539:SER:H | 1.48 | 0.78 |
| 2:B:204:LYS:HE2 | 2:B:241:GLU:OE1 | 1.84 | 0.78 |
| 2:A:345:LYS:O | 2:A:395:VAL:HG13 | 1.83 | 0.78 |
| 2:A:290:LYS:O | 2:A:474:GLY:HA2 | 1.83 | 0.78 |
| 2:B:411:LEU:HB2 | 2:B:413:LEU:HD12 | 1.65 | 0.78 |
| 2:A:568:GLU:OE1 | 2:A:571:ARG:HD2 | 1.82 | 0.78 |
| 2:B:277:LEU:HD11 | 2:B:281:GLU:HG2 | 1.65 | 0.78 |
| 2:B:326:PRO:HA | 2:B:384:ASP:OD1 | 1.83 | 0.78 |
| 2:B:112:ALA:HB3 | 2:B:119:GLU:HG2 | 1.66 | 0.77 |
| 2:B:393:ARG:HG2 | 3:B:2039:HOH:O | 1.83 | 0.77 |
| 2:B:449:HIS:CD2 | 2:B:464:ARG:NH1 | 2.51 | 0.77 |
| 2:B:452:ASP:HA | 2:B:455:LEU:HD23 | 1.66 | 0.77 |
| 2:A:568:GLU:OE1 | 2:A:571:ARG:CD | 2.31 | 0.77 |
| 2:A:254:ASN:ND2 | 2:A:525:ILE:HG21 | 2.00 | 0.77 |
| 2:A:292:ASP:OD1 | 2:A:294:ARG:HD3 | 1.84 | 0.77 |
| 2:B:499:ILE:H | 2:B:499:ILE:HD12 | 1.50 | 0.77 |
| 2:A:228:ARG:NH1 | 2:A:228:ARG:HA | 1.99 | 0.77 |
| 1:C:1:G:O2' | 1:C:2:G:H5' | 1.85 | 0.77 |
| 2:A:447:SER:HA | 2:A:484:ILE:CD1 | 2.16 | 0.76 |
| 1:C:71:C:H2' | 1:C:72:C:C6 | 2.20 | 0.76 |
| 1:D:6:G:O2' | 1:D:7:G:H5' | 1.84 | 0.76 |
| 2:B:343:ARG:HA | 2:B:343:ARG:NH1 | 1.99 | 0.76 |
| 2:B:10:LEU:H | 2:B:10:LEU:CD1 | 1.98 | 0.76 |
| 2:A:297:LEU:O | 2:A:404:ARG:HD2 | 1.85 | 0.76 |
| 2:B:276:ARG:HG3 | 2:B:422:TRP:HB2 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:431:TRP:CH2 | 2:A:436:GLU:HB3 | 2.21 | 0.75 |
| 2:A:443:HIS:CG | 2:A:444:PRO:HD2 | 2.21 | 0.75 |
| 2:A:559:THR:HG23 | 2:B:173:LYS:HB2 | 1.69 | 0.75 |
| 1:D:2:G:N1 | 1:D:71:C:N4 | 2.25 | 0.75 |
| 2:A:228:ARG:CZ | 2:A:228:ARG:HA | 2.16 | 0.75 |
| 1:C:15:G:H5'' | 1:C:16:H2U:H5' | 1.68 | 0.75 |
| 1:D:69:U:H2' | 1:D:70:U:C6 | 2.22 | 0.75 |
| 2:A:109:PRO:CG | 2:A:120:LYS:HE2 | 2.17 | 0.75 |
| 2:A:59:THR:O | 2:A:63:VAL:HG23 | 1.86 | 0.75 |
| 1:D:36:C:N4 | 2:B:80:GLU:HB3 | 2.00 | 0.75 |
| 2:A:240:LEU:HD22 | 2:A:525:ILE:HG22 | 1.69 | 0.75 |
| 2:A:429:LEU:HD13 | 2:A:438:TRP:HB3 | 1.68 | 0.74 |
| 1:D:34:QUO:H4' | 1:D:35:U:C5' | 2.16 | 0.74 |
| 2:A:25:VAL:HG21 | 2:A:63:VAL:HG11 | 1.69 | 0.74 |
| 2:A:321:LYS:HD2 | 2:A:397:ALA:HB2 | 1.69 | 0.74 |
| 2:A:241:GLU:HA | 2:A:241:GLU:OE1 | 1.86 | 0.74 |
| 2:B:220:ARG:HD3 | 2:B:235:PHE:O | 1.87 | 0.74 |
| 2:B:27:ARG:HD3 | 2:B:115:ARG:HE | 1.49 | 0.74 |
| 2:B:343:ARG:HA | 2:B:343:ARG:CZ | 2.18 | 0.74 |
| 2:B:349:LEU:HD12 | 2:B:350:ALA:N | 2.01 | 0.74 |
| 2:B:318:GLU:OE2 | 2:B:393:ARG:HB2 | 1.88 | 0.74 |
| 1:C:42:G:O2' | 1:C:43:G:H5' | 1.88 | 0.74 |
| 2:A:147:ARG:HD2 | 2:A:533:LEU:HD13 | 1.67 | 0.73 |
| 2:A:7:ALA:N | 2:A:41:ASP:OD2 | 2.21 | 0.73 |
| 2:A:326:PRO:HD2 | 2:A:411:LEU:HD21 | 1.71 | 0.73 |
| 2:B:10:LEU:N | 2:B:10:LEU:HD12 | 1.97 | 0.73 |
| 2:B:299:LEU:HD23 | 2:B:299:LEU:N | 2.03 | 0.73 |
| 2:B:475:VAL:CG2 | 2:B:535:LEU:HD11 | 2.18 | 0.72 |
| 2:A:421:LEU:HD23 | 2:A:471:VAL:HG22 | 1.70 | 0.72 |
| 1:D:62:C:H2' | 1:D:63:C:C6 | 2.25 | 0.72 |
| 2:A:220:ARG:HG2 | 2:B:170:PHE:CE1 | 2.25 | 0.72 |
| 2:A:4:THR:HG1 | 2:A:5:HIS:HD1 | 1.38 | 0.72 |
| 2:A:226:ASP:CB | 2:A:228:ARG:HG2 | 2.19 | 0.72 |
| 1:C:3:A:H2' | 1:C:4:G:C8 | 2.25 | 0.72 |
| 2:B:49:VAL:HG21 | 2:B:91:GLU:OE2 | 1.89 | 0.71 |
| 2:A:238:LEU:HB3 | 2:A:527:TRP:HB2 | 1.72 | 0.71 |
| 2:B:307:ARG:HD2 | 2:B:315:GLN:O | 1.90 | 0.71 |
| 2:B:120:LYS:HD2 | 2:B:120:LYS:N | 2.06 | 0.71 |
| 2:B:27:ARG:HD2 | 2:B:115:ARG:HE | 1.55 | 0.71 |
| 2:B:78:ARG:HD3 | 2:B:88:GLY:O | 1.91 | 0.71 |
| 1:C:36:C:O2 | 2:A:78:ARG:NH2 | 2.23 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:4:THR:HG23 | 2:B:20:VAL:HB | 1.71 | 0.71 |
| 1:C:66:C:H2' | 1:C:67:C:H6 | 1.55 | 0.71 |
| 1:C:72:C:O3' | 2:A:343:ARG:HD2 | 1.90 | 0.71 |
| 2:B:266:LEU:HB3 | 2:B:268:VAL:HG23 | 1.72 | 0.71 |
| 2:B:1:MET:N | 2:B:70:ARG:HD3 | 2.04 | 0.70 |
| 1:C:11:U:O2' | 1:C:12:U:H5' | 1.90 | 0.70 |
| 2:A:165:GLN:C | 2:A:165:GLN:HE21 | 1.94 | 0.70 |
| 2:A:227:LEU:HD22 | 2:A:227:LEU:H | 1.56 | 0.70 |
| 1:D:3:A:C2 | 1:D:71:C:N4 | 2.60 | 0.70 |
| 1:D:70:U:H6 | 1:D:70:U:O5' | 1.73 | 0.70 |
| 2:A:440:TYR:HB3 | 2:A:497:LEU:HD11 | 1.73 | 0.70 |
| 1:D:38:C:OP2 | 2:B:27:ARG:NH2 | 2.25 | 0.70 |
| 2:B:27:ARG:HH21 | 2:B:29:ARG:HH11 | 0.75 | 0.70 |
| 2:B:147:ARG:HG3 | 2:B:533:LEU:HD11 | 1.71 | 0.70 |
| 2:B:561:ALA:HA | 2:B:562:PRO:C | 2.11 | 0.70 |
| 2:A:129:LYS:O | 2:A:129:LYS:HG3 | 1.90 | 0.70 |
| 2:A:550:LYS:HD2 | 2:A:554:GLY:O | 1.91 | 0.70 |
| 2:A:76:ARG:HH11 | 2:A:76:ARG:HG2 | 1.57 | 0.69 |
| 2:B:266:LEU:CB | 2:B:268:VAL:HG23 | 2.22 | 0.69 |
| 2:A:139:ARG:HH22 | 2:A:537:THR:HG23 | 1.55 | 0.69 |
| 2:B:394:LYS:O | 2:B:398:THR:HG23 | 1.92 | 0.69 |
| 1:D:1:G:H2' | 1:D:2:G:C4' | 2.22 | 0.69 |
| 2:A:226:ASP:C | 2:A:228:ARG:H | 1.96 | 0.69 |
| 2:A:575:LEU:HD23 | 2:B:577:VAL:HA | 1.73 | 0.69 |
| 2:A:500:GLY:O | 2:A:504:GLN:HB2 | 1.91 | 0.69 |
| 2:B:198:GLN:O | 2:B:221:CYS:HB3 | 1.92 | 0.69 |
| 2:B:251:LEU:O | 2:B:255:GLU:HG3 | 1.93 | 0.69 |
| 2:B:111:ASP:OD1 | 2:B:115:ARG:NH2 | 2.26 | 0.69 |
| 2:A:173:LYS:HB2 | 2:B:559:THR:HG23 | 1.74 | 0.69 |
| 1:D:48:C:C4' | 1:D:49:G:OP2 | 2.36 | 0.69 |
| 1:D:65:PSU:H2' | 1:D:66:C:C6 | 2.28 | 0.69 |
| 2:B:386:LEU:HB3 | 2:B:388:PHE:CE1 | 2.27 | 0.69 |
| 2:A:371:ARG:HG3 | 2:A:375:LEU:CD2 | 2.23 | 0.69 |
| 2:B:299:LEU:O | 2:B:300:LYS:HG2 | 1.93 | 0.69 |
| 1:C:2:G:H1 | 1:C:71:C:H42 | 1.40 | 0.69 |
| 2:B:389:VAL:HG23 | 2:B:400:LEU:HD23 | 1.74 | 0.68 |
| 2:A:351:TRP:HA | 2:A:386:LEU:O | 1.92 | 0.68 |
| 2:A:421:LEU:HD21 | 2:A:471:VAL:CG2 | 2.23 | 0.68 |
| 2:B:533:LEU:O | 2:B:537:THR:HG22 | 1.94 | 0.68 |
| 2:B:561:ALA:HA | 2:B:562:PRO:O | 1.93 | 0.68 |
| 2:A:231:ARG:HG3 | 2:A:231:ARG:NH1 | 2.00 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:8:4SU:H1' | 1:D:48:C:H1' | 1.75 | 0.68 |
| 2:A:263:ARG:HD3 | 2:A:269:GLU:OE1 | 1.94 | 0.68 |
| 2:A:483:ARG:HE | 2:A:523:GLY:HA2 | 1.58 | 0.68 |
| 2:B:27:ARG:HH11 | 2:B:115:ARG:HE | 1.42 | 0.68 |
| 2:B:558:LEU:O | 2:B:558:LEU:HD12 | 1.94 | 0.68 |
| 2:A:488:ARG:O | 2:A:491:ALA:HB3 | 1.93 | 0.68 |
| 2:B:368:GLU:N | 2:B:369:PRO:HD2 | 2.09 | 0.68 |
| 1:D:65:PSU:H2' | 1:D:66:C:H6 | 1.59 | 0.68 |
| 2:A:184:VAL:HB | 2:A:194:TYR:HB2 | 1.75 | 0.68 |
| 2:A:345:LYS:O | 2:A:395:VAL:CG1 | 2.42 | 0.67 |
| 2:B:255:GLU:HG2 | 2:B:422:TRP:HE1 | 1.59 | 0.67 |
| 2:A:445:PHE:HD2 | 2:A:490:GLN:OE1 | 1.77 | 0.67 |
| 1:C:21:A:H2' | 1:C:46:G7M:O6 | 1.94 | 0.67 |
| 1:C:22:G:O2' | 1:C:23:A:C5' | 2.42 | 0.67 |
| 2:A:440:TYR:CE1 | 2:A:444:PRO:HD3 | 2.28 | 0.67 |
| 2:B:7:ALA:N | 2:B:41:ASP:OD2 | 2.28 | 0.67 |
| 1:D:36:C:O2 | 2:B:78:ARG:NH2 | 2.27 | 0.67 |
| 2:A:447:SER:HA | 2:A:484:ILE:HD13 | 1.75 | 0.67 |
| 2:A:578:VAL:HG11 | 2:B:576:MET:SD | 2.34 | 0.67 |
| 2:B:277:LEU:HB2 | 2:B:421:LEU:HD11 | 1.77 | 0.67 |
| 1:D:17:C:H4' | 1:D:18:G:OP2 | 1.93 | 0.67 |
| 2:B:48:LEU:HB3 | 2:B:94:LEU:HD21 | 1.74 | 0.67 |
| 2:A:451:GLU:O | 2:A:454:PRO:HD2 | 1.95 | 0.67 |
| 1:D:1:G:C2' | 1:D:2:G:C5' | 2.72 | 0.67 |
| 2:A:109:PRO:HG3 | 2:A:120:LYS:HE2 | 1.76 | 0.66 |
| 2:B:296:GLY:O | 2:B:404:ARG:NH1 | 2.29 | 0.66 |
| 2:B:429:LEU:HB3 | 2:B:438:TRP:HB3 | 1.78 | 0.66 |
| 1:D:63:C:O2' | 1:D:64:G:H5' | 1.95 | 0.66 |
| 2:B:168:THR:HG23 | 2:B:169:PRO:HD2 | 1.76 | 0.66 |
| 1:C:66:C:H2' | 1:C:67:C:C6 | 2.29 | 0.66 |
| 2:B:329:LEU:HA | 2:B:333:GLU:OE1 | 1.94 | 0.66 |
| 1:D:70:U:H2' | 1:D:71:C:C6 | 2.30 | 0.66 |
| 2:A:302:VAL:HG12 | 2:A:305:LEU:HD12 | 1.76 | 0.66 |
| 2:B:354:VAL:HG21 | 2:B:381:ARG:O | 1.96 | 0.66 |
| 1:C:48:C:H4' | 1:C:49:G:OP2 | 1.96 | 0.66 |
| 1:D:12:U:H2' | 1:D:13:C:O4' | 1.95 | 0.66 |
| 2:A:443:HIS:CD2 | 2:A:444:PRO:HD2 | 2.31 | 0.66 |
| 1:D:30:G:H2' | 1:D:31:C:H6 | 1.60 | 0.66 |
| 2:B:127:ARG:CZ | 2:B:137:ARG:HH22 | 2.09 | 0.66 |
| 2:B:268:VAL:HG12 | 2:B:269:GLU:H | 1.61 | 0.66 |
| 2:B:327:LYS:CG | 2:B:328:ALA:H | 2.09 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:1:G:H2' | 1:D:2:G:C5' | 2.25 | 0.66 |
| 1:D:9:A:H5'' | 1:D:46:G7M:H22 | 1.60 | 0.65 |
| 2:B:497:LEU:HB3 | 2:B:499:ILE:CD1 | 2.26 | 0.65 |
| 2:A:115:ARG:HH11 | 2:A:117:GLU:CD | 1.99 | 0.65 |
| 1:D:30:G:H2' | 1:D:31:C:C6 | 2.31 | 0.65 |
| 2:B:221:CYS:SG | 2:B:237:GLN:HG3 | 2.37 | 0.65 |
| 2:B:487:PRO:HG3 | 2:B:515:LEU:HB3 | 1.78 | 0.65 |
| 2:A:227:LEU:CA | 2:A:231:ARG:HB2 | 2.26 | 0.65 |
| 1:D:11:U:H2' | 1:D:12:U:C6 | 2.31 | 0.65 |
| 1:D:34:QUO:H14 | 2:B:51:HIS:CE1 | 2.32 | 0.65 |
| 1:D:63:C:H2' | 1:D:64:G:C8 | 2.32 | 0.65 |
| 2:A:115:ARG:HD2 | 2:A:117:GLU:OE2 | 1.97 | 0.65 |
| 2:B:214:ARG:NH1 | 3:B:2066:HOH:O | 2.30 | 0.64 |
| 2:B:276:ARG:HG3 | 2:B:422:TRP:CB | 2.27 | 0.64 |
| 1:C:71:C:H2' | 1:C:72:C:H6 | 1.60 | 0.64 |
| 2:A:76:ARG:NH1 | 2:A:76:ARG:HG2 | 2.11 | 0.64 |
| 2:B:313:VAL:HG12 | 2:B:314:PHE:N | 2.12 | 0.64 |
| 2:B:206:MET:HE1 | 2:B:510:PHE:HD1 | 1.62 | 0.64 |
| 1:C:61:C:HO2' | 1:C:62:C:H5' | 1.62 | 0.64 |
| 2:A:42:ARG:HD3 | 2:A:145:ARG:HH22 | 1.59 | 0.64 |
| 2:B:27:ARG:NH1 | 2:B:115:ARG:NE | 2.43 | 0.64 |
| 1:D:8:4SU:C5' | 1:D:49:G:OP2 | 2.45 | 0.64 |
| 2:B:227:LEU:HA | 2:B:231:ARG:HB2 | 1.78 | 0.64 |
| 1:C:21:A:O2' | 1:C:22:G:C8 | 2.48 | 0.64 |
| 2:B:281:GLU:CG | 2:B:285:ARG:HD3 | 2.28 | 0.64 |
| 2:B:321:LYS:O | 2:B:388:PHE:HA | 1.98 | 0.64 |
| 2:B:325:LEU:O | 2:B:384:ASP:HB3 | 1.96 | 0.64 |
| 1:C:1:G:H2' | 1:C:2:G:H8 | 1.62 | 0.64 |
| 2:A:39:LEU:HB3 | 2:A:46:VAL:HG23 | 1.80 | 0.64 |
| 2:B:6:TYR:HB2 | 2:B:9:SER:OG | 1.98 | 0.64 |
| 1:C:28:C:H2' | 1:C:29:U:C6 | 2.33 | 0.64 |
| 2:A:36:PHE:CD2 | 2:A:49:VAL:HG23 | 2.32 | 0.63 |
| 2:B:68:VAL:HB | 2:B:101:ALA:HB3 | 1.81 | 0.63 |
| 1:C:28:C:H2' | 1:C:29:U:H6 | 1.62 | 0.63 |
| 1:D:2:G:C2 | 1:D:3:A:C4 | 2.85 | 0.63 |
| 2:B:226:ASP:C | 2:B:228:ARG:H | 2.01 | 0.63 |
| 2:B:77:LEU:HD23 | 2:B:89:ARG:O | 1.98 | 0.63 |
| 1:C:2:G:N1 | 1:C:72:C:N4 | 2.46 | 0.63 |
| 2:A:455:LEU:HB2 | 2:A:463:VAL:HG22 | 1.78 | 0.63 |
