



Full wwPDB X-ray Structure Validation Report i

Jun 17, 2024 – 03:40 PM EDT

PDB ID : 3A2K
Title : Crystal structure of TilS complexed with tRNA
Authors : Nakanishi, K.; Bonnefond, L.; Ishitani, R.; Nureki, O.
Deposited on : 2009-05-23
Resolution : 3.65 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 i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

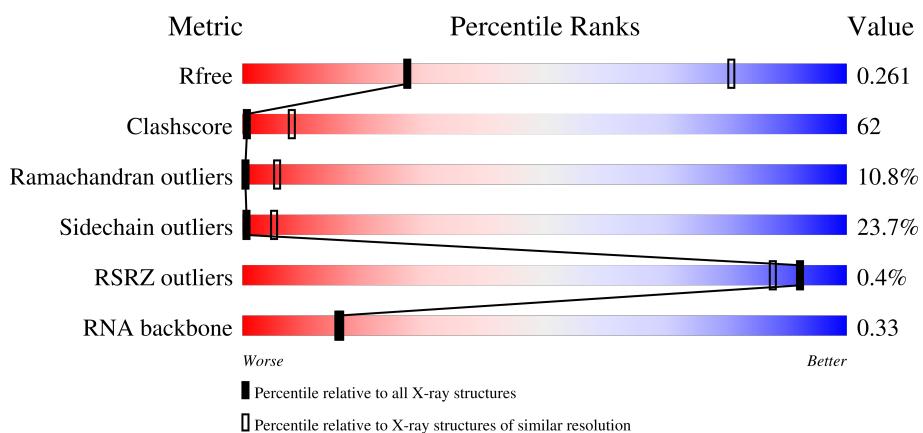
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

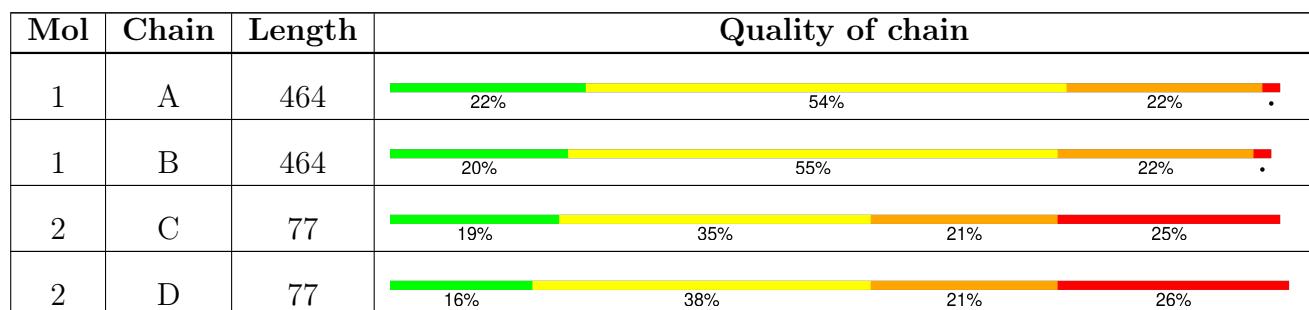
The reported resolution of this entry is 3.65 Å.

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 | 1557 (3.82-3.50) |
| Clashscore | 141614 | 1037 (3.80-3.52) |
| Ramachandran outliers | 138981 | 1004 (3.80-3.52) |
| Sidechain outliers | 138945 | 1002 (3.80-3.52) |
| RSRZ outliers | 127900 | 1441 (3.82-3.50) |
| RNA backbone | 3102 | 1024 (4.30-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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.



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10724 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 protein called tRNA(Ile)-lysidine synthase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 462 | 3724 | 2366 | 687 | 650 | 21 | 0 | 0 | 0 |
| 1 | B | 462 | 3724 | 2366 | 687 | 650 | 21 | 0 | 0 | 0 |

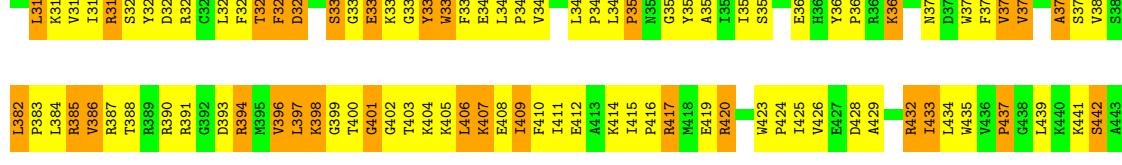
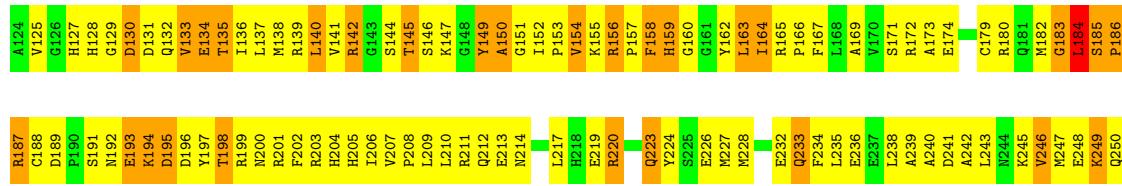
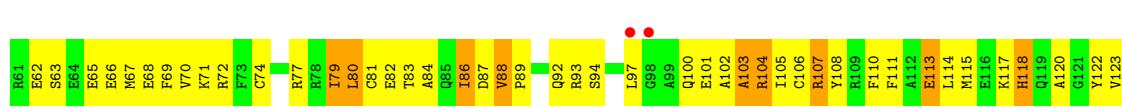
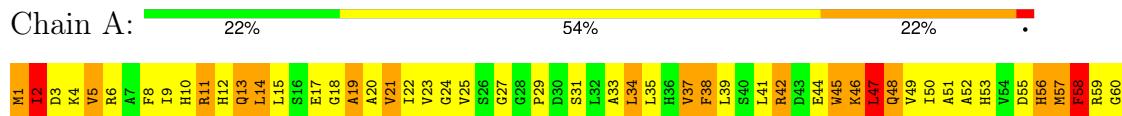
- Molecule 2 is a RNA chain called bacterial tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 2 | C | 77 | 1638 | 731 | 290 | 540 | 77 | 0 | 0 | 0 |
| 2 | D | 77 | 1638 | 731 | 290 | 540 | 77 | 0 | 0 | 0 |

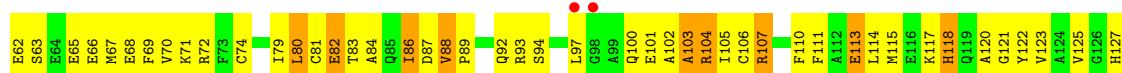
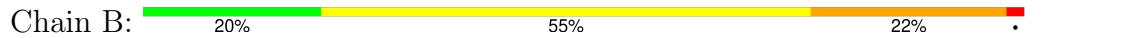
3 Residue-property plots

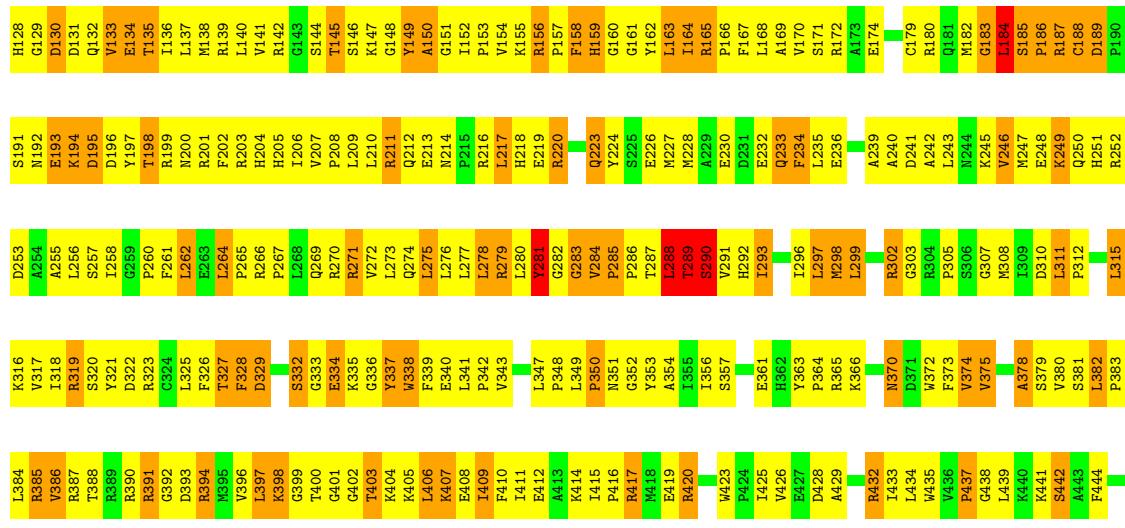
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: tRNA(Ile)-lysidine synthase