| 2:B:109:PRO:HG2 | 2:B:120:LYS:HD3 | 1.78 | 0.63 |
| 2:A:359:PHE:HB2 | 2:A:364:ALA:HB1 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:421:LEU:HD23 | 2:B:471:VAL:HG21 | 1.80 | 0.63 |
| 2:B:293:LEU:HD11 | 2:B:421:LEU:HD13 | 1.80 | 0.63 |
| 2:B:312:ARG:HH11 | 2:B:312:ARG:HA | 1.63 | 0.63 |
| 1:C:24:A:H2' | 1:C:25:U:O4' | 1.99 | 0.63 |
| 2:A:576:MET:HB2 | 2:B:578:VAL:HG21 | 1.81 | 0.62 |
| 2:A:240:LEU:HD22 | 2:A:525:ILE:CG2 | 2.29 | 0.62 |
| 1:D:38:C:OP2 | 2:B:27:ARG:CZ | 2.47 | 0.62 |
| 2:B:41:ASP:O | 2:B:43:GLU:N | 2.32 | 0.62 |
| 2:A:168:THR:HG23 | 2:A:169:PRO:CD | 2.29 | 0.62 |
| 2:A:172:THR:HG22 | 2:A:173:LYS:H | 1.64 | 0.62 |
| 2:A:534:ALA:O | 2:A:537:THR:HG22 | 2.00 | 0.62 |
| 2:A:277:LEU:HD12 | 2:A:421:LEU:CD1 | 2.30 | 0.62 |
| 2:B:166:VAL:CG1 | 2:B:207:LEU:HD21 | 2.28 | 0.62 |
| 1:C:4:G:N2 | 1:C:70:U:O2 | 2.33 | 0.62 |
| 1:D:2:G:C6 | 1:D:3:A:C6 | 2.88 | 0.62 |
| 2:A:251:LEU:HD12 | 2:A:276:ARG:NH2 | 2.14 | 0.62 |
| 2:A:266:LEU:HD11 | 2:A:536:MET:HB3 | 1.82 | 0.62 |
| 2:A:579:ARG:CB | 2:A:580:PRO:HD3 | 2.29 | 0.62 |
| 2:B:329:LEU:HD22 | 2:B:333:GLU:HB3 | 1.82 | 0.62 |
| 2:A:302:VAL:HG12 | 2:A:305:LEU:CD1 | 2.30 | 0.62 |
| 2:B:323:LEU:CB | 2:B:400:LEU:HD11 | 2.25 | 0.62 |
| 2:A:109:PRO:HG2 | 2:A:120:LYS:HE2 | 1.80 | 0.62 |
| 2:A:326:PRO:HD2 | 2:A:411:LEU:CD2 | 2.30 | 0.62 |
| 2:A:490:GLN:HG3 | 2:A:494:PHE:CE1 | 2.35 | 0.61 |
| 1:C:12:U:H5 | 3:C:2011:HOH:O | 1.83 | 0.61 |
| 2:A:244:PHE:CE2 | 2:A:521:PRO:HD2 | 2.34 | 0.61 |
| 2:A:168:THR:HB | 2:A:217:GLN:NE2 | 2.01 | 0.61 |
| 2:B:327:LYS:CG | 2:B:328:ALA:N | 2.63 | 0.61 |
| 2:B:332:LYS:O | 2:B:335:ALA:HB3 | 2.01 | 0.61 |
| 2:B:354:VAL:CG2 | 2:B:384:ASP:H | 2.13 | 0.61 |
| 2:B:354:VAL:HG23 | 2:B:383:GLY:H | 1.63 | 0.61 |
| 2:A:533:LEU:O | 2:A:537:THR:HB | 2.00 | 0.61 |
| 1:C:30:G:O2' | 1:C:31:C:H5' | 2.00 | 0.61 |
| 2:A:155:TRP:CH2 | 2:A:165:GLN:HG3 | 2.35 | 0.61 |
| 1:D:28:C:O2' | 1:D:29:U:H5' | 2.01 | 0.61 |
| 1:D:70:U:H3' | 1:D:70:U:C6 | 2.35 | 0.61 |
| 2:B:336:GLU:O | 2:B:339:GLU:N | 2.32 | 0.61 |
| 2:B:556:ASP:CG | 2:B:559:THR:HB | 2.20 | 0.61 |
| 2:B:155:TRP:CZ2 | 2:B:165:GLN:HG3 | 2.35 | 0.61 |
| 2:B:74:LEU:HD23 | 2:B:76:ARG:HH21 | 1.64 | 0.61 |
| 2:A:483:ARG:NE | 2:A:523:GLY:HA2 | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:442:HIS:HB2 | 2:B:446:THR:OG1 | 2.00 | 0.61 |
| 2:B:320:VAL:HG22 | 2:B:390:ALA:HB1 | 1.81 | 0.61 |
| 2:B:226:ASP:OD1 | 2:B:228:ARG:CG | 2.48 | 0.60 |
| 2:B:290:LYS:N | 2:B:291:PRO:HD3 | 2.16 | 0.60 |
| 2:A:25:VAL:HG21 | 2:A:63:VAL:CG1 | 2.31 | 0.60 |
| 2:B:139:ARG:NH2 | 2:B:544:GLU:HB3 | 2.15 | 0.60 |
| 2:B:440:TYR:HD1 | 2:B:442:HIS:O | 1.83 | 0.60 |
| 2:B:525:ILE:HG12 | 2:B:526:ALA:H | 1.65 | 0.60 |
| 2:A:7:ALA:HA | 2:A:21:LEU:HD13 | 1.83 | 0.60 |
| 2:B:313:VAL:HG12 | 2:B:314:PHE:HD1 | 1.65 | 0.60 |
| 2:B:566:PRO:O | 2:B:569:GLN:N | 2.32 | 0.60 |
| 2:A:17:GLU:O | 2:A:75:VAL:HG23 | 2.00 | 0.60 |
| 2:B:372:GLU:O | 2:B:376:GLN:HB2 | 2.02 | 0.60 |
| 2:A:213:ASP:OD1 | 2:B:3:ARG:NH1 | 2.31 | 0.60 |
| 2:A:215:TYR:CE1 | 2:A:217:GLN:HB3 | 2.37 | 0.60 |
| 2:A:81:PRO:O | 2:A:83:PRO:HD3 | 2.01 | 0.60 |
| 2:B:311:PHE:HB2 | 2:B:366:PHE:CD2 | 2.35 | 0.60 |
| 2:B:369:PRO:O | 2:B:370:VAL:HG13 | 2.02 | 0.60 |
| 2:B:108:PHE:HD2 | 2:B:126:LEU:HD13 | 1.67 | 0.60 |
| 1:C:7:G:C2 | 1:C:49:G:C8 | 2.90 | 0.60 |
| 1:D:1:G:O2' | 1:D:2:G:H5' | 2.02 | 0.60 |
| 1:D:5:C:O2' | 1:D:6:G:H5' | 2.01 | 0.60 |
| 2:B:262:PHE:CZ | 2:B:536:MET:HG2 | 2.36 | 0.60 |
| 2:B:205:GLN:HE22 | 2:B:445:PHE:HD1 | 1.48 | 0.60 |
| 2:B:202:LEU:CD2 | 2:B:445:PHE:HE1 | 2.09 | 0.60 |
| 2:A:499:ILE:HG23 | 2:A:503:GLU:HG3 | 1.84 | 0.59 |
| 2:A:501:GLU:O | 2:A:505:ARG:HD3 | 2.01 | 0.59 |
| 2:A:132:TYR:CD2 | 2:B:206:MET:HE2 | 2.37 | 0.59 |
| 2:A:452:ASP:OD1 | 2:A:464:ARG:NE | 2.35 | 0.59 |
| 2:B:1:MET:H1 | 2:B:70:ARG:HD3 | 1.65 | 0.59 |
| 2:B:336:GLU:O | 2:B:337:LEU:C | 2.39 | 0.59 |
| 2:B:51:HIS:O | 2:B:57:TYR:HB2 | 2.03 | 0.59 |
| 2:B:315:GLN:HE21 | 2:B:316:GLU:HG2 | 1.68 | 0.59 |
| 2:B:57:TYR:HA | 2:B:60:ALA:HB3 | 1.82 | 0.59 |
| 1:C:4:G:H2' | 1:C:5:C:O4' | 2.02 | 0.59 |
| 1:D:2:G:H2' | 1:D:3:A:H8 | 1.67 | 0.59 |
| 2:B:299:LEU:HD23 | 2:B:299:LEU:H | 1.67 | 0.59 |
| 2:A:154:ILE:HG21 | 2:A:238:LEU:HD13 | 1.83 | 0.59 |
| 2:A:568:GLU:OE1 | 2:A:571:ARG:NH1 | 2.33 | 0.59 |
| 2:A:497:LEU:O | 2:A:499:ILE:HG13 | 2.03 | 0.59 |
| 2:B:331:ARG:HA | 2:B:331:ARG:NE | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:491:ALA:O | 2:B:495:ARG:HG3 | 2.02 | 0.59 |
| 2:B:78:ARG:HG2 | 2:B:91:GLU:OE1 | 2.03 | 0.59 |
| 1:D:49:G:O2' | 1:D:50:C:H5' | 2.03 | 0.59 |
| 2:A:254:ASN:HD21 | 2:A:525:ILE:CG2 | 2.13 | 0.59 |
| 2:B:354:VAL:HG23 | 2:B:384:ASP:H | 1.68 | 0.59 |
| 2:B:39:LEU:HG | 2:B:48:LEU:HD11 | 1.85 | 0.59 |
| 2:A:146:LEU:HD12 | 2:A:149:ARG:NH1 | 2.18 | 0.58 |
| 2:B:483:ARG:HG2 | 2:B:523:GLY:HA2 | 1.83 | 0.58 |
| 1:C:2:G:H2' | 1:C:3:A:H8 | 1.64 | 0.58 |
| 1:D:1:G:C3' | 1:D:2:G:H5' | 2.25 | 0.58 |
| 2:A:331:ARG:NE | 2:A:331:ARG:H | 1.91 | 0.58 |
| 2:B:119:GLU:OE2 | 2:B:137:ARG:HD2 | 2.02 | 0.58 |
| 2:B:386:LEU:HD13 | 2:B:388:PHE:CZ | 2.37 | 0.58 |
| 2:B:330:SER:OG | 2:B:331:ARG:N | 2.36 | 0.58 |
| 1:D:2:G:H2' | 1:D:3:A:C8 | 2.39 | 0.58 |
| 2:A:371:ARG:HG3 | 2:A:375:LEU:HD23 | 1.85 | 0.58 |
| 2:B:201:GLN:HG3 | 2:B:202:LEU:H | 1.67 | 0.58 |
| 1:D:38:C:N3 | 2:B:31:LEU:HD13 | 2.18 | 0.58 |
| 2:B:235:PHE:CD1 | 2:B:235:PHE:N | 2.71 | 0.58 |
| 1:C:1:G:H2' | 1:C:2:G:C8 | 2.38 | 0.58 |
| 2:A:135:LEU:HD23 | 2:A:140:MET:HB3 | 1.86 | 0.58 |
| 2:A:220:ARG:NH1 | 2:A:234:ASP:OD1 | 2.35 | 0.58 |
| 2:B:238:LEU:HB3 | 2:B:527:TRP:HB2 | 1.85 | 0.58 |
| 2:B:277:LEU:CD1 | 2:B:281:GLU:HG2 | 2.31 | 0.58 |
| 2:A:155:TRP:CZ2 | 2:A:165:GLN:HG3 | 2.39 | 0.58 |
| 2:A:440:TYR:HD2 | 2:A:440:TYR:H | 1.50 | 0.58 |
| 2:B:180:ARG:NH1 | 2:B:224:ASP:O | 2.36 | 0.58 |
| 2:A:186:TYR:CG | 2:B:562:PRO:HG3 | 2.38 | 0.58 |
| 1:D:3:A:C2 | 1:D:4:G:C5 | 2.92 | 0.58 |
| 1:D:37:2MA:C5' | 2:B:27:ARG:NH1 | 2.55 | 0.58 |
| 2:B:556:ASP:OD1 | 2:B:559:THR:HB | 2.03 | 0.58 |
| 2:A:290:LYS:HD3 | 3:A:2048:HOH:O | 2.03 | 0.58 |
| 2:A:139:ARG:NH2 | 2:A:537:THR:HG23 | 2.18 | 0.58 |
| 2:B:39:LEU:HB2 | 2:B:48:LEU:HD21 | 1.85 | 0.58 |
| 1:D:15:G:H5'' | 1:D:16:H2U:H5' | 1.86 | 0.58 |
| 1:D:36:C:H41 | 2:B:80:GLU:HB3 | 1.65 | 0.58 |
| 1:D:8:4SU:C4' | 1:D:49:G:OP2 | 2.52 | 0.58 |
| 1:D:71:C:H2' | 1:D:72:C:O4' | 2.04 | 0.58 |
| 2:A:438:TRP:CZ3 | 2:A:460:PRO:HG2 | 2.39 | 0.57 |
| 2:B:184:VAL:HB | 2:B:194:TYR:HB2 | 1.86 | 0.57 |
| 2:B:276:ARG:NH1 | 3:B:2081:HOH:O | 2.36 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:320:VAL:HG22 | 2:B:390:ALA:CB | 2.34 | 0.57 |
| 2:A:303:GLY:N | 2:A:304:PRO:HD2 | 2.19 | 0.57 |
| 2:A:252:GLU:OE1 | 2:A:256:ARG:HD3 | 2.03 | 0.57 |
| 2:B:7:ALA:O | 2:B:10:LEU:HD13 | 2.04 | 0.57 |
| 2:A:109:PRO:HG3 | 2:A:120:LYS:CE | 2.34 | 0.57 |
| 2:A:532:LEU:O | 2:A:536:MET:HG3 | 2.04 | 0.57 |
| 2:B:227:LEU:O | 2:B:229:ALA:O | 2.23 | 0.57 |
| 2:B:341:ALA:O | 2:B:344:HIS:O | 2.22 | 0.57 |
| 2:B:449:HIS:CD2 | 2:B:464:ARG:HH12 | 2.22 | 0.57 |
| 2:B:499:ILE:HG22 | 2:B:504:GLN:HG3 | 1.86 | 0.57 |
| 2:A:428:LEU:HD22 | 2:A:448:PRO:HB3 | 1.87 | 0.57 |
| 2:B:205:GLN:HB3 | 2:B:522:HIS:HE2 | 1.69 | 0.57 |
| 2:B:432:ASP:HB2 | 2:B:439:THR:OG1 | 2.04 | 0.57 |
| 2:B:499:ILE:HD12 | 2:B:499:ILE:N | 2.18 | 0.57 |
| 2:B:176:PRO:HB2 | 2:B:507:LYS:HE2 | 1.87 | 0.57 |
| 2:B:257:LEU:HD13 | 2:B:527:TRP:CH2 | 2.39 | 0.57 |
| 2:A:40:ARG:HG2 | 2:A:41:ASP:N | 2.19 | 0.57 |
| 2:A:556:ASP:OD1 | 2:A:559:THR:HB | 2.04 | 0.57 |
| 2:B:421:LEU:HD23 | 2:B:471:VAL:CG2 | 2.35 | 0.57 |
| 1:D:47:U:H1' | 1:D:48:C:OP1 | 2.05 | 0.57 |
| 2:A:176:PRO:HD2 | 2:A:507:LYS:HG2 | 1.86 | 0.57 |
| 2:A:7:ALA:CB | 2:A:21:LEU:HD13 | 2.35 | 0.57 |
| 2:B:458:LYS:C | 2:B:460:PRO:HD3 | 2.25 | 0.57 |
| 2:A:278:SER:HA | 2:A:424:VAL:O | 2.05 | 0.57 |
| 1:C:31:C:H2' | 1:C:32:C:C6 | 2.40 | 0.57 |
| 1:C:70:U:H2' | 1:C:71:C:C6 | 2.40 | 0.57 |
| 2:A:341:ALA:O | 2:A:344:HIS:O | 2.22 | 0.57 |
| 2:B:289:ASP:C | 2:B:291:PRO:HD3 | 2.25 | 0.57 |
| 2:B:525:ILE:HG12 | 2:B:526:ALA:N | 2.19 | 0.57 |
| 2:B:556:ASP:O | 2:B:560:GLY:N | 2.28 | 0.57 |
| 1:D:63:C:H6 | 1:D:63:C:O5' | 1.87 | 0.56 |
| 2:A:106:PRO:HB2 | 2:A:108:PHE:O | 2.05 | 0.56 |
| 2:A:447:SER:HA | 2:A:484:ILE:HD11 | 1.87 | 0.56 |
| 1:D:70:U:H2' | 1:D:71:C:C5 | 2.40 | 0.56 |
| 2:A:104:LYS:HD3 | 2:B:516:GLU:HG2 | 1.87 | 0.56 |
| 2:A:452:ASP:HA | 2:A:455:LEU:HD12 | 1.87 | 0.56 |
| 2:B:27:ARG:HD2 | 2:B:115:ARG:HH21 | 1.70 | 0.56 |
| 2:B:36:PHE:CE2 | 2:B:49:VAL:HG22 | 2.40 | 0.56 |
| 2:B:40:ARG:HG3 | 2:B:45:LEU:HD23 | 1.87 | 0.56 |
| 2:B:421:LEU:HB3 | 2:B:471:VAL:CG2 | 2.36 | 0.56 |
| 2:B:166:VAL:HB | 2:B:215:TYR:CD1 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:563:SER:O | 2:B:193:PHE:N | 2.31 | 0.56 |
| 2:B:108:PHE:CD2 | 2:B:126:LEU:HD13 | 2.40 | 0.56 |
| 1:C:52:G:O2' | 1:C:53:G:H5' | 2.04 | 0.56 |
| 2:B:230:ASP:HB3 | 2:B:531:ARG:HH22 | 1.69 | 0.56 |
| 1:D:34:QUO:C4' | 1:D:35:U:H5' | 2.22 | 0.56 |
| 1:C:44:G:O2' | 1:C:45:G:H5' | 2.06 | 0.56 |
| 2:A:45:LEU:O | 2:A:87:THR:OG1 | 2.23 | 0.56 |
| 2:B:112:ALA:CB | 2:B:119:GLU:HG2 | 2.35 | 0.56 |
| 1:C:34:QUO:H4' | 1:C:35:U:C5' | 2.34 | 0.56 |
| 2:B:227:LEU:HB3 | 2:B:231:ARG:O | 2.05 | 0.56 |
| 1:D:36:C:O2' | 2:B:27:ARG:NH2 | 2.39 | 0.56 |
| 2:B:306:PHE:CD2 | 2:B:314:PHE:HD2 | 2.24 | 0.56 |
| 2:B:359:PHE:CE1 | 2:B:371:ARG:HG2 | 2.40 | 0.56 |
| 1:D:13:C:O2' | 1:D:14:A:H5' | 2.06 | 0.56 |
| 2:A:235:PHE:HB2 | 2:A:530:ASP:OD2 | 2.05 | 0.56 |
| 2:A:419:ARG:HG3 | 2:A:419:ARG:HH11 | 1.71 | 0.56 |
| 2:A:554:GLY:O | 2:B:194:TYR:OH | 2.22 | 0.56 |
| 2:B:331:ARG:O | 2:B:335:ALA:HB2 | 2.05 | 0.56 |
| 2:B:374:LEU:O | 2:B:378:THR:HG23 | 2.05 | 0.56 |