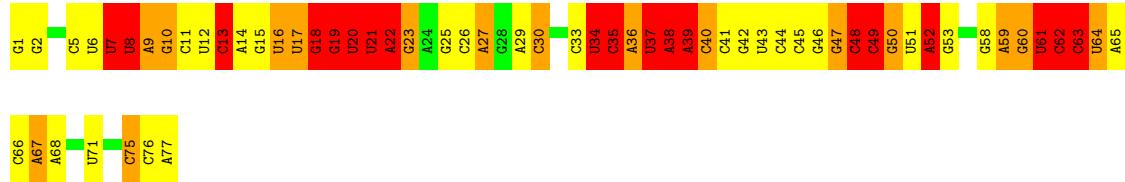
- Molecule 1: tRNA(Ile)-lysidine synthase





- Molecule 2: bacterial tRNA

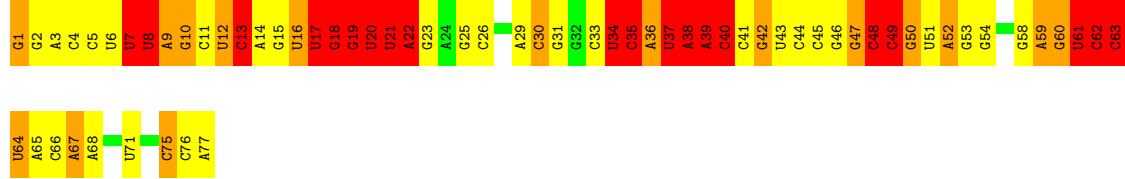
Chain C: 19% 35% 21% 25%



- Molecule 2: bacterial tRNA

Chain D: 16% 38% 21% 26%

A horizontal progress bar divided into four colored segments: green (16%), yellow (38%), orange (21%), and red (26%). The total length of the bar represents 100% completion.



4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 85.73 Å 157.40 Å 208.18 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 43.75 – 3.65 43.75 – 3.64 | Depositor EDS |
| % Data completeness (in resolution range) | 96.8 (43.75-3.65) 96.4 (43.75-3.64) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.06 | Depositor |
| $< I/\sigma(I) >$ ¹ | 2.58 (at 3.66 Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine) | Depositor |
| R , R_{free} | 0.216 , 0.266 0.209 , 0.261 | Depositor DCC |
| R_{free} test set | 1563 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 117.5 | Xtriage |
| Anisotropy | 0.179 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.23 , 62.3 | EDS |
| L-test for twinning ² | $< L > = 0.38$, $< L^2 > = 0.21$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 10724 | wwPDB-VP |
| Average B, all atoms (Å ²) | 157.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.48 | 0/3810 | 0.72 | 1/5137 (0.0%) |
| 1 | B | 0.48 | 0/3810 | 0.72 | 1/5137 (0.0%) |
| 2 | C | 0.81 | 1/1829 (0.1%) | 1.76 | 59/2846 (2.1%) |
| 2 | D | 0.75 | 1/1829 (0.1%) | 1.72 | 58/2846 (2.0%) |
| All | All | 0.59 | 2/11278 (0.0%) | 1.19 | 119/15966 (0.7%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2 | C | 1 | G | OP3-P | -10.56 | 1.48 | 1.61 |
| 2 | D | 1 | G | OP3-P | -9.32 | 1.50 | 1.61 |