| 1:D:4:G:H2' | 1:D:5:C:O4' | 2.06 | 0.56 |
| 2:A:154:ILE:HD13 | 2:A:238:LEU:HD13 | 1.89 | 0.55 |
| 2:A:6:TYR:CE2 | 2:B:213:ASP:OD1 | 2.59 | 0.55 |
| 2:B:268:VAL:HG12 | 2:B:269:GLU:N | 2.21 | 0.55 |
| 2:B:344:HIS:O | 2:B:346:ALA:N | 2.39 | 0.55 |
| 1:C:8:4SU:H5'' | 1:C:49:G:OP2 | 2.04 | 0.55 |
| 2:A:42:ARG:CD | 2:A:145:ARG:NH2 | 2.65 | 0.55 |
| 2:B:532:LEU:O | 2:B:536:MET:HG3 | 2.06 | 0.55 |
| 1:D:51:G:O2' | 1:D:52:G:H5' | 2.06 | 0.55 |
| 2:B:12:GLU:O | 2:B:15:VAL:HG23 | 2.06 | 0.55 |
| 2:B:299:LEU:C | 2:B:300:LYS:HG2 | 2.26 | 0.55 |
| 2:B:2:ARG:HG2 | 3:B:2085:HOH:O | 2.06 | 0.55 |
| 2:B:315:GLN:HG3 | 2:B:316:GLU:N | 2.20 | 0.55 |
| 2:B:483:ARG:HH21 | 2:B:524:GLY:N | 2.03 | 0.55 |
| 1:D:59:G:H2' | 1:D:60:U:H5' | 1.88 | 0.55 |
| 2:A:293:LEU:O | 2:A:419:ARG:NH1 | 2.39 | 0.55 |
| 1:D:43:G:H2' | 1:D:44:G:C8 | 2.42 | 0.55 |
| 2:A:462:ARG:HG3 | 2:A:462:ARG:O | 2.07 | 0.55 |
| 2:A:176:PRO:HD2 | 2:A:507:LYS:HE2 | 1.88 | 0.55 |
| 2:B:155:TRP:HH2 | 2:B:165:GLN:HE21 | 1.55 | 0.55 |
| 2:B:302:VAL:O | 2:B:303:GLY:C | 2.45 | 0.55 |
| 2:A:292:ASP:OD2 | 2:A:294:ARG:NH1 | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:20(A):H2U:H3' | 1:C:21:A:H5' | 1.88 | 0.55 |
| 2:A:198:GLN:O | 2:A:221:CYS:HB3 | 2.06 | 0.55 |
| 2:A:325:LEU:HD12 | 2:A:329:LEU:HD11 | 1.87 | 0.55 |
| 2:A:173:LYS:HB2 | 2:B:559:THR:CG2 | 2.37 | 0.55 |
| 2:B:227:LEU:H | 2:B:227:LEU:CD2 | 1.94 | 0.55 |
| 1:D:11:U:H2' | 1:D:12:U:H6 | 1.72 | 0.55 |
| 2:B:361:GLY:O | 2:B:364:ALA:N | 2.35 | 0.54 |
| 2:A:168:THR:CB | 2:A:217:GLN:HE22 | 2.05 | 0.54 |
| 2:A:251:LEU:HD22 | 2:A:422:TRP:CD2 | 2.42 | 0.54 |
| 2:A:433:GLU:O | 2:A:435:GLU:N | 2.40 | 0.54 |
| 2:B:209:VAL:HG22 | 2:B:519:ALA:CB | 2.38 | 0.54 |
| 2:B:537:THR:HG23 | 2:B:539:SER:HG | 1.72 | 0.54 |
| 1:C:39:G:O2' | 1:C:40:C:H5' | 2.08 | 0.54 |
| 2:A:450:PRO:O | 2:A:453:LEU:HB2 | 2.07 | 0.54 |
| 2:B:311:PHE:CE1 | 2:B:313:VAL:HB | 2.42 | 0.54 |
| 2:B:411:LEU:HB2 | 2:B:413:LEU:HD11 | 1.88 | 0.54 |
| 2:B:208:MET:HG3 | 2:B:522:HIS:CD2 | 2.42 | 0.54 |
| 2:A:222:PHE:N | 2:A:222:PHE:CD1 | 2.75 | 0.54 |
| 2:B:307:ARG:CD | 2:B:315:GLN:O | 2.54 | 0.54 |
| 2:B:323:LEU:HD12 | 2:B:324:ALA:H | 1.71 | 0.54 |
| 2:A:111:ASP:OD1 | 2:A:115:ARG:NH2 | 2.41 | 0.54 |
| 2:B:277:LEU:O | 2:B:423:VAL:HA | 2.06 | 0.54 |
| 2:B:542:ILE:O | 2:B:545:VAL:HG22 | 2.07 | 0.54 |
| 1:C:3:A:H2' | 1:C:4:G:H8 | 1.72 | 0.54 |
| 1:D:59:G:C2' | 1:D:60:U:H5' | 2.37 | 0.54 |
| 2:A:508:PHE:HB2 | 2:A:512:LEU:CD2 | 2.38 | 0.54 |
| 2:B:551:ASN:O | 2:B:553:GLU:N | 2.40 | 0.54 |
| 2:A:146:LEU:CD1 | 2:A:149:ARG:HH12 | 2.21 | 0.54 |
| 2:A:457:GLU:OE2 | 2:A:492:ARG:HD3 | 2.07 | 0.54 |
| 2:A:505:ARG:CD | 2:A:505:ARG:N | 2.71 | 0.54 |
| 2:B:163:PHE:HA | 2:B:214:ARG:CG | 2.37 | 0.54 |
| 2:B:449:HIS:ND1 | 2:B:451:GLU:HB2 | 2.22 | 0.54 |
| 2:A:419:ARG:HG3 | 2:A:419:ARG:NH1 | 2.22 | 0.54 |
| 2:A:578:VAL:HG11 | 2:B:576:MET:CB | 2.38 | 0.54 |
| 2:B:326:PRO:HD2 | 2:B:411:LEU:CD1 | 2.38 | 0.54 |
| 1:C:53:G:O2' | 1:C:54:5MU:H5'' | 2.08 | 0.54 |
| 2:A:440:TYR:HB3 | 2:A:497:LEU:CD1 | 2.38 | 0.53 |
| 2:A:71:ALA:HB1 | 2:A:94:LEU:CD2 | 2.38 | 0.53 |
| 2:B:292:ASP:CG | 2:B:294:ARG:HE | 2.12 | 0.53 |
| 1:C:68:G:H4' | 2:A:125:GLU:OE1 | 2.08 | 0.53 |
| 2:A:418:PHE:O | 2:A:419:ARG:HD2 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:451:GLU:O | 2:A:453:LEU:N | 2.42 | 0.53 |
| 2:A:568:GLU:OE1 | 2:A:571:ARG:HD3 | 2.08 | 0.53 |
| 2:B:228:ARG:HG2 | 2:B:228:ARG:HH11 | 1.74 | 0.53 |
| 2:B:182:PHE:CZ | 2:B:233:PRO:HB3 | 2.43 | 0.53 |
| 2:B:327:LYS:HG3 | 2:B:328:ALA:H | 1.72 | 0.53 |
| 2:B:392:PRO:HB2 | 2:B:395:VAL:HG23 | 1.90 | 0.53 |
| 2:A:189:GLU:HB3 | 2:A:192:LEU:HD13 | 1.91 | 0.53 |
| 2:A:461:GLY:O | 2:A:463:VAL:N | 2.41 | 0.53 |
| 2:A:137:ARG:O | 2:A:141:GLN:HG3 | 2.08 | 0.53 |
| 2:A:517:TYR:CZ | 2:B:104:LYS:HE2 | 2.43 | 0.53 |
| 2:B:36:PHE:CD2 | 2:B:49:VAL:HG22 | 2.44 | 0.53 |
| 2:A:283:MET:O | 2:A:287:GLY:HA2 | 2.08 | 0.53 |
| 2:A:543:ARG:HH21 | 2:A:552:LYS:HG3 | 1.73 | 0.53 |
| 2:B:109:PRO:CG | 2:B:120:LYS:HD3 | 2.39 | 0.53 |
| 1:D:2:G:C2 | 1:D:3:A:C5 | 2.96 | 0.53 |
| 2:A:321:LYS:HB3 | 2:A:400:LEU:HD12 | 1.91 | 0.53 |
| 2:A:513:GLU:O | 2:A:516:GLU:HB2 | 2.08 | 0.53 |
| 2:B:89:ARG:HG3 | 2:B:89:ARG:HH11 | 1.74 | 0.53 |
| 2:A:302:VAL:CG1 | 2:A:305:LEU:HD12 | 2.39 | 0.53 |
| 2:A:324:ALA:HB2 | 2:A:386:LEU:CD2 | 2.38 | 0.53 |
| 2:A:42:ARG:HD3 | 2:A:145:ARG:HH21 | 1.69 | 0.53 |
| 2:A:457:GLU:OE1 | 2:A:492:ARG:NH1 | 2.38 | 0.53 |
| 2:A:472:LEU:HD23 | 2:A:535:LEU:HD12 | 1.90 | 0.53 |
| 2:A:537:THR:HG23 | 2:A:539:SER:H | 1.74 | 0.53 |
| 2:B:39:LEU:CB | 2:B:48:LEU:HD21 | 2.39 | 0.53 |
| 2:B:551:ASN:ND2 | 2:B:557:PRO:HG3 | 2.24 | 0.53 |
| 2:A:163:PHE:CD2 | 2:A:214:ARG:HB2 | 2.44 | 0.53 |
| 2:A:230:ASP:OD1 | 2:A:542:ILE:N | 2.38 | 0.53 |
| 2:A:63:VAL:HA | 2:A:67:TRP:CE3 | 2.43 | 0.53 |
| 2:B:127:ARG:CZ | 2:B:137:ARG:NH2 | 2.70 | 0.53 |
| 2:B:408:ALA:CA | 2:B:413:LEU:HD13 | 2.25 | 0.53 |
| 2:A:112:ALA:HA | 2:A:115:ARG:NH1 | 2.24 | 0.53 |
| 2:A:235:PHE:N | 2:A:235:PHE:CD1 | 2.77 | 0.53 |
| 2:A:438:TRP:CZ2 | 2:A:460:PRO:HB2 | 2.44 | 0.53 |
| 2:B:223:ARG:CD | 2:B:225:GLU:HG2 | 2.38 | 0.53 |
| 2:B:430:GLU:HG3 | 2:B:431:TRP:N | 2.24 | 0.53 |
| 1:D:66:C:H2' | 1:D:67:C:C6 | 2.43 | 0.52 |
| 2:B:290:LYS:HA | 2:B:471:VAL:HG11 | 1.90 | 0.52 |
| 2:B:72:LYS:HB3 | 2:B:96:ALA:HB3 | 1.91 | 0.52 |
| 2:A:45:LEU:HD21 | 2:A:114:TRP:HB3 | 1.91 | 0.52 |
| 2:B:166:VAL:HB | 2:B:215:TYR:HD1 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:4:THR:HG23 | 2:A:20:VAL:HB | 1.92 | 0.52 |
| 2:A:179:ALA:HA | 2:A:225:GLU:OE2 | 2.08 | 0.52 |
| 1:C:47:U:C2' | 1:C:48:C:OP1 | 2.57 | 0.52 |
| 2:A:226:ASP:C | 2:A:228:ARG:N | 2.61 | 0.52 |
| 2:A:475:VAL:HG11 | 2:A:531:ARG:HG2 | 1.92 | 0.52 |
| 2:B:108:PHE:HD2 | 2:B:126:LEU:CD1 | 2.22 | 0.52 |
| 2:B:237:GLN:HA | 2:B:527:TRP:O | 2.09 | 0.52 |
| 2:B:311:PHE:C | 2:B:311:PHE:CD1 | 2.81 | 0.52 |
| 1:C:11:U:H2' | 1:C:12:U:C6 | 2.45 | 0.52 |
| 2:A:194:TYR:OH | 2:B:554:GLY:O | 2.23 | 0.52 |
| 2:A:571:ARG:NE | 2:B:580:PRO:O | 2.43 | 0.52 |
| 1:D:2:G:N1 | 1:D:3:A:C5 | 2.78 | 0.52 |
| 2:A:452:ASP:OD2 | 2:A:464:ARG:HD3 | 2.10 | 0.52 |
| 2:B:409:ASP:O | 2:B:412:GLY:N | 2.29 | 0.52 |
| 1:D:46:G7M:H4' | 1:D:47:U:OP1 | 2.09 | 0.52 |
| 2:A:230:ASP:HB3 | 2:A:531:ARG:HH22 | 1.74 | 0.52 |
| 2:A:563:SER:CB | 2:B:173:LYS:HE3 | 2.39 | 0.52 |
| 2:B:364:ALA:O | 2:B:365:LYS:C | 2.46 | 0.52 |
| 1:C:37:2MA:H4' | 2:A:27:ARG:NH1 | 2.25 | 0.52 |
| 1:D:70:U:C3' | 1:D:70:U:C6 | 2.93 | 0.52 |
| 2:A:49:VAL:HG12 | 2:A:93:GLU:HA | 1.91 | 0.52 |
| 2:B:115:ARG:NH1 | 2:B:117:GLU:CD | 2.64 | 0.52 |
| 2:B:493:VAL:O | 2:B:497:LEU:HD13 | 2.09 | 0.52 |
| 2:B:513:GLU:CG | 3:B:2071:HOH:O | 2.58 | 0.52 |
| 2:B:406:ARG:HG3 | 2:B:410:LEU:HG | 1.92 | 0.51 |
| 2:B:410:LEU:C | 2:B:411:LEU:HD23 | 2.30 | 0.51 |
| 2:B:429:LEU:HA | 2:B:439:THR:O | 2.10 | 0.51 |
| 2:B:206:MET:HE1 | 2:B:510:PHE:CD1 | 2.45 | 0.51 |
| 2:A:324:ALA:HB2 | 2:A:386:LEU:HD23 | 1.91 | 0.51 |
| 2:B:200:PRO:HG2 | 2:B:239:ASP:OD1 | 2.11 | 0.51 |
| 2:B:27:ARG:HD3 | 2:B:115:ARG:NE | 2.24 | 0.51 |
| 2:B:470:LEU:O | 2:B:477:VAL:HG22 | 2.11 | 0.51 |
| 2:B:59:THR:C | 2:B:61:GLU:H | 2.13 | 0.51 |
| 2:B:76:ARG:NH1 | 2:B:93:GLU:OE1 | 2.43 | 0.51 |
| 2:A:337:LEU:CD1 | 2:A:387:LEU:HD21 | 2.41 | 0.51 |
| 2:B:182:PHE:HZ | 2:B:233:PRO:HB3 | 1.75 | 0.51 |
| 2:B:290:LYS:N | 2:B:291:PRO:CD | 2.72 | 0.51 |
| 2:B:368:GLU:N | 2:B:369:PRO:CD | 2.73 | 0.51 |
| 1:C:34:QUO:H5' | 2:A:31:LEU:HD23 | 1.91 | 0.51 |
| 2:B:327:LYS:HG2 | 2:B:328:ALA:N | 2.24 | 0.51 |
| 2:B:459:ASP:OD1 | 2:B:462:ARG:HB2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:C:20:H2U:H5' | 1:C:20(A):H2U:H5'' | 1.92 | 0.51 |
| 2:B:163:PHE:HA | 2:B:214:ARG:HG2 | 1.92 | 0.51 |
| 2:B:340:VAL:HG12 | 2:B:341:ALA:N | 2.26 | 0.51 |
| 2:B:28:ARG:NE | 2:B:64:ARG:HE | 2.08 | 0.51 |
| 1:C:27:C:H2' | 1:C:28:C:C6 | 2.46 | 0.51 |
| 1:C:64:G:H2' | 1:C:65:PSU:O4' | 2.11 | 0.51 |
| 2:A:440:TYR:HE1 | 2:A:444:PRO:HD3 | 1.72 | 0.51 |
| 2:B:227:LEU:HD13 | 2:B:227:LEU:N | 2.24 | 0.51 |
| 2:B:48:LEU:HD23 | 2:B:48:LEU:N | 2.25 | 0.51 |
| 1:D:18:G:H21 | 1:D:58:A:H5' | 1.76 | 0.51 |
| 1:D:44:G:O2' | 1:D:45:G:H5' | 2.11 | 0.51 |
| 2:A:252:GLU:OE1 | 2:A:256:ARG:CD | 2.59 | 0.51 |
| 2:A:561:ALA:HA | 2:A:562:PRO:C | 2.31 | 0.51 |
| 2:A:457:GLU:OE1 | 2:A:492:ARG:HD3 | 2.11 | 0.51 |
| 2:A:543:ARG:NH2 | 2:A:552:LYS:HG3 | 2.25 | 0.51 |
| 2:B:164:VAL:O | 2:B:166:VAL:HG23 | 2.11 | 0.51 |
| 2:B:320:VAL:HG13 | 2:B:390:ALA:HB2 | 1.93 | 0.51 |
| 2:B:325:LEU:HD12 | 2:B:387:LEU:HD21 | 1.93 | 0.51 |
| 2:B:389:VAL:CG2 | 2:B:400:LEU:HD23 | 2.41 | 0.51 |
| 1:C:53:G:H2' | 1:C:54:5MU:H6 | 1.74 | 0.51 |
| 2:A:182:PHE:HB2 | 2:A:196:LEU:HD12 | 1.93 | 0.51 |
| 2:A:449:HIS:CE1 | 2:A:451:GLU:HG3 | 2.46 | 0.51 |
| 2:A:567:GLU:HG3 | 2:A:568:GLU:N | 2.25 | 0.51 |
| 2:B:451:GLU:O | 2:B:454:PRO:HD2 | 2.11 | 0.51 |
| 2:B:456:LEU:HG | 2:B:496:LEU:HD22 | 1.93 | 0.51 |
| 1:D:54:5MU:C5M | 1:D:55:PSU:C2 | 2.94 | 0.51 |
| 1:D:8:4SU:C1' | 1:D:48:C:H1' | 2.41 | 0.51 |
| 2:A:10:LEU:HD23 | 2:A:46:VAL:CG1 | 2.39 | 0.50 |
| 2:A:175:THR:HB | 2:A:507:LYS:CE | 2.41 | 0.50 |
| 2:B:566:PRO:O | 2:B:567:GLU:C | 2.50 | 0.50 |
| 2:B:566:PRO:O | 2:B:568:GLU:N | 2.45 | 0.50 |
| 2:B:7:ALA:O | 2:B:10:LEU:CD1 | 2.59 | 0.50 |
| 2:B:168:THR:HG23 | 2:B:169:PRO:CD | 2.41 | 0.50 |
| 2:B:209:VAL:HG22 | 2:B:519:ALA:HB2 | 1.94 | 0.50 |
| 2:A:154:ILE:HG21 | 2:A:238:LEU:CD1 | 2.42 | 0.50 |
| 1:C:2:G:H1 | 1:C:71:C:N4 | 2.08 | 0.50 |
| 2:A:39:LEU:HG | 2:A:48:LEU:HD11 | 1.91 | 0.50 |
| 2:B:67:TRP:CH2 | 2:B:102:GLU:HG2 | 2.46 | 0.50 |
| 2:B:172:THR:OG1 | 2:B:173:LYS:N | 2.42 | 0.50 |
| 2:B:311:PHE:O | 2:B:312:ARG:C | 2.48 | 0.50 |
| 2:B:361:GLY:O | 2:B:363:VAL:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:7:ALA:O | 2:B:46:VAL:HB | 2.11 | 0.50 |
| 2:B:4:THR:C | 2:B:5:HIS:ND1 | 2.65 | 0.50 |
| 1:C:27:C:H2' | 1:C:28:C:H6 | 1.77 | 0.50 |
| 1:C:36:C:C2 | 2:A:78:ARG:NH2 | 2.79 | 0.50 |
| 2:A:186:TYR:CD2 | 2:B:562:PRO:HG3 | 2.46 | 0.50 |
| 2:B:201:GLN:HA | 2:B:204:LYS:CD | 2.42 | 0.50 |
| 1:C:12:U:H2' | 1:C:13:C:O4' | 2.10 | 0.50 |
| 1:D:63:C:H2' | 1:D:64:G:H8 | 1.74 | 0.50 |
| 2:A:42:ARG:CD | 2:A:145:ARG:HH21 | 2.25 | 0.50 |
| 2:B:115:ARG:NH1 | 2:B:117:GLU:OE2 | 2.45 | 0.50 |
| 2:A:558:LEU:HD21 | 2:B:206:MET:SD | 2.52 | 0.50 |
| 2:B:354:VAL:HG23 | 2:B:383:GLY:N | 2.27 | 0.50 |
| 2:B:435:GLU:O | 2:B:436:GLU:OE1 | 2.29 | 0.50 |
| 2:B:483:ARG:HH21 | 2:B:524:GLY:CA | 2.24 | 0.50 |
| 1:C:4:G:N2 | 1:C:70:U:C2 | 2.80 | 0.50 |
| 1:D:2:G:N3 | 1:D:3:A:C8 | 2.79 | 0.50 |
| 2:A:1:MET:O | 2:A:1:MET:HG2 | 2.11 | 0.50 |
| 2:A:290:LYS:N | 2:A:291:PRO:HD3 | 2.27 | 0.50 |
| 2:B:429:LEU:HB3 | 2:B:438:TRP:CB | 2.40 | 0.50 |
| 2:B:147:ARG:NH1 | 2:B:533:LEU:HD12 | 2.26 | 0.50 |
| 1:C:20(A):H2U:H3' | 1:C:21:A:C5' | 2.42 | 0.50 |
| 1:D:29:U:H2' | 1:D:30:G:H8 | 1.75 | 0.50 |
| 1:C:53:G:C2 | 1:C:62:C:C2 | 3.00 | 0.50 |
| 2:A:112:ALA:HB1 | 2:A:117:GLU:HB2 | 1.94 | 0.49 |
| 2:A:4:THR:CG2 | 2:A:20:VAL:HB | 2.42 | 0.49 |
| 2:A:562:PRO:HG3 | 2:B:186:TYR:CG | 2.47 | 0.49 |
| 2:B:223:ARG:HD2 | 2:B:225:GLU:HG2 | 1.93 | 0.49 |
| 2:B:266:LEU:HB2 | 2:B:268:VAL:HG23 | 1.93 | 0.49 |
| 2:B:334:VAL:HG11 | 2:B:351:TRP:CD1 | 2.47 | 0.49 |
| 2:B:255:GLU:CG | 2:B:422:TRP:HE1 | 2.22 | 0.49 |
| 2:A:7:ALA:HB1 | 2:A:46:VAL:HG22 | 1.94 | 0.49 |
| 2:B:351:TRP:HA | 2:B:386:LEU:O | 2.12 | 0.49 |
| 1:C:3:A:H2' | 1:C:4:G:O4' | 2.12 | 0.49 |
| 2:B:18:GLU:HA | 2:B:74:LEU:HA | 1.94 | 0.49 |
| 2:A:358:GLY:HA2 | 2:A:371:ARG:HD3 | 1.93 | 0.49 |
| 2:A:326:PRO:CD | 2:A:411:LEU:HD21 | 2.41 | 0.49 |
| 2:A:499:ILE:HA | 2:A:503:GLU:OE1 | 2.12 | 0.49 |
| 2:B:325:LEU:HD22 | 2:B:411:LEU:HD11 | 1.95 | 0.49 |
| 2:B:570:LEU:HD13 | 2:B:575:LEU:O | 2.12 | 0.49 |
| 2:B:325:LEU:O | 2:B:384:ASP:CB | 2.60 | 0.49 |
| 2:A:251:LEU:HD22 | 2:A:422:TRP:CE3 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:39:LEU:HB2 | 2:A:48:LEU:HG | 1.95 | 0.49 |
| 2:A:457:GLU:CD | 2:A:492:ARG:HD3 | 2.33 | 0.49 |
| 2:A:77:LEU:HD23 | 2:A:89:ARG:O | 2.12 | 0.49 |
| 2:B:331:ARG:CA | 2:B:331:ARG:HE | 2.08 | 0.49 |
| 1:C:47:U:H2' | 1:C:50:C:OP1 | 2.13 | 0.49 |
| 2:A:539:SER:OG | 2:A:544:GLU:HB2 | 2.13 | 0.49 |
| 2:B:299:LEU:CD2 | 2:B:299:LEU:N | 2.74 | 0.49 |
| 2:B:323:LEU:HD12 | 2:B:324:ALA:N | 2.27 | 0.49 |
| 2:B:543:ARG:HD3 | 2:B:550:LYS:O | 2.13 | 0.49 |
| 2:A:213:ASP:OD1 | 2:A:214:ARG:HD3 | 2.12 | 0.49 |
| 2:B:472:LEU:O | 2:B:475:VAL:HG23 | 2.13 | 0.49 |
| 2:B:291:PRO:HB2 | 2:B:421:LEU:HD22 | 1.94 | 0.49 |
| 2:B:89:ARG:CG | 2:B:89:ARG:HH11 | 2.26 | 0.49 |
| 1:C:61:C:C2' | 1:C:62:C:H5' | 2.43 | 0.49 |
| 2:A:455:LEU:CB | 2:A:463:VAL:HG22 | 2.42 | 0.49 |
| 2:B:312:ARG:HH12 | 2:B:316:GLU:CG | 2.26 | 0.49 |
| 2:B:341:ALA:HB2 | 2:B:403:VAL:CG2 | 2.43 | 0.49 |
| 2:B:537:THR:O | 2:B:538:GLY:C | 2.51 | 0.49 |
| 2:A:155:TRP:O | 2:A:156:ASP:C | 2.52 | 0.48 |
| 2:A:21:LEU:HD12 | 2:A:39:LEU:HD12 | 1.94 | 0.48 |
| 2:A:283:MET:O | 2:A:287:GLY:N | 2.46 | 0.48 |
| 2:A:490:GLN:HG3 | 2:A:494:PHE:CD1 | 2.48 | 0.48 |
| 2:A:514:ALA:HB2 | 2:B:132:TYR:CZ | 2.48 | 0.48 |
| 2:A:546:ILE:O | 2:A:547:ALA:C | 2.51 | 0.48 |
| 2:B:119:GLU:OE2 | 2:B:137:ARG:CD | 2.61 | 0.48 |
| 2:B:4:THR:CG2 | 2:B:20:VAL:HB | 2.43 | 0.48 |
| 2:B:497:LEU:CB | 2:B:499:ILE:CD1 | 2.91 | 0.48 |
| 2:B:513:GLU:HG2 | 3:B:2071:HOH:O | 2.13 | 0.48 |
| 1:D:43:G:H2' | 1:D:44:G:H8 | 1.77 | 0.48 |
| 2:A:268:VAL:HG12 | 2:A:269:GLU:N | 2.29 | 0.48 |
| 2:A:241:GLU:OE1 | 2:A:524:GLY:N | 2.46 | 0.48 |
| 2:A:558:LEU:HD11 | 2:B:206:MET:CE | 2.42 | 0.48 |
| 2:B:134:ASP:CG | 2:B:137:ARG:HH21 | 2.17 | 0.48 |
| 2:A:359:PHE:HB2 | 2:A:364:ALA:CB | 2.43 | 0.48 |
| 2:A:311:PHE:HB2 | 2:A:366:PHE:CD2 | 2.49 | 0.48 |
| 2:A:74:LEU:HD21 | 2:A:76:ARG:NH2 | 2.29 | 0.48 |
| 2:B:123:SER:O | 2:B:124:GLU:C | 2.51 | 0.48 |
| 2:B:155:TRP:O | 2:B:159:ASP:HB2 | 2.13 | 0.48 |
| 2:B:339:GLU:O | 2:B:343:ARG:N | 2.43 | 0.48 |
| 2:B:39:LEU:HD22 | 2:B:40:ARG:H | 1.78 | 0.48 |
| 2:B:69:VAL:HG12 | 2:B:99:VAL:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:70:U:C6 | 1:D:70:U:O5' | 2.62 | 0.48 |
| 2:A:36:PHE:CE2 | 2:A:49:VAL:HG23 | 2.48 | 0.48 |
| 2:A:63:VAL:HG12 | 2:A:64:ARG:N | 2.29 | 0.48 |
| 2:B:120:LYS:CD | 2:B:120:LYS:H | 2.18 | 0.48 |
| 2:A:559:THR:CG2 | 2:B:173:LYS:HB2 | 2.41 | 0.48 |
| 2:B:434:GLU:O | 2:B:436:GLU:N | 2.43 | 0.48 |
| 1:D:33:U:C6 | 2:B:33:GLY:O | 2.67 | 0.48 |
| 2:A:204:LYS:O | 2:A:208:MET:HG2 | 2.13 | 0.48 |
| 2:B:146:LEU:CD1 | 2:B:149:ARG:HH12 | 2.20 | 0.48 |
| 2:B:449:HIS:HD2 | 2:B:464:ARG:NH1 | 2.10 | 0.48 |
| 2:A:452:ASP:O | 2:A:455:LEU:HB2 | 2.14 | 0.48 |
| 2:B:312:ARG:HH12 | 2:B:316:GLU:HG3 | 1.77 | 0.48 |
| 2:B:452:ASP:CA | 2:B:455:LEU:HD23 | 2.40 | 0.48 |
| 1:D:34:QUO:N2 | 2:B:91:GLU:OE1 | 2.42 | 0.48 |
| 1:C:20:H2U:H5' | 1:C:20(A):H2U:C5' | 2.43 | 0.48 |
| 2:A:200:PRO:O | 2:A:201:GLN:C | 2.51 | 0.48 |
| 2:A:198:GLN:NE2 | 2:A:223:ARG:HB2 | 2.29 | 0.48 |
| 2:B:28:ARG:CG | 2:B:28:ARG:NH1 | 2.59 | 0.48 |
| 2:B:321:LYS:HG3 | 2:B:397:ALA:HA | 1.96 | 0.48 |
| 1:D:66:C:H2' | 1:D:67:C:H6 | 1.78 | 0.48 |
| 2:A:7:ALA:CA | 2:A:21:LEU:HD13 | 2.43 | 0.48 |
| 2:B:173:LYS:HD3 | 2:B:174:SER:N | 2.29 | 0.48 |
| 2:B:78:ARG:HD2 | 2:B:90:VAL:O | 2.13 | 0.48 |
| 2:A:105:THR:HA | 2:A:106:PRO:HD3 | 1.77 | 0.48 |
| 2:A:234:ASP:OD1 | 2:A:234:ASP:O | 2.32 | 0.48 |
| 2:A:428:LEU:HA | 2:A:465:ALA:HB2 | 1.96 | 0.48 |
| 2:A:503:GLU:O | 2:A:507:LYS:HB2 | 2.14 | 0.48 |
| 2:B:202:LEU:HA | 2:B:202:LEU:HD23 | 1.61 | 0.48 |
| 2:B:235:PHE:HE2 | 2:B:237:GLN:NE2 | 2.11 | 0.48 |
| 2:B:246:GLU:O | 2:B:247:VAL:C | 2.52 | 0.48 |
| 2:B:28:ARG:NE | 2:B:64:ARG:NE | 2.61 | 0.48 |
| 1:D:52:G:H2' | 1:D:53:G:O4' | 2.14 | 0.48 |
| 2:A:431:TRP:CD1 | 2:A:438:TRP:NE1 | 2.82 | 0.48 |
| 2:B:123:SER:O | 2:B:126:LEU:N | 2.45 | 0.48 |
| 1:C:15:G:C5' | 1:C:16:H2U:H5' | 2.42 | 0.48 |
| 1:C:35:U:O2' | 2:A:29:ARG:HD2 | 2.14 | 0.48 |
| 1:C:49:G:H2' | 1:C:50:C:C6 | 2.49 | 0.48 |
| 1:C:49:G:N2 | 1:C:50:C:C2 | 2.81 | 0.48 |
| 1:C:53:G:H2' | 1:C:54:5MU:C6 | 2.49 | 0.48 |
| 1:C:65:PSU:H2' | 1:C:66:C:H6 | 1.78 | 0.48 |
| 1:D:28:C:H2' | 1:D:29:U:H6 | 1.76 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:9:A:H5'' | 1:D:46:G7M:N2 | 2.28 | 0.48 |
| 2:A:182:PHE:HB3 | 2:B:184:VAL:CG1 | 2.44 | 0.47 |
| 2:A:230:ASP:HB3 | 2:A:531:ARG:HH12 | 1.79 | 0.47 |
| 2:A:508:PHE:O | 2:A:512:LEU:HD22 | 2.14 | 0.47 |
| 2:B:39:LEU:HD22 | 2:B:40:ARG:N | 2.28 | 0.47 |
| 1:D:29:U:H2' | 1:D:30:G:C8 | 2.48 | 0.47 |
| 2:A:133:LEU:HD11 | 2:B:517:TYR:CG | 2.50 | 0.47 |
| 2:A:64:ARG:O | 2:A:67:TRP:HB2 | 2.14 | 0.47 |
| 2:B:128:LEU:O | 2:B:558:LEU:HB2 | 2.15 | 0.47 |
| 1:D:22:G:O2' | 1:D:23:A:H5' | 2.13 | 0.47 |
| 2:A:4:THR:HG1 | 2:A:5:HIS:CE1 | 2.32 | 0.47 |
| 2:B:140:MET:O | 2:B:143:ASN:HB2 | 2.14 | 0.47 |
| 2:B:534:ALA:O | 2:B:537:THR:HG22 | 2.14 | 0.47 |
| 2:B:139:ARG:HH21 | 2:B:544:GLU:HB3 | 1.79 | 0.47 |
| 2:B:551:ASN:HD22 | 2:B:557:PRO:HG3 | 1.77 | 0.47 |
| 2:A:505:ARG:N | 2:A:505:ARG:HD2 | 2.28 | 0.47 |
| 2:B:63:VAL:HA | 2:B:67:TRP:CE3 | 2.49 | 0.47 |
| 2:B:77:LEU:HD23 | 2:B:78:ARG:N | 2.29 | 0.47 |
| 1:D:34:QUO:HN22 | 2:B:91:GLU:CD | 2.18 | 0.47 |
| 2:A:147:ARG:HD2 | 2:A:533:LEU:HD11 | 1.94 | 0.47 |
| 2:A:339:GLU:O | 2:A:339:GLU:HG3 | 2.15 | 0.47 |
| 2:A:371:ARG:HG3 | 2:A:375:LEU:HD21 | 1.96 | 0.47 |
| 2:A:461:GLY:C | 2:A:463:VAL:H | 2.17 | 0.47 |
| 2:A:579:ARG:HB2 | 2:A:580:PRO:HD3 | 1.95 | 0.47 |
| 2:B:114:TRP:CZ2 | 2:B:138:ARG:HA | 2.49 | 0.47 |
| 2:B:120:LYS:O | 2:B:120:LYS:HG2 | 2.14 | 0.47 |
| 2:B:260:HIS:HA | 2:B:263:ARG:NH2 | 2.30 | 0.47 |
| 2:B:361:GLY:H | 2:B:364:ALA:CB | 2.28 | 0.47 |
| 1:D:24:A:H2' | 1:D:25:U:O4' | 2.14 | 0.47 |
| 2:A:212:LEU:HD23 | 2:A:212:LEU:HA | 1.71 | 0.47 |
| 2:A:139:ARG:HH21 | 2:A:539:SER:HG | 1.61 | 0.47 |
| 2:A:517:TYR:CG | 2:B:133:LEU:HD11 | 2.50 | 0.47 |
| 2:B:171:LEU:HB3 | 2:B:194:TYR:CD1 | 2.50 | 0.47 |
| 2:B:226:ASP:O | 2:B:228:ARG:N | 2.42 | 0.47 |
| 2:A:433:GLU:C | 2:A:435:GLU:H | 2.18 | 0.47 |
| 2:A:494:PHE:HD2 | 2:A:499:ILE:HB | 1.80 | 0.47 |
| 2:B:354:VAL:CG2 | 2:B:381:ARG:O | 2.62 | 0.47 |
| 1:D:70:U:H5 | 1:D:70:U:OP2 | 1.98 | 0.47 |
| 2:B:250:VAL:HG11 | 2:B:468:TYR:OH | 2.14 | 0.47 |
| 2:B:287:GLY:O | 2:B:398:THR:HA | 2.15 | 0.47 |
| 2:B:372:GLU:HA | 2:B:375:LEU:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:284:GLU:HA | 2:A:284:GLU:OE1 | 2.14 | 0.47 |
| 2:A:449:HIS:HE1 | 2:A:451:GLU:HG3 | 1.79 | 0.47 |
| 3:A:2016:HOH:O | 2:B:147:ARG:HD3 | 2.14 | 0.47 |
| 2:B:386:LEU:HD13 | 2:B:388:PHE:HZ | 1.80 | 0.47 |
| 2:A:303:GLY:HA2 | 2:A:320:VAL:HG23 | 1.97 | 0.47 |
| 2:A:426:PHE:CD2 | 2:A:441:MET:HE2 | 2.50 | 0.47 |
| 2:A:10:LEU:O | 2:A:87:THR:HG22 | 2.14 | 0.47 |
| 2:B:435:GLU:HA | 2:B:435:GLU:OE1 | 2.15 | 0.47 |
| 1:C:22:G:H2' | 1:C:23:A:H8 | 1.80 | 0.47 |
| 2:A:349:LEU:HD22 | 2:A:350:ALA:O | 2.15 | 0.47 |
| 1:D:2:G:C6 | 1:D:3:A:C5 | 3.03 | 0.47 |
| 2:A:275:PRO:HD2 | 2:A:420:PHE:O | 2.14 | 0.46 |
| 2:A:320:VAL:HG13 | 2:A:390:ALA:HB2 | 1.98 | 0.46 |
| 2:A:517:TYR:CE2 | 2:B:107:PRO:HD3 | 2.50 | 0.46 |
| 2:B:205:GLN:O | 2:B:208:MET:HB2 | 2.15 | 0.46 |
| 2:B:300:LYS:HE2 | 2:B:377:ALA:O | 2.15 | 0.46 |
| 2:A:204:LYS:HE3 | 2:A:241:GLU:HB2 | 1.97 | 0.46 |
| 2:A:409:ASP:O | 2:A:410:LEU:C | 2.53 | 0.46 |
| 2:A:576:MET:HB2 | 2:B:578:VAL:CG2 | 2.45 | 0.46 |
| 2:B:296:GLY:O | 2:B:297:LEU:HB2 | 2.15 | 0.46 |
| 2:B:73:GLY:HA2 | 2:B:95:SER:H | 1.81 | 0.46 |
| 2:A:179:ALA:HB1 | 2:A:198:GLN:NE2 | 2.29 | 0.46 |