All (119) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | C | 7 | U | P-O3'-C3' | 12.86 | 135.13 | 119.70 |
| 2 | C | 63 | C | N1-C1'-C2' | -12.09 | 98.29 | 114.00 |
| 2 | D | 63 | C | N1-C1'-C2' | -11.65 | 98.85 | 114.00 |
| 2 | D | 7 | U | P-O3'-C3' | 11.50 | 133.50 | 119.70 |
| 2 | C | 37 | U | P-O3'-C3' | 11.19 | 133.13 | 119.70 |
| 2 | C | 61 | U | P-O3'-C3' | 10.81 | 132.68 | 119.70 |
| 2 | D | 61 | U | P-O3'-C3' | 10.69 | 132.53 | 119.70 |
| 2 | D | 37 | U | O4'-C1'-N1 | -10.63 | 99.69 | 108.20 |
| 2 | D | 16 | U | O4'-C1'-N1 | -10.30 | 99.96 | 108.20 |
| 2 | C | 37 | U | O4'-C1'-N1 | -10.18 | 100.06 | 108.20 |
| 2 | D | 7 | U | N1-C1'-C2' | 9.83 | 126.78 | 114.00 |
| 2 | C | 34 | U | O4'-C1'-N1 | 9.71 | 115.97 | 108.20 |
| 2 | C | 63 | C | O4'-C1'-N1 | 9.65 | 115.92 | 108.20 |
| 2 | C | 7 | U | N1-C1'-C2' | 9.43 | 126.26 | 114.00 |
| 2 | D | 63 | C | O4'-C1'-N1 | 9.10 | 115.48 | 108.20 |
| 2 | D | 20 | U | O4'-C1'-N1 | 9.05 | 115.44 | 108.20 |
| 2 | D | 37 | U | P-O3'-C3' | 8.99 | 130.49 | 119.70 |
| 2 | C | 16 | U | O4'-C1'-N1 | -8.97 | 101.02 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 38 | A | P-O3'-C3' | -8.68 | 109.28 | 119.70 |
| 2 | C | 21 | U | O4'-C1'-N1 | 8.57 | 115.06 | 108.20 |
| 2 | C | 8 | U | P-O3'-C3' | -8.50 | 109.50 | 119.70 |
| 2 | D | 62 | C | N1-C1'-C2' | -8.47 | 102.69 | 112.00 |
| 2 | C | 20 | U | O4'-C1'-N1 | 8.42 | 114.94 | 108.20 |
| 2 | C | 62 | C | N1-C1'-C2' | -8.32 | 102.85 | 112.00 |
| 2 | C | 20 | U | P-O3'-C3' | 8.00 | 129.31 | 119.70 |
| 2 | C | 48 | C | P-O3'-C3' | -7.96 | 110.15 | 119.70 |
| 2 | C | 8 | U | O4'-C1'-N1 | -7.94 | 101.85 | 108.20 |
| 2 | D | 8 | U | P-O3'-C3' | -7.91 | 110.21 | 119.70 |
| 2 | C | 39 | A | C3'-C2'-C1' | 7.89 | 107.81 | 101.50 |
| 2 | D | 21 | U | O4'-C1'-N1 | 7.86 | 114.49 | 108.20 |
| 2 | D | 49 | C | N1-C2-O2 | 7.82 | 123.59 | 118.90 |
| 2 | D | 8 | U | O4'-C1'-N1 | -7.62 | 102.10 | 108.20 |
| 2 | D | 20 | U | P-O3'-C3' | 7.62 | 128.84 | 119.70 |
| 2 | D | 39 | A | C3'-C2'-C1' | 7.43 | 107.45 | 101.50 |
| 2 | D | 34 | U | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 2 | D | 50 | G | P-O5'-C5' | -7.35 | 109.14 | 120.90 |
| 2 | C | 75 | C | P-O3'-C3' | -7.34 | 110.89 | 119.70 |
| 2 | C | 36 | A | O4'-C1'-N9 | 7.29 | 114.03 | 108.20 |
| 2 | C | 61 | U | N1-C1'-C2' | 7.04 | 123.15 | 114.00 |
| 2 | C | 38 | A | P-O3'-C3' | -6.78 | 111.56 | 119.70 |
| 2 | C | 13 | C | O4'-C1'-N1 | -6.78 | 102.78 | 108.20 |
| 2 | C | 39 | A | C8-N9-C4 | -6.74 | 103.11 | 105.80 |
| 