| 2:A:289:ASP:C | 2:A:291:PRO:HD3 | 2.36 | 0.46 |
| 2:A:361:GLY:O | 2:A:362:GLY:C | 2.54 | 0.46 |
| 2:B:115:ARG:HH11 | 2:B:117:GLU:CD | 2.18 | 0.46 |
| 1:C:15:G:H2' | 1:C:59:G:C6 | 2.49 | 0.46 |
| 2:A:517:TYR:HB3 | 2:B:133:LEU:HD21 | 1.97 | 0.46 |
| 2:B:452:ASP:OD1 | 2:B:464:ARG:NE | 2.49 | 0.46 |
| 2:A:111:ASP:CG | 2:A:115:ARG:NH2 | 2.69 | 0.46 |
| 2:A:539:SER:CB | 2:A:544:GLU:HB2 | 2.45 | 0.46 |
| 2:A:406:ARG:O | 2:A:409:ASP:HB2 | 2.15 | 0.46 |
| 2:A:534:ALA:O | 2:A:538:GLY:N | 2.47 | 0.46 |
| 2:B:242:MET:O | 2:B:522:HIS:HB2 | 2.14 | 0.46 |
| 1:C:65:PSU:H2' | 1:C:66:C:C6 | 2.50 | 0.46 |
| 2:A:175:THR:HB | 2:A:507:LYS:HE2 | 1.97 | 0.46 |
| 2:A:426:PHE:HD2 | 2:A:441:MET:HE1 | 1.81 | 0.46 |
| 2:A:311:PHE:HB2 | 2:A:366:PHE:CG | 2.51 | 0.46 |
| 2:A:147:ARG:NH1 | 2:A:545:VAL:O | 2.49 | 0.46 |
| 2:B:170:PHE:O | 2:B:197:PRO:HD3 | 2.16 | 0.46 |
| 2:B:297:LEU:O | 2:B:404:ARG:HD2 | 2.16 | 0.46 |
| 2:B:360:SER:O | 2:B:360:SER:OG | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:429:LEU:HD13 | 2:B:438:TRP:HB2 | 1.98 | 0.46 |
| 2:B:311:PHE:O | 2:B:313:VAL:N | 2.49 | 0.46 |
| 1:D:2:G:C4 | 1:D:3:A:N7 | 2.84 | 0.46 |
| 1:D:48:C:H5'' | 1:D:49:G:H5'' | 1.98 | 0.46 |
| 1:C:33:U:C6 | 2:A:33:GLY:HA3 | 2.51 | 0.46 |
| 2:A:165:GLN:HE22 | 2:A:167:GLU:HG3 | 1.80 | 0.45 |
| 2:A:169:PRO:HG2 | 2:A:203:PHE:CE2 | 2.51 | 0.45 |
| 2:A:185:PRO:HA | 2:A:193:PHE:CD1 | 2.52 | 0.45 |
| 1:C:18:G:H1' | 1:C:57:G:N2 | 2.32 | 0.45 |
| 1:D:49:G:H2' | 1:D:50:C:H6 | 1.80 | 0.45 |
| 2:A:331:ARG:HE | 2:A:331:ARG:N | 1.92 | 0.45 |
| 2:A:405:LEU:HD22 | 2:A:415:ARG:NH2 | 2.31 | 0.45 |
| 2:A:426:PHE:HD2 | 2:A:441:MET:CE | 2.28 | 0.45 |
| 2:B:292:ASP:OD1 | 2:B:294:ARG:NE | 2.47 | 0.45 |
| 2:B:327:LYS:HE2 | 2:B:333:GLU:OE1 | 2.16 | 0.45 |
| 2:A:130:TYR:O | 2:A:132:TYR:N | 2.50 | 0.45 |
| 2:A:409:ASP:O | 2:A:412:GLY:N | 2.45 | 0.45 |
| 2:A:501:GLU:OE2 | 2:A:505:ARG:CZ | 2.64 | 0.45 |
| 2:B:147:ARG:NH1 | 2:B:533:LEU:CD1 | 2.79 | 0.45 |
| 2:B:155:TRP:CH2 | 2:B:165:GLN:HG3 | 2.51 | 0.45 |
| 1:C:13:C:O2' | 1:C:14:A:H5' | 2.17 | 0.45 |
| 2:A:182:PHE:CB | 2:A:196:LEU:HD12 | 2.47 | 0.45 |
| 2:A:208:MET:HG3 | 2:A:241:GLU:HG3 | 1.99 | 0.45 |
| 2:A:232:GLN:O | 2:A:233:PRO:C | 2.55 | 0.45 |
| 2:A:433:GLU:C | 2:A:435:GLU:N | 2.70 | 0.45 |
| 2:A:445:PHE:O | 2:A:484:ILE:HG12 | 2.17 | 0.45 |
| 2:B:114:TRP:CE2 | 2:B:138:ARG:HB2 | 2.51 | 0.45 |
| 2:B:226:ASP:C | 2:B:228:ARG:N | 2.69 | 0.45 |
| 2:B:27:ARG:NH1 | 2:B:115:ARG:CD | 2.79 | 0.45 |
| 2:B:307:ARG:HG3 | 2:B:315:GLN:HB2 | 1.99 | 0.45 |
| 2:B:449:HIS:CE1 | 2:B:451:GLU:HB2 | 2.51 | 0.45 |
| 2:B:454:PRO:HG2 | 2:B:455:LEU:HD22 | 1.98 | 0.45 |
| 2:B:6:TYR:O | 2:B:7:ALA:C | 2.55 | 0.45 |
| 2:A:41:ASP:C | 2:A:41:ASP:OD1 | 2.54 | 0.45 |
| 2:A:508:PHE:HB2 | 2:A:512:LEU:HD22 | 1.99 | 0.45 |
| 2:B:84:ARG:O | 2:B:85:LEU:HD23 | 2.17 | 0.45 |
| 1:C:52:G:N2 | 1:C:63:C:C2 | 2.85 | 0.45 |
| 1:D:9:A:C5' | 1:D:46:G7M:H22 | 2.29 | 0.45 |
| 2:A:165:GLN:NE2 | 2:A:165:GLN:C | 2.67 | 0.45 |
| 2:A:206:MET:HE1 | 2:A:510:PHE:HD1 | 1.81 | 0.45 |
| 2:A:7:ALA:HB1 | 2:A:46:VAL:CG2 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:177:GLU:H | 2:A:507:LYS:HE3 | 1.81 | 0.45 |
| 2:A:558:LEU:HD11 | 2:B:206:MET:HE1 | 1.99 | 0.45 |
| 2:A:57:TYR:O | 2:A:61:GLU:HG3 | 2.16 | 0.45 |
| 2:B:163:PHE:HA | 2:B:214:ARG:O | 2.16 | 0.45 |
| 2:B:437:ALA:HB1 | 2:B:496:LEU:O | 2.16 | 0.45 |
| 2:A:112:ALA:HA | 2:A:115:ARG:CZ | 2.46 | 0.45 |
| 2:A:244:PHE:CD2 | 2:A:521:PRO:HD2 | 2.52 | 0.45 |
| 2:A:257:LEU:HD13 | 2:A:527:TRP:CH2 | 2.52 | 0.45 |
| 2:A:453:LEU:HD12 | 2:A:453:LEU:HA | 1.81 | 0.45 |
| 2:A:490:GLN:CG | 2:A:494:PHE:HE1 | 2.30 | 0.45 |
| 2:A:240:LEU:CD2 | 2:A:525:ILE:HG22 | 2.42 | 0.45 |
| 2:B:185:PRO:HG3 | 2:B:193:PHE:HE1 | 1.82 | 0.45 |
| 2:B:499:ILE:CD1 | 2:B:499:ILE:H | 2.26 | 0.45 |
| 1:C:11:U:H2' | 1:C:12:U:H6 | 1.81 | 0.45 |
| 1:C:35:U:O2 | 2:A:29:ARG:NE | 2.39 | 0.45 |
| 2:A:165:GLN:HA | 2:A:216:PHE:O | 2.17 | 0.45 |
| 2:A:214:ARG:HG2 | 2:A:214:ARG:H | 1.63 | 0.45 |
| 2:A:297:LEU:HB3 | 2:A:323:LEU:HD11 | 1.99 | 0.45 |
| 2:A:371:ARG:O | 2:A:375:LEU:HD23 | 2.17 | 0.45 |
| 2:B:335:ALA:O | 2:B:338:GLU:HB3 | 2.17 | 0.45 |
| 1:D:22:G:H2' | 1:D:23:A:C8 | 2.50 | 0.45 |
| 2:A:297:LEU:H | 2:A:404:ARG:NH1 | 2.15 | 0.45 |
| 2:B:371:ARG:O | 2:B:375:LEU:HB2 | 2.16 | 0.45 |
| 1:C:71:C:N4 | 1:C:72:C:N4 | 2.65 | 0.45 |
| 1:D:30:G:O2' | 1:D:31:C:H5' | 2.17 | 0.45 |
| 2:A:230:ASP:OD1 | 2:A:541:SER:HA | 2.17 | 0.44 |
| 2:A:246:GLU:O | 2:A:249:ASP:HB2 | 2.17 | 0.44 |
| 2:B:513:GLU:O | 2:B:516:GLU:HB2 | 2.17 | 0.44 |
| 1:D:38:C:OP2 | 2:B:29:ARG:HD3 | 2.17 | 0.44 |
| 2:A:192:LEU:HD23 | 2:B:563:SER:N | 2.32 | 0.44 |
| 2:A:351:TRP:HB3 | 2:A:387:LEU:HD12 | 1.99 | 0.44 |
| 2:A:8:GLY:HA3 | 2:A:44:GLY:N | 2.33 | 0.44 |
| 2:B:23:GLY:HA3 | 2:B:40:ARG:O | 2.16 | 0.44 |
| 2:B:321:LYS:HD3 | 2:B:321:LYS:HA | 1.69 | 0.44 |
| 2:B:371:ARG:O | 2:B:375:LEU:N | 2.40 | 0.44 |
| 2:B:480:GLY:HA3 | 2:B:525:ILE:HA | 1.99 | 0.44 |
| 2:B:561:ALA:CA | 2:B:562:PRO:O | 2.64 | 0.44 |
| 2:B:1:MET:H2 | 2:B:70:ARG:HD3 | 1.81 | 0.44 |
| 2:B:74:LEU:CD2 | 2:B:76:ARG:HE | 2.30 | 0.44 |
| 1:C:34:QUO:H101 | 1:C:34:QUO:O6 | 2.17 | 0.44 |
| 2:A:375:LEU:HD12 | 2:A:380:ALA:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:350:ALA:HB3 | 2:A:388:PHE:HB2 | 1.99 | 0.44 |
| 2:A:487:PRO:HG3 | 2:A:515:LEU:HB3 | 1.99 | 0.44 |
| 2:B:532:LEU:HD13 | 2:B:536:MET:SD | 2.57 | 0.44 |
| 2:B:551:ASN:O | 2:B:554:GLY:N | 2.50 | 0.44 |
| 1:C:3:A:O2' | 1:C:4:G:O4' | 2.28 | 0.44 |
| 2:A:52:PRO:HA | 2:A:57:TYR:CG | 2.52 | 0.44 |
| 2:B:509:GLY:O | 2:B:510:PHE:C | 2.56 | 0.44 |
| 2:A:193:PHE:N | 2:B:563:SER:O | 2.45 | 0.44 |
| 1:C:64:G:O2' | 1:C:65:PSU:H5'' | 2.17 | 0.44 |
| 2:A:20:VAL:HG13 | 2:A:72:LYS:HG2 | 1.99 | 0.44 |
| 2:A:504:GLN:HE21 | 2:A:504:GLN:HB2 | 1.68 | 0.44 |
| 2:A:82:ASN:C | 2:A:82:ASN:OD1 | 2.54 | 0.44 |
| 2:B:67:TRP:CZ3 | 2:B:102:GLU:HG2 | 2.52 | 0.44 |
| 1:C:61:C:H2' | 1:C:62:C:H6 | 1.83 | 0.44 |
| 2:B:306:PHE:CB | 2:B:314:PHE:HB3 | 2.47 | 0.44 |
| 2:B:287:GLY:HA3 | 2:B:397:ALA:O | 2.18 | 0.44 |
| 2:B:482:ILE:HA | 2:B:523:GLY:HA3 | 1.99 | 0.44 |
| 2:A:157:PHE:HD1 | 2:A:160:ARG:HH12 | 1.62 | 0.44 |
| 2:A:443:HIS:CD2 | 2:A:445:PHE:H | 2.35 | 0.44 |
| 2:B:261:VAL:C | 2:B:263:ARG:H | 2.19 | 0.44 |
| 2:B:536:MET:HE2 | 2:B:536:MET:HB3 | 1.66 | 0.44 |
| 2:A:140:MET:O | 2:A:141:GLN:C | 2.55 | 0.44 |
| 2:A:189:GLU:OE2 | 2:A:192:LEU:HD11 | 2.18 | 0.44 |
| 2:A:216:PHE:HA | 2:A:239:ASP:O | 2.16 | 0.44 |
| 2:A:451:GLU:C | 2:A:453:LEU:H | 2.21 | 0.44 |
| 2:A:508:PHE:HB2 | 2:A:512:LEU:HD21 | 1.98 | 0.44 |
| 2:B:337:LEU:HB3 | 2:B:349:LEU:CD2 | 2.48 | 0.44 |
| 2:B:495:ARG:O | 2:B:498:GLY:N | 2.50 | 0.44 |
| 2:A:20:VAL:O | 2:A:21:LEU:HD23 | 2.18 | 0.44 |
| 2:A:327:LYS:HG2 | 2:A:329:LEU:HD23 | 2.00 | 0.44 |
| 2:A:73:GLY:HA3 | 2:A:92:VAL:HG12 | 1.99 | 0.44 |
| 2:B:48:LEU:HB3 | 2:B:94:LEU:CD2 | 2.47 | 0.44 |
| 2:A:144:LEU:O | 2:A:147:ARG:HB3 | 2.17 | 0.43 |
| 2:A:490:GLN:HG3 | 2:A:494:PHE:HE1 | 1.82 | 0.43 |
| 2:B:127:ARG:NE | 2:B:137:ARG:NH2 | 2.65 | 0.43 |
| 2:B:313:VAL:CG1 | 2:B:314:PHE:N | 2.81 | 0.43 |
| 1:D:3:A:O2' | 1:D:4:G:H5' | 2.18 | 0.43 |
| 2:A:115:ARG:NH1 | 2:A:117:GLU:OE1 | 2.50 | 0.43 |
| 2:B:154:ILE:HD13 | 2:B:238:LEU:HD22 | 1.99 | 0.43 |
| 2:B:543:ARG:HH21 | 2:B:552:LYS:HG3 | 1.83 | 0.43 |
| 1:C:40:C:O2' | 1:C:41:A:H5' | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:110:VAL:HG13 | 2:B:110:VAL:O | 2.18 | 0.43 |
| 2:B:279:TYR:O | 2:B:283:MET:HB2 | 2.16 | 0.43 |
| 2:B:350:ALA:O | 2:B:388:PHE:HD1 | 2.01 | 0.43 |
| 2:B:361:GLY:N | 2:B:364:ALA:HB2 | 2.33 | 0.43 |
| 2:B:552:LYS:HE3 | 2:B:552:LYS:HB2 | 1.74 | 0.43 |
| 2:B:72:LYS:HB2 | 2:B:72:LYS:HE3 | 1.68 | 0.43 |
| 1:C:70:U:H2' | 1:C:71:C:C5 | 2.52 | 0.43 |
| 1:D:46:G7M:O2' | 1:D:47:U:H3' | 2.18 | 0.43 |
| 2:A:182:PHE:HB3 | 2:B:184:VAL:HG11 | 2.00 | 0.43 |
| 2:A:211:GLY:HA2 | 2:B:24:TRP:CH2 | 2.53 | 0.43 |
| 2:A:216:PHE:CD1 | 2:A:216:PHE:C | 2.92 | 0.43 |
| 2:A:308:GLN:HB3 | 2:A:308:GLN:HE21 | 1.54 | 0.43 |
| 2:A:12:GLU:CD | 2:A:89:ARG:HD3 | 2.39 | 0.43 |
| 2:B:361:GLY:H | 2:B:364:ALA:HB2 | 1.83 | 0.43 |
| 1:D:16:H2U:H3' | 1:D:17:C:C5' | 2.48 | 0.43 |
| 2:B:483:ARG:HB2 | 2:B:522:HIS:CE1 | 2.54 | 0.43 |
| 2:A:192:LEU:CD2 | 2:B:562:PRO:HG2 | 2.39 | 0.43 |
| 2:B:8:GLY:O | 2:B:11:ARG:NH2 | 2.52 | 0.43 |
| 1:C:2:G:H1 | 1:C:72:C:N4 | 2.16 | 0.43 |
| 2:A:543:ARG:HH22 | 2:A:552:LYS:HE3 | 1.83 | 0.43 |
| 2:B:117:GLU:O | 2:B:118:GLU:C | 2.57 | 0.43 |
| 2:B:540:PRO:HG2 | 2:B:541:SER:H | 1.83 | 0.43 |
| 1:C:26:A:C6 | 1:C:27:C:C4 | 3.07 | 0.43 |
| 2:A:148:HIS:C | 2:A:148:HIS:CD2 | 2.92 | 0.43 |
| 2:A:227:LEU:N | 2:A:227:LEU:HD22 | 2.30 | 0.43 |
| 2:A:579:ARG:HB3 | 2:A:580:PRO:HD3 | 2.00 | 0.43 |
| 2:A:71:ALA:HB1 | 2:A:94:LEU:HD21 | 2.01 | 0.43 |
| 2:B:76:ARG:CZ | 2:B:93:GLU:OE1 | 2.66 | 0.43 |
| 1:C:19:G:N2 | 1:C:57:G:H1' | 2.34 | 0.43 |
| 1:C:68:G:H2' | 1:C:69:U:C6 | 2.53 | 0.43 |
| 2:A:170:PHE:HD1 | 2:B:220:ARG:NH1 | 2.16 | 0.43 |
| 2:A:40:ARG:HG3 | 2:A:45:LEU:HD23 | 2.00 | 0.43 |
| 2:A:71:ALA:HB2 | 2:A:97:LEU:CD1 | 2.49 | 0.43 |
| 2:A:6:TYR:HE2 | 2:B:213:ASP:OD1 | 2.00 | 0.43 |
| 2:B:443:HIS:C | 2:B:445:PHE:N | 2.72 | 0.43 |
| 2:B:556:ASP:OD2 | 2:B:559:THR:N | 2.51 | 0.43 |
| 2:A:202:LEU:HD23 | 2:A:202:LEU:HA | 1.67 | 0.43 |
| 2:A:266:LEU:HB3 | 2:A:268:VAL:HG23 | 1.99 | 0.43 |
| 2:A:349:LEU:HD22 | 2:A:349:LEU:C | 2.39 | 0.43 |
| 2:A:368:GLU:N | 2:A:369:PRO:HD2 | 2.33 | 0.43 |
| 2:A:494:PHE:CD2 | 2:A:499:ILE:HG21 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:152:LYS:HD3 | 2:B:155:TRP:CE3 | 2.54 | 0.43 |
| 2:B:381:ARG:O | 2:B:384:ASP:OD2 | 2.37 | 0.43 |
| 2:B:278:SER:HA | 2:B:424:VAL:O | 2.19 | 0.43 |
| 1:C:20(A):H2U:C3' | 1:C:21:A:C5' | 2.97 | 0.43 |
| 1:C:8:4SU:HO2' | 1:C:21:A:H2 | 1.63 | 0.43 |
| 2:A:343:ARG:HA | 2:A:343:ARG:NE | 2.33 | 0.43 |
| 2:A:407:ALA:O | 2:A:411:LEU:HB2 | 2.18 | 0.43 |
| 2:A:529:LEU:HA | 2:A:529:LEU:HD12 | 1.90 | 0.43 |
| 2:B:409:ASP:C | 2:B:411:LEU:N | 2.72 | 0.43 |
| 2:B:443:HIS:C | 2:B:445:PHE:H | 2.22 | 0.43 |
| 2:B:528:GLY:O | 2:B:529:LEU:C | 2.57 | 0.43 |
| 2:B:543:ARG:HG2 | 2:B:549:PRO:HB2 | 2.00 | 0.43 |
| 2:A:351:TRP:O | 2:A:363:VAL:HG12 | 2.18 | 0.42 |
| 2:A:426:PHE:CD2 | 2:A:441:MET:CE | 3.02 | 0.42 |
| 2:A:443:HIS:HD2 | 2:A:445:PHE:H | 1.67 | 0.42 |
| 2:B:294:ARG:NH1 | 2:B:294:ARG:HG2 | 2.34 | 0.42 |
| 2:B:570:LEU:HD22 | 2:B:575:LEU:HB2 | 2.01 | 0.42 |
| 1:C:30:G:C6 | 1:C:31:C:C4 | 3.06 | 0.42 |
| 2:A:42:ARG:NE | 2:A:145:ARG:HH21 | 2.17 | 0.42 |
| 2:A:299:LEU:HD23 | 2:A:299:LEU:N | 2.33 | 0.42 |
| 2:A:242:MET:O | 2:A:522:HIS:HB2 | 2.19 | 0.42 |
| 2:B:330:SER:H | 2:B:333:GLU:HB2 | 1.84 | 0.42 |
| 1:D:34:QUO:H14 | 2:B:51:HIS:ND1 | 2.34 | 0.42 |
| 2:A:443:HIS:CG | 2:A:444:PRO:CD | 2.99 | 0.42 |
| 2:A:486:ASP:OD1 | 2:A:486:ASP:C | 2.57 | 0.42 |
| 2:A:74:LEU:N | 2:A:92:VAL:HG12 | 2.34 | 0.42 |
| 2:B:25:VAL:HG21 | 2:B:63:VAL:HG22 | 2.02 | 0.42 |
| 2:A:225:GLU:O | 2:A:226:ASP:C | 2.57 | 0.42 |
| 2:A:241:GLU:OE1 | 2:A:524:GLY:HA3 | 2.19 | 0.42 |
| 2:A:571:ARG:O | 2:A:574:GLY:N | 2.42 | 0.42 |
| 2:A:97:LEU:HD12 | 2:A:97:LEU:HA | 1.88 | 0.42 |
| 2:B:107:PRO:HD2 | 2:B:133:LEU:HD13 | 2.00 | 0.42 |
| 2:B:163:PHE:CE1 | 2:B:253:LEU:HD11 | 2.54 | 0.42 |
| 2:B:201:GLN:HA | 2:B:204:LYS:HD3 | 2.01 | 0.42 |
| 2:B:240:LEU:HD23 | 2:B:240:LEU:C | 2.39 | 0.42 |
| 2:B:410:LEU:O | 2:B:411:LEU:HD23 | 2.19 | 0.42 |
| 2:B:512:LEU:HA | 2:B:512:LEU:HD12 | 1.76 | 0.42 |
| 1:C:14:A:C2 | 1:C:22:G:C4 | 3.08 | 0.42 |
| 1:D:18:G:N2 | 1:D:57:G:H2' | 2.35 | 0.42 |
| 1:D:71:C:C2' | 1:D:72:C:H5' | 2.49 | 0.42 |
| 2:B:483:ARG:HE | 2:B:523:GLY:HA2 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:63:C:O2' | 1:C:64:G:H5' | 2.20 | 0.42 |
| 1:C:71:C:C4 | 1:C:72:C:N4 | 2.87 | 0.42 |
| 2:A:190:PRO:HB3 | 2:B:577:VAL:HG12 | 2.02 | 0.42 |
| 2:A:292:ASP:CG | 2:A:294:ARG:HH11 | 2.22 | 0.42 |
| 2:A:432:ASP:O | 2:A:433:GLU:OE2 | 2.37 | 0.42 |
| 2:A:452:ASP:HB3 | 2:A:463:VAL:HG13 | 2.02 | 0.42 |
| 2:A:570:LEU:O | 2:A:573:LEU:HB2 | 2.19 | 0.42 |
| 2:B:70:ARG:NH2 | 2:B:100:LEU:HD22 | 2.33 | 0.42 |
| 2:B:235:PHE:HE2 | 2:B:237:GLN:HE21 | 1.66 | 0.42 |
| 2:B:294:ARG:HG2 | 2:B:294:ARG:HH11 | 1.83 | 0.42 |
| 2:B:453:LEU:N | 2:B:454:PRO:HD2 | 2.35 | 0.42 |
| 2:B:579:ARG:HA | 2:B:580:PRO:HD3 | 1.88 | 0.42 |
| 2:A:226:ASP:CG | 2:A:228:ARG:HG2 | 2.40 | 0.42 |
| 2:A:283:MET:O | 2:A:287:GLY:CA | 2.67 | 0.42 |
| 2:A:8:GLY:HA3 | 2:A:44:GLY:CA | 2.49 | 0.42 |
| 2:B:232:GLN:HG2 | 2:B:542:ILE:HD11 | 2.01 | 0.42 |
| 2:B:59:THR:C | 2:B:61:GLU:N | 2.73 | 0.42 |
| 1:C:2:G:O2' | 1:C:3:A:O4' | 2.34 | 0.42 |
| 1:D:20:H2U:O2' | 1:D:20(A):H2U:OP1 | 2.34 | 0.42 |
| 1:D:52:G:C2 | 1:D:53:G:H1' | 2.54 | 0.42 |
| 1:D:70:U:C2 | 1:D:71:C:C5 | 3.07 | 0.42 |
| 2:A:153:ALA:HB1 | 2:A:260:HIS:CD2 | 2.55 | 0.42 |
| 2:A:548:PHE:HB2 | 2:B:169:PRO:HG3 | 2.02 | 0.42 |
| 1:C:22:G:C2 | 1:C:23:A:C5 | 3.07 | 0.42 |
| 1:C:29:U:O2' | 1:C:30:G:H5' | 2.20 | 0.42 |
| 1:C:4:G:C2 | 1:C:70:U:O2 | 2.72 | 0.42 |
| 1:D:31:C:O2' | 1:D:32:C:H5' | 2.19 | 0.42 |
| 2:A:192:LEU:HD23 | 2:B:562:PRO:C | 2.39 | 0.42 |
| 2:A:486:ASP:HA | 2:A:487:PRO:HD3 | 1.86 | 0.42 |
| 1:D:25:U:H2' | 1:D:26:A:C8 | 2.55 | 0.42 |
| 2:A:20:VAL:C | 2:A:21:LEU:HD23 | 2.40 | 0.42 |
| 2:A:246:GLU:O | 2:A:249:ASP:N | 2.52 | 0.42 |
| 2:A:405:LEU:HA | 2:A:405:LEU:HD23 | 1.70 | 0.42 |
| 2:A:183:LEU:HD12 | 2:B:573:LEU:HD11 | 2.01 | 0.42 |
| 1:C:39:G:H2' | 1:C:40:C:C6 | 2.55 | 0.42 |
| 1:D:37:2MA:H4' | 2:B:27:ARG:NH1 | 2.34 | 0.42 |
| 1:D:48:C:O2' | 1:D:49:G:P | 2.77 | 0.42 |
| 1:D:57:G:H2' | 1:D:58:A:H5' | 2.01 | 0.42 |
| 2:A:342:LYS:O | 2:A:344:HIS:O | 2.37 | 0.41 |
| 2:A:326:PRO:HG2 | 2:A:411:LEU:CD2 | 2.49 | 0.41 |
| 1:C:33:U:O2 | 1:C:34:QUO:H14 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:38:C:C2' | 1:D:39:G:H5' | 2.50 | 0.41 |
| 1:D:53:G:C5 | 1:D:54:5MU:C5 | 3.07 | 0.41 |
| 2:A:447:SER:CA | 2:A:484:ILE:HD13 | 2.46 | 0.41 |
| 2:B:182:PHE:HB3 | 2:B:196:LEU:HD12 | 2.01 | 0.41 |
| 2:B:189:GLU:HB3 | 2:B:192:LEU:HD22 | 2.01 | 0.41 |
| 2:B:414:LYS:HD2 | 2:B:414:LYS:HA | 1.80 | 0.41 |
| 2:B:513:GLU:HG3 | 3:B:2071:HOH:O | 2.17 | 0.41 |
| 2:B:77:LEU:HA | 2:B:90:VAL:HG12 | 2.01 | 0.41 |
| 2:A:263:ARG:HA | 2:A:268:VAL:O | 2.19 | 0.41 |
| 2:A:452:ASP:OD2 | 2:A:464:ARG:CD | 2.69 | 0.41 |
| 2:B:149:ARG:HD2 | 2:B:265:ALA:HA | 2.02 | 0.41 |
| 2:B:302:VAL:O | 2:B:304:PRO:N | 2.53 | 0.41 |
| 1:C:3:A:C2' | 1:C:4:G:O4' | 2.68 | 0.41 |
| 2:A:160:ARG:NH2 | 2:A:161:GLU:OE2 | 2.53 | 0.41 |
| 2:A:28:ARG:HA | 2:A:37:LEU:HD23 | 2.01 | 0.41 |
| 2:A:326:PRO:O | 2:A:327:LYS:HB2 | 2.20 | 0.41 |
| 2:A:512:LEU:O | 2:A:515:LEU:HB2 | 2.19 | 0.41 |
| 2:B:66:GLU:O | 2:B:103:ALA:HB2 | 2.20 | 0.41 |
| 2:B:424:VAL:O | 2:B:425:ASP:HB2 | 2.21 | 0.41 |
| 2:A:541:SER:OG | 2:A:543:ARG:HG3 | 2.20 | 0.41 |
| 1:D:6:G:C2' | 1:D:7:G:H5' | 2.51 | 0.41 |
| 2:A:172:THR:CG2 | 2:A:173:LYS:H | 2.25 | 0.41 |
| 2:A:485:HIS:O | 2:A:515:LEU:HD23 | 2.20 | 0.41 |
| 2:B:110:VAL:CG1 | 2:B:110:VAL:O | 2.68 | 0.41 |
| 2:B:252:GLU:OE1 | 2:B:256:ARG:HD3 | 2.20 | 0.41 |
| 2:B:430:GLU:O | 2:B:438:TRP:CD1 | 2.73 | 0.41 |
| 2:B:537:THR:CG2 | 2:B:539:SER:OG | 2.61 | 0.41 |
| 2:B:68:VAL:HG12 | 2:B:100:LEU:HD12 | 2.01 | 0.41 |
| 2:B:73:GLY:HA3 | 2:B:92:VAL:HG12 | 2.02 | 0.41 |
| 1:C:67:C:O2' | 1:C:68:G:H5' | 2.19 | 0.41 |
| 2:B:163:PHE:HA | 2:B:214:ARG:HG3 | 2.02 | 0.41 |
| 2:B:333:GLU:C | 2:B:335:ALA:N | 2.73 | 0.41 |
| 2:B:421:LEU:HB3 | 2:B:471:VAL:HG22 | 2.02 | 0.41 |
| 1:C:34:QUO:H13 | 2:A:51:HIS:ND1 | 2.36 | 0.41 |
| 2:A:512:LEU:HA | 2:A:515:LEU:HD12 | 2.02 | 0.41 |
| 2:B:522:HIS:ND1 | 2:B:522:HIS:N | 2.68 | 0.41 |
| 1:C:24:A:C6 | 1:C:25:U:N3 | 2.89 | 0.41 |
| 2:A:299:LEU:HD13 | 2:A:400:LEU:HB3 | 2.02 | 0.41 |
| 2:A:578:VAL:HG11 | 2:B:576:MET:HB3 | 2.03 | 0.41 |
| 2:A:504:GLN:HB3 | 2:A:505:ARG:HH11 | 1.86 | 0.41 |
| 2:B:440:TYR:CD2 | 2:B:440:TYR:N | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:31:C:H2' | 1:D:32:C:O4' | 2.21 | 0.41 |
| 1:D:2:G:N1 | 1:D:3:A:C6 | 2.89 | 0.41 |
| 1:D:70:U:OP2 | 1:D:70:U:C5 | 2.74 | 0.41 |
| 2:A:134:ASP:O | 2:A:137:ARG:HG3 | 2.21 | 0.41 |
| 2:A:371:ARG:O | 2:A:375:LEU:CD2 | 2.68 | 0.41 |
| 2:A:39:LEU:HD22 | 2:A:40:ARG:N | 2.36 | 0.41 |
| 2:A:48:LEU:HB3 | 2:A:94:LEU:HD11 | 2.03 | 0.41 |
| 2:A:206:MET:CE | 2:A:510:PHE:HD1 | 2.34 | 0.41 |
| 2:A:579:ARG:CB | 2:A:580:PRO:CD | 2.97 | 0.41 |
| 2:B:27:ARG:HD2 | 2:B:115:ARG:NE | 2.28 | 0.41 |
| 2:B:330:SER:O | 2:B:334:VAL:HG23 | 2.20 | 0.41 |
| 2:B:409:ASP:C | 2:B:411:LEU:H | 2.23 | 0.41 |
| 2:B:42:ARG:HD3 | 2:B:145:ARG:HH21 | 1.86 | 0.41 |
| 1:D:47:U:C1' | 1:D:48:C:OP1 | 2.69 | 0.41 |
| 1:D:49:G:N3 | 1:D:50:C:C6 | 2.89 | 0.41 |
| 2:A:363:VAL:O | 2:A:363:VAL:HG22 | 2.21 | 0.40 |
| 2:A:206:MET:HE1 | 2:A:510:PHE:CD1 | 2.56 | 0.40 |
| 2:A:517:TYR:HE2 | 2:B:107:PRO:HD3 | 1.85 | 0.40 |
| 2:B:208:MET:HG3 | 2:B:522:HIS:CB | 2.51 | 0.40 |
| 2:B:154:ILE:HG21 | 2:B:238:LEU:HD13 | 2.03 | 0.40 |
| 2:A:118:GLU:HG3 | 2:A:118:GLU:O | 2.22 | 0.40 |
| 2:A:77:LEU:HD23 | 2:A:78:ARG:N | 2.37 | 0.40 |
| 2:B:237:GLN:HB3 | 2:B:527:TRP:O | 2.22 | 0.40 |
| 2:B:392:PRO:HB2 | 2:B:395:VAL:CG2 | 2.51 | 0.40 |
| 2:B:440:TYR:CD1 | 2:B:442:HIS:O | 2.70 | 0.40 |
| 1:C:51:G:H2' | 1:C:52:G:O4' | 2.21 | 0.40 |
| 1:C:52:G:H1 | 1:C:62:C:H42 | 1.68 | 0.40 |
| 1:D:22:G:H2' | 1:D:23:A:H8 | 1.85 | 0.40 |
| 1:D:56:C:H6 | 1:D:56:C:O5' | 2.04 | 0.40 |
| 2:A:414:LYS:HD3 | 2:A:414:LYS:HA | 1.99 | 0.40 |
| 2:A:429:LEU:HD13 | 2:A:438:TRP:CB | 2.46 | 0.40 |
| 2:A:422:TRP:CZ3 | 2:A:470:LEU:HB2 | 2.56 | 0.40 |
| 2:A:486:ASP:OD1 | 2:A:488:ARG:N | 2.55 | 0.40 |
| 2:B:118:GLU:HG2 | 2:B:119:GLU:N | 2.35 | 0.40 |
| 2:B:395:VAL:O | 2:B:396:ALA:C | 2.57 | 0.40 |
| 2:B:78:ARG:HA | 2:B:79:PRO:HD3 | 1.88 | 0.40 |
| 1:C:51:G:C4 | 1:C:64:G:N2 | 2.89 | 0.40 |
| 1:D:5:C:O5' | 1:D:5:C:H6 | 2.04 | 0.40 |
| 1:D:69:U:H2' | 1:D:70:U:C5 | 2.55 | 0.40 |
| 2:A:386:LEU:HA | 2:A:386:LEU:HD23 | 1.98 | 0.40 |
| 2:A:287:GLY:HA3 | 2:A:397:ALA:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:C:6:G:C2 | 1:C:7:G:C4 | 3.09 | 0.40 |
| 2:A:168:THR:CG2 | 2:A:169:PRO:N | 2.85 | 0.40 |
| 2:A:27:ARG:HB2 | 3:A:2026:HOH:O | 2.22 | 0.40 |
| 2:A:175:THR:HB | 2:A:507:LYS:NZ | 2.37 | 0.40 |
| 2:B:467:ALA:HA | 2:B:481:SER:CB | 2.52 | 0.40 |
| 2:B:501:GLU:O | 2:B:504:GLN:N | 2.53 | 0.40 |
| 1:C:48:C:C4' | 1:C:49:G:OP2 | 2.68 | 0.40 |
| 1:D:28:C:H2' | 1:D:29:U:C6 | 2.54 | 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 | A | 578/580 (100%) | 499 (86%) | 64 (11%) | 15 (3%) | 5 | 27 |
| 2 | B | 578/580 (100%) | 459 (79%) | 93 (16%) | 26 (4%) | 2 | 14 |
| All | All | 1156/1160 (100%) | 958 (83%) | 157 (14%) | 41 (4%) | 3 | 20 |

All (41) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 188 | HIS |
| 2 | A | 462 | ARG |
| 2 | A | 579 | ARG |
| 2 | B | 42 | ARG |
| 2 | B | 227 | LEU |
| 2 | B | 312 | ARG |
| 2 | B | 345 | LYS |
| 2 | B | 362 | GLY |
| 2 | B | 435 | GLU |
| 2 | B | 501 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 552 | LYS |
| 2 | A | 42 | ARG |
| 2 | A | 131 | ARG |
| 2 | A | 434 | GLU |
| 2 | A | 452 | ASP |
| 2 | A | 509 | GLY |
| 2 | B | 370 | VAL |
| 2 | B | 377 | ALA |
| 2 | B | 433 | GLU |
| 2 | B | 437 | ALA |
| 2 | B | 509 | GLY |
| 2 | B | 567 | GLU |
| 2 | A | 362 | GLY |
| 2 | A | 413 | LEU |
| 2 | B | 60 | ALA |
| 2 | B | 94 | LEU |
| 2 | B | 303 | GLY |
| 2 | B | 336 | GLU |
| 2 | B | 438 | TRP |
| 2 | A | 229 | ALA |
| 2 | A | 502 | GLU |
| 2 | B | 299 | LEU |
| 2 | B | 314 | PHE |
| 2 | B | 337 | LEU |
| 2 | B | 396 | ALA |
| 2 | B | 525 | ILE |
| 2 | A | 226 | ASP |
| 2 | A | 255 | GLU |
| 2 | B | 122 | ALA |
| 2 | B | 291 | PRO |
| 2 | A | 247 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 2 | A | 483/483 (100%) | 410 (85%) | 73 (15%) | 3 | 14 |
| 2 | B | 483/483 (100%) | 414 (86%) | 69 (14%) | 3 | 15 |
| All | All | 966/966 (100%) | 824 (85%) | 142 (15%) | 3 | 15 |

All (142) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 2 | ARG |
| 2 | A | 4 | THR |
| 2 | A | 10 | LEU |
| 2 | A | 11 | ARG |
| 2 | A | 28 | ARG |
| 2 | A | 39 | LEU |
| 2 | A | 42 | ARG |
| 2 | A | 46 | VAL |
| 2 | A | 49 | VAL |
| 2 | A | 65 | PRO |
| 2 | A | 66 | GLU |
| 2 | A | 92 | VAL |
| 2 | A | 119 | GLU |
| 2 | A | 120 | LYS |
| 2 | A | 124 | GLU |
| 2 | A | 125 | GLU |
| 2 | A | 126 | LEU |
| 2 | A | 139 | ARG |
| 2 | A | 165 | GLN |
| 2 | A | 168 | THR |
| 2 | A | 172 | THR |
| 2 | A | 177 | GLU |
| 2 | A | 181 | ASP |
| 2 | A | 190 | PRO |
| 2 | A | 192 | LEU |
| 2 | A | 199 | SER |
| 2 | A | 201 | GLN |
| 2 | A | 207 | LEU |
| 2 | A | 214 | ARG |
| 2 | A | 215 | TYR |
| 2 | A | 216 | PHE |
| 2 | A | 217 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 227 | LEU |
| 2 | A | 228 | ARG |
| 2 | A | 234 | ASP |
| 2 | A | 240 | LEU |
| 2 | A | 253 | LEU |
| 2 | A | 257 | LEU |
| 2 | A | 272 | LEU |
| 2 | A | 276 | ARG |
| 2 | A | 302 | VAL |
| 2 | A | 307 | ARG |
| 2 | A | 331 | ARG |
| 2 | A | 339 | GLU |
| 2 | A | 343 | ARG |
| 2 | A | 349 | LEU |
| 2 | A | 372 | GLU |
| 2 | A | 387 | LEU |
| 2 | A | 393 | ARG |
| 2 | A | 400 | LEU |
| 2 | A | 411 | LEU |
| 2 | A | 431 | TRP |
| 2 | A | 434 | GLU |
| 2 | A | 435 | GLU |
| 2 | A | 436 | GLU |
| 2 | A | 438 | TRP |
| 2 | A | 440 | TYR |
| 2 | A | 453 | LEU |
| 2 | A | 464 | ARG |
| 2 | A | 485 | HIS |
| 2 | A | 489 | LEU |
| 2 | A | 492 | ARG |
| 2 | A | 505 | ARG |
| 2 | A | 506 | GLU |
| 2 | A | 507 | LYS |
| 2 | A | 515 | LEU |
| 2 | A | 516 | GLU |
| 2 | A | 537 | THR |
| 2 | A | 559 | THR |
| 2 | A | 565 | VAL |
| 2 | A | 568 | GLU |
| 2 | A | 570 | LEU |
| 2 | A | 579 | ARG |
| 2 | B | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 2 | ARG |
| 2 | B | 11 | ARG |
| 2 | B | 13 | THR |
| 2 | B | 27 | ARG |
| 2 | B | 28 | ARG |
| 2 | B | 39 | LEU |
| 2 | B | 42 | ARG |
| 2 | B | 48 | LEU |
| 2 | B | 54 | SER |
| 2 | B | 80 | GLU |
| 2 | B | 89 | ARG |
| 2 | B | 107 | PRO |
| 2 | B | 115 | ARG |
| 2 | B | 120 | LYS |
| 2 | B | 124 | GLU |
| 2 | B | 126 | LEU |
| 2 | B | 128 | LEU |
| 2 | B | 131 | ARG |
| 2 | B | 142 | GLU |
| 2 | B | 145 | ARG |
| 2 | B | 168 | THR |
| 2 | B | 177 | GLU |
| 2 | B | 214 | ARG |
| 2 | B | 215 | TYR |
| 2 | B | 227 | LEU |
| 2 | B | 228 | ARG |
| 2 | B | 235 | PHE |
| 2 | B | 240 | LEU |
| 2 | B | 257 | LEU |
| 2 | B | 272 | LEU |
| 2 | B | 277 | LEU |
| 2 | B | 285 | ARG |
| 2 | B | 288 | SER |
| 2 | B | 290 | LYS |
| 2 | B | 294 | ARG |
| 2 | B | 299 | LEU |
| 2 | B | 307 | ARG |
| 2 | B | 311 | PHE |
| 2 | B | 326 | PRO |
| 2 | B | 331 | ARG |
| 2 | B | 339 | GLU |
| 2 | B | 340 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 342 | LYS |
| 2 | B | 343 | ARG |
| 2 | B | 345 | LYS |
| 2 | B | 360 | SER |
| 2 | B | 363 | VAL |
| 2 | B | 368 | GLU |
| 2 | B | 370 | VAL |
| 2 | B | 375 | LEU |
| 2 | B | 394 | LYS |
| 2 | B | 400 | LEU |
| 2 | B | 432 | ASP |
| 2 | B | 436 | GLU |
| 2 | B | 447 | SER |
| 2 | B | 451 | GLU |
| 2 | B | 459 | ASP |
| 2 | B | 462 | ARG |
| 2 | B | 489 | LEU |
| 2 | B | 492 | ARG |
| 2 | B | 501 | GLU |
| 2 | B | 516 | GLU |
| 2 | B | 522 | HIS |
| 2 | B | 559 | THR |
| 2 | B | 571 | ARG |
| 2 | B | 577 | VAL |
| 2 | B | 579 | ARG |
| 2 | B | 580 | PRO |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 143 | ASN |
| 2 | A | 165 | GLN |
| 2 | A | 198 | GLN |
| 2 | A | 205 | GLN |
| 2 | A | 217 | GLN |
| 2 | A | 254 | ASN |
| 2 | A | 308 | GLN |
| 2 | A | 443 | HIS |
| 2 | A | 504 | GLN |
| 2 | B | 143 | ASN |
| 2 | B | 237 | GLN |
| 2 | B | 260 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 315 | GLN |
| 2 | B | 443 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1 | C | 70/73 (95%) | 9 (12%) | 3 (4%) |
| 1 | D | 70/73 (95%) | 13 (18%) | 3 (4%) |
| All | All | 140/146 (95%) | 22 (15%) | 6 (4%) |

All (22) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 1 | C | 9 | A |
| 1 | C | 16 | H2U |
| 1 | C | 17 | C |
| 1 | C | 18 | G |
| 1 | C | 20 | H2U |
| 1 | C | 38 | C |
| 1 | C | 48 | C |
| 1 | C | 49 | G |
| 1 | C | 55 | PSU |
| 1 | D | 9 | A |
| 1 | D | 13 | C |
| 1 | D | 16 | H2U |
| 1 | D | 17 | C |
| 1 | D | 18 | G |
| 1 | D | 20 | H2U |
| 1 | D | 20(A) | H2U |
| 1 | D | 22 | G |
| 1 | D | 38 | C |
| 1 | D | 47 | U |
| 1 | D | 48 | C |
| 1 | D | 49 | G |
| 1 | D | 71 | C |

All (6) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 17 | C |
| 1 | C | 47 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 48 | C |
| 1 | D | 17 | C |
| 1 | D | 47 | U |
| 1 | D | 48 | C |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-------|------|--------------|------|----------|-------------|-------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | H2U | C | 20(A) | 1 | 18,21,22 | 0.53 | 0 | 21,30,33 | 0.79 | 0 |
| 1 | 4SU | D | 8 | 1 | 14,21,22 | 6.17 | 2 (14%) | 15,30,33 | 2.84 | 2 (13%) |
| 1 | H2U | C | 20 | 1 | 18,21,22 | 0.90 | 1 (5%) | 21,30,33 | 0.71 | 0 |
| 1 | QUO | C | 34 | 1 | 28,35,36 | 1.36 | 5 (17%) | 32,52,55 | 4.03 | 12 (37%) |
| 1 | 5MU | D | 54 | 1 | 15,22,23 | 1.92 | 4 (26%) | 16,32,35 | 11.08 | 4 (25%) |
| 1 | G7M | D | 46 | 1 | 20,26,27 | 1.19 | 2 (10%) | 20,39,42 | 2.72 | 6 (30%) |
| 1 | PSU | C | 65 | 1 | 17,21,22 | 2.25 | 4 (23%) | 20,30,33 | 5.77 | 5 (25%) |
| 1 | PSU | D | 65 | 1 | 17,21,22 | 1.94 | 4 (23%) | 20,30,33 | 5.68 | 5 (25%) |
| 1 | G7M | C | 46 | 1 | 20,26,27 | 1.22 | 2 (10%) | 20,39,42 | 2.62 | 5 (25%) |
| 1 | QUO | D | 34 | 1 | 28,35,36 | 1.22 | 3 (10%) | 32,52,55 | 3.94 | 12 (37%) |
| 1 | H2U | D | 16 | 1 | 18,21,22 | 0.66 | 1 (5%) | 21,30,33 | 0.81 | 0 |
| 1 | 5MU | C | 54 | 1 | 15,22,23 | 1.17 | 2 (13%) | 16,32,35 | 3.69 | 2 (12%) |
| 1 | 2MA | C | 37 | 1 | 17,25,26 | 0.75 | 1 (5%) | 19,37,40 | 2.01 | 2 (10%) |
| 1 | PSU | D | 55 | 1 | 17,21,22 | 1.94 | 4 (23%) | 20,30,33 | 5.76 | 5 (25%) |
| 1 | H2U | C | 16 | 1 | 18,21,22 | 0.93 | 1 (5%) | 21,30,33 | 0.82 | 1 (4%) |
| 1 | H2U | D | 20(A) | 1 | 18,21,22 | 0.81 | 1 (5%) | 21,30,33 | 0.82 | 0 |
| 1 | H2U | D | 20 | 1 | 18,21,22 | 0.70 | 1 (5%) | 21,30,33 | 0.83 | 1 (4%) |
| 1 | 4SU | C | 8 | 1 | 14,21,22 | 6.10 | 2 (14%) | 15,30,33 | 2.86 | 2 (13%) |
| 1 | PSU | C | 55 | 1 | 17,21,22 | 1.99 | 4 (23%) | 20,30,33 | 5.80 | 5 (25%) |
| 1 | 2MA | D | 37 | 1 | 17,25,26 | 0.64 | 0 | 19,37,40 | 2.04 | 2 (10%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-------|------|---------|-----------|---------|
| 1 | H2U | C | 20(A) | 1 | - | 1/7/38/39 | 0/2/2/2 |
| 1 | 4SU | D | 8 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | H2U | C | 20 | 1 | - | 0/7/38/39 | 0/2/2/2 |
| 1 | QUO | C | 34 | 1 | - | 2/6/43/44 | 0/4/4/4 |
| 1 | 5MU | D | 54 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | G7M | D | 46 | 1 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | PSU | C | 65 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | D | 65 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | G7M | C | 46 | 1 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | QUO | D | 34 | 1 | - | 1/6/43/44 | 0/4/4/4 |
| 1 | H2U | D | 16 | 1 | - | 2/7/38/39 | 0/2/2/2 |
| 1 | 5MU | C | 54 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 2MA | C | 37 | 1 | - | 1/3/25/26 | 0/3/3/3 |
| 1 | PSU | D | 55 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | H2U | C | 16 | 1 | - | 2/7/38/39 | 0/2/2/2 |
| 1 | H2U | D | 20(A) | 1 | - | 3/7/38/39 | 0/2/2/2 |
| 1 | H2U | D | 20 | 1 | - | 7/7/38/39 | 0/2/2/2 |
| 1 | 4SU | C | 8 | 1 | - | 1/5/25/26 | 0/2/2/2 |
| 1 | PSU | C | 55 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | D | 37 | 1 | - | 1/3/25/26 | 0/3/3/3 |

All (44) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | D | 8 | 4SU | C4-S4 | -22.45 | 1.26 | 1.67 |
| 1 | C | 8 | 4SU | C4-S4 | -22.17 | 1.26 | 1.67 |
| 1 | C | 65 | PSU | C5-C1' | -6.42 | 1.46 | 1.52 |
| 1 | C | 55 | PSU | C5-C1' | -5.07 | 1.47 | 1.52 |
| 1 | C | 65 | PSU | C6-N1 | -4.96 | 1.23 | 1.34 |
| 1 | D | 65 | PSU | C6-N1 | -4.85 | 1.24 | 1.34 |
| 1 | C | 55 | PSU | C6-N1 | -4.73 | 1.24 | 1.34 |
| 1 | D | 55 | PSU | C6-N1 | -4.66 | 1.24 | 1.34 |
| 1 | D | 65 | PSU | C5-C1' | -4.65 | 1.48 | 1.52 |
| 1 | D | 55 | PSU | C5-C1' | -4.60 | 1.48 | 1.52 |
| 1 | D | 54 | 5MU | C4-N3 | 4.44 | 1.40 | 1.33 |
| 1 | D | 8 | 4SU | C5-C4 | 4.36 | 1.43 | 1.38 |
| 1 | C | 8 | 4SU | C5-C4 | 4.31 | 1.43 | 1.38 |
| 1 | C | 34 | QUO | C6-N1 | 4.23 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 1 | D | 34 | QUO | C6-N1 | 4.05 | 1.40 | 1.33 |
| 1 | C | 46 | G7M | C6-N1 | 3.99 | 1.40 | 1.33 |
| 1 | D | 46 | G7M | C6-N1 | 3.78 | 1.39 | 1.33 |
| 1 | C | 34 | QUO | C7-C5 | -3.65 | 1.35 | 1.41 |
| 1 | D | 54 | 5MU | C2-N3 | 3.48 | 1.45 | 1.38 |
| 1 | C | 54 | 5MU | C4-N3 | 3.21 | 1.38 | 1.33 |
| 1 | C | 16 | H2U | C2-N1 | 3.17 | 1.40 | 1.35 |
| 1 | C | 20 | H2U | C2-N1 | 3.15 | 1.40 | 1.35 |
| 1 | D | 54 | 5MU | C6-C5 | -2.96 | 1.31 | 1.40 |
| 1 | C | 65 | PSU | C6-C5 | -2.92 | 1.34 | 1.38 |
| 1 | D | 34 | QUO | C7-C5 | -2.84 | 1.36 | 1.41 |
| 1 | C | 55 | PSU | C6-C5 | -2.78 | 1.34 | 1.38 |
| 1 | D | 20(A) | H2U | C2-N1 | 2.77 | 1.39 | 1.35 |
| 1 | D | 55 | PSU | C6-C5 | -2.71 | 1.34 | 1.38 |
| 1 | D | 46 | G7M | C8-N9 | 2.67 | 1.38 | 1.33 |
| 1 | C | 46 | G7M | C8-N9 | 2.62 | 1.38 | 1.33 |
| 1 | D | 55 | PSU | C4-N3 | 2.59 | 1.37 | 1.33 |
| 1 | D | 65 | PSU | C6-C5 | -2.57 | 1.34 | 1.38 |
| 1 | D | 65 | PSU | C4-N3 | 2.47 | 1.37 | 1.33 |
| 1 | D | 20 | H2U | C2-N1 | 2.36 | 1.39 | 1.35 |
| 1 | C | 65 | PSU | C4-N3 | 2.32 | 1.37 | 1.33 |
| 1 | C | 55 | PSU | C4-N3 | 2.30 | 1.37 | 1.33 |
| 1 | C | 34 | QUO | C5-C4 | -2.20 | 1.37 | 1.43 |
| 1 | D | 34 | QUO | C5-C4 | -2.19 | 1.37 | 1.43 |
| 1 | D | 54 | 5MU | C2'-C1' | -2.18 | 1.50 | 1.53 |
| 1 | C | 34 | QUO | C2-N1 | 2.18 | 1.39 | 1.35 |
| 1 | C | 54 | 5MU | C6-C5 | -2.09 | 1.34 | 1.40 |
| 1 | C | 37 | 2MA | CM2-C2 | -2.08 | 1.43 | 1.49 |
| 1 | D | 16 | H2U | C2-N1 | 2.01 | 1.38 | 1.35 |
| 1 | C | 34 | QUO | C10-C7 | -2.01 | 1.46 | 1.52 |

All (71) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | D | 54 | 5MU | C5M-C5-C4 | -42.38 | 45.44 | 121.37 |
| 1 | D | 55 | PSU | N1-C2-N3 | -17.60 | 114.44 | 128.43 |
| 1 | C | 65 | PSU | N1-C2-N3 | -17.41 | 114.59 | 128.43 |
| 1 | C | 55 | PSU | N1-C2-N3 | -17.35 | 114.63 | 128.43 |
| 1 | D | 65 | PSU | N1-C2-N3 | -17.18 | 114.77 | 128.43 |
| 1 | D | 34 | QUO | C5-C6-N1 | -15.10 | 110.69 | 124.09 |
| 1 | C | 34 | QUO | C5-C6-N1 | -15.09 | 110.70 | 124.09 |
| 1 | C | 54 | 5MU | C4-N3-C2 | 14.29 | 127.21 | 115.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | D | 55 | PSU | C4-N3-C2 | 12.47 | 125.67 | 115.14 |
| 1 | C | 55 | PSU | C4-N3-C2 | 12.29 | 125.52 | 115.14 |
| 1 | D | 65 | PSU | C4-N3-C2 | 12.26 | 125.50 | 115.14 |
| 1 | C | 65 | PSU | C4-N3-C2 | 12.26 | 125.49 | 115.14 |
| 1 | D | 54 | 5MU | C4-N3-C2 | 10.95 | 124.39 | 115.14 |
| 1 | C | 55 | PSU | O4'-C1'-C5 | 10.82 | 126.69 | 109.93 |
| 1 | C | 65 | PSU | O4'-C1'-C5 | 10.31 | 125.90 | 109.93 |
| 1 | D | 55 | PSU | O4'-C1'-C5 | 9.90 | 125.27 | 109.93 |
| 1 | D | 65 | PSU | O4'-C1'-C5 | 9.83 | 125.15 | 109.93 |
| 1 | C | 34 | QUO | C6-C5-C4 | 9.55 | 120.40 | 115.01 |
| 1 | D | 34 | QUO | C6-C5-C4 | 8.99 | 120.09 | 115.01 |
| 1 | D | 65 | PSU | C5-C4-N3 | -8.85 | 113.96 | 125.36 |
| 1 | C | 46 | G7M | C5-C6-N1 | -8.70 | 111.54 | 123.43 |
| 1 | D | 55 | PSU | C5-C4-N3 | -8.68 | 114.17 | 125.36 |
| 1 | C | 55 | PSU | C5-C4-N3 | -8.68 | 114.18 | 125.36 |
| 1 | C | 65 | PSU | C5-C4-N3 | -8.68 | 114.18 | 125.36 |
| 1 | D | 46 | G7M | C5-C6-N1 | -8.61 | 111.66 | 123.43 |
| 1 | C | 34 | QUO | C10-N11-C12 | 8.44 | 132.63 | 114.90 |
| 1 | C | 8 | 4SU | C2-N3-C4 | 8.32 | 127.22 | 115.15 |
| 1 | D | 8 | 4SU | C2-N3-C4 | 8.29 | 127.16 | 115.15 |
| 1 | D | 34 | QUO | C10-N11-C12 | 7.69 | 131.06 | 114.90 |
| 1 | C | 8 | 4SU | C5-C4-N3 | -7.07 | 114.37 | 123.83 |
| 1 | D | 8 | 4SU | C5-C4-N3 | -6.99 | 114.48 | 123.83 |
| 1 | D | 37 | 2MA | C2-N3-C4 | -6.08 | 110.58 | 115.52 |
| 1 | C | 37 | 2MA | C2-N3-C4 | -5.89 | 110.74 | 115.52 |
| 1 | C | 46 | G7M | C6-N1-C2 | 5.87 | 125.26 | 115.93 |
| 1 | D | 46 | G7M | C6-N1-C2 | 5.82 | 125.18 | 115.93 |
| 1 | C | 34 | QUO | C6-N1-C2 | 5.71 | 125.00 | 115.93 |
| 1 | D | 34 | QUO | C6-N1-C2 | 5.62 | 124.86 | 115.93 |
| 1 | D | 54 | 5MU | C6-N1-C1' | 5.20 | 130.92 | 119.24 |
| 1 | D | 37 | 2MA | C5-C6-N1 | -5.02 | 117.79 | 123.06 |
| 1 | C | 37 | 2MA | C5-C6-N1 | -4.93 | 117.88 | 123.06 |
| 1 | D | 55 | PSU | C6-N1-C2 | 4.59 | 122.93 | 115.36 |
| 1 | C | 55 | PSU | C6-N1-C2 | 4.52 | 122.82 | 115.36 |
| 1 | C | 65 | PSU | C6-N1-C2 | 4.49 | 122.77 | 115.36 |
| 1 | D | 65 | PSU | C6-N1-C2 | 4.33 | 122.50 | 115.36 |
| 1 | D | 34 | QUO | C7-C10-N11 | 4.31 | 125.29 | 112.75 |
| 1 | D | 54 | 5MU | C5-C6-N1 | -3.95 | 117.94 | 122.19 |
| 1 | C | 34 | QUO | C8-N9-C1' | 3.92 | 128.96 | 125.48 |
| 1 | C | 34 | QUO | O14-C14-C13 | 3.81 | 118.48 | 111.27 |
| 1 | D | 34 | QUO | C8-N9-C1' | 3.78 | 128.83 | 125.48 |
| 1 | D | 34 | QUO | O14-C14-C15 | 3.72 | 120.39 | 111.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | D | 34 | QUO | C16-C15-C14 | -3.67 | 99.40 | 105.68 |
| 1 | C | 34 | QUO | C16-C15-C14 | -3.60 | 99.51 | 105.68 |
| 1 | C | 34 | QUO | C7-C10-N11 | 3.48 | 122.88 | 112.75 |
| 1 | C | 34 | QUO | C2-N3-C4 | -3.17 | 111.74 | 115.36 |
| 1 | D | 34 | QUO | C2-N3-C4 | -3.09 | 111.83 | 115.36 |
| 1 | D | 46 | G7M | C2-N3-C4 | -2.88 | 112.07 | 115.36 |
| 1 | C | 46 | G7M | C2-N3-C4 | -2.79 | 112.18 | 115.36 |
| 1 | C | 34 | QUO | N3-C2-N1 | -2.76 | 123.55 | 127.22 |
| 1 | D | 34 | QUO | O14-C14-C13 | 2.65 | 116.28 | 111.27 |
| 1 | C | 46 | G7M | N3-C2-N1 | -2.62 | 123.73 | 127.22 |
| 1 | D | 46 | G7M | C6-C5-C4 | -2.60 | 118.31 | 120.80 |
| 1 | D | 46 | G7M | N3-C2-N1 | -2.59 | 123.76 | 127.22 |
| 1 | C | 34 | QUO | O14-C14-C15 | 2.53 | 117.57 | 111.54 |
| 1 | D | 20 | H2U | N3-C2-N1 | -2.44 | 114.07 | 116.65 |
| 1 | D | 34 | QUO | C16-C12-C13 | 2.44 | 106.81 | 103.18 |
| 1 | D | 34 | QUO | N3-C2-N1 | -2.40 | 124.02 | 127.22 |
| 1 | C | 46 | G7M | C6-C5-C4 | -2.31 | 118.59 | 120.80 |
| 1 | C | 34 | QUO | C16-C12-C13 | 2.19 | 106.43 | 103.18 |
| 1 | D | 46 | G7M | O4'-C1'-C2' | 2.14 | 110.06 | 106.93 |
| 1 | C | 16 | H2U | C4-N3-C2 | 2.11 | 127.54 | 125.79 |
| 1 | C | 54 | 5MU | C5M-C5-C6 | 2.05 | 123.00 | 118.68 |

There are no chirality outliers.

All (22) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-------|------|-----------------|
| 1 | C | 34 | QUO | C13-C12-N11-C10 |
| 1 | C | 34 | QUO | C16-C12-N11-C10 |
| 1 | D | 16 | H2U | O4'-C1'-N1-C6 |
| 1 | C | 16 | H2U | O4'-C1'-N1-C2 |
| 1 | C | 16 | H2U | O4'-C1'-N1-C6 |
| 1 | D | 20 | H2U | O4'-C1'-N1-C6 |
| 1 | D | 20 | H2U | C2'-C1'-N1-C2 |
| 1 | D | 20 | H2U | C2'-C1'-N1-C6 |
| 1 | C | 8 | 4SU | C2'-C1'-N1-C6 |
| 1 | D | 20 | H2U | O4'-C4'-C5'-O5' |
| 1 | D | 20(A) | H2U | C2'-C1'-N1-C6 |
| 1 | D | 16 | H2U | O4'-C1'-N1-C2 |
| 1 | D | 20 | H2U | C4'-C5'-O5'-P |
| 1 | D | 20 | H2U | O4'-C1'-N1-C2 |
| 1 | D | 20 | H2U | C3'-C4'-C5'-O5' |
| 1 | D | 55 | PSU | O4'-C1'-C5-C4 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-------|------|-----------------|
| 1 | D | 20(A) | H2U | O4'-C1'-N1-C2 |
| 1 | D | 37 | 2MA | C4'-C5'-O5'-P |
| 1 | D | 20(A) | H2U | C2'-C1'-N1-C2 |
| 1 | D | 34 | QUO | C16-C12-N11-C10 |
| 1 | C | 20(A) | H2U | C4'-C5'-O5'-P |
| 1 | C | 37 | 2MA | C4'-C5'-O5'-P |

There are no ring outliers.

19 monomers are involved in 53 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-------|------|---------|--------------|
| 1 | C | 20(A) | H2U | 5 | 0 |
| 1 | D | 8 | 4SU | 5 | 0 |
| 1 | C | 20 | H2U | 2 | 0 |
| 1 | C | 34 | QUO | 6 | 0 |
| 1 | D | 54 | 5MU | 2 | 0 |
| 1 | D | 46 | G7M | 5 | 0 |
| 1 | C | 65 | PSU | 4 | 0 |
| 1 | D | 65 | PSU | 2 | 0 |
| 1 | C | 46 | G7M | 1 | 0 |
| 1 | D | 34 | QUO | 7 | 0 |
| 1 | D | 16 | H2U | 2 | 0 |
| 1 | C | 54 | 5MU | 3 | 0 |
| 1 | C | 37 | 2MA | 1 | 0 |
| 1 | D | 55 | PSU | 1 | 0 |
| 1 | C | 16 | H2U | 2 | 0 |
| 1 | D | 20(A) | H2U | 1 | 0 |
| 1 | D | 20 | H2U | 1 | 0 |
| 1 | C | 8 | 4SU | 2 | 0 |
| 1 | D | 37 | 2MA | 5 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 | C | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | C | 59:G | O3' | 60:U | P | 1.76 |

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 | C | 63/73 (86%) | -0.15 | 0 100 100 | 26, 56, 90, 102 | 0 |
| 1 | D | 63/73 (86%) | -0.13 | 1 (1%) 72 44 | 32, 52, 96, 101 | 0 |
| 2 | A | 580/580 (100%) | 0.01 | 3 (0%) 91 75 | 7, 26, 64, 102 | 0 |
| 2 | B | 580/580 (100%) | 0.08 | 8 (1%) 75 49 | 6, 34, 68, 102 | 0 |
| All | All | 1286/1306 (98%) | 0.03 | 12 (0%) 84 63 | 6, 31, 71, 102 | 0 |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 437 | ALA | 5.7 |
| 2 | A | 432 | ASP | 5.0 |
| 2 | B | 580 | PRO | 5.0 |
| 2 | B | 435 | GLU | 4.9 |
| 1 | D | 72 | C | 2.6 |
| 2 | B | 307 | ARG | 2.5 |
| 2 | B | 439 | THR | 2.5 |
| 2 | B | 436 | GLU | 2.5 |
| 2 | A | 580 | PRO | 2.5 |
| 2 | B | 201 | GLN | 2.4 |
| 2 | A | 579 | ARG | 2.2 |
| 2 | B | 329 | LEU | 2.1 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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 |
|-----|------|-------|-------|-------|------|------|-----------------------------|-------|
| 1 | PSU | D | 65 | 20/21 | 0.86 | 0.15 | 76,79,82,83 | 0 |
| 1 | H2U | C | 20 | 20/21 | 0.88 | 0.24 | 61,72,77,77 | 0 |
| 1 | 5MU | D | 54 | 21/22 | 0.89 | 0.15 | 54,60,64,65 | 0 |
| 1 | H2U | D | 20 | 20/21 | 0.89 | 0.20 | 49,68,72,73 | 0 |
| 1 | QUO | D | 34 | 32/33 | 0.90 | 0.23 | 48,63,72,73 | 0 |
| 1 | 4SU | C | 8 | 20/21 | 0.90 | 0.19 | 52,56,60,61 | 0 |
| 1 | 5MU | C | 54 | 21/22 | 0.91 | 0.16 | 79,81,81,82 | 0 |
| 1 | H2U | D | 20(A) | 20/21 | 0.93 | 0.15 | 57,61,66,67 | 0 |
| 1 | PSU | D | 55 | 20/21 | 0.93 | 0.15 | 48,53,65,65 | 0 |
| 1 | H2U | C | 16 | 20/21 | 0.93 | 0.14 | 60,66,70,73 | 0 |
| 1 | PSU | C | 55 | 20/21 | 0.93 | 0.10 | 74,75,82,82 | 0 |
| 1 | QUO | C | 34 | 32/33 | 0.94 | 0.25 | 23,35,51,53 | 0 |
| 1 | G7M | D | 46 | 24/25 | 0.94 | 0.16 | 43,47,49,53 | 0 |
| 1 | PSU | C | 65 | 20/21 | 0.94 | 0.12 | 72,75,80,82 | 0 |
| 1 | H2U | D | 16 | 20/21 | 0.95 | 0.18 | 51,65,67,71 | 0 |
| 1 | 4SU | D | 8 | 20/21 | 0.95 | 0.20 | 39,43,47,48 | 0 |
| 1 | G7M | C | 46 | 24/25 | 0.95 | 0.18 | 36,42,48,50 | 0 |
| 1 | H2U | C | 20(A) | 20/21 | 0.95 | 0.14 | 57,63,73,73 | 0 |
| 1 | 2MA | D | 37 | 23/24 | 0.95 | 0.17 | 50,60,67,68 | 0 |
| 1 | 2MA | C | 37 | 23/24 | 0.96 | 0.18 | 25,41,44,64 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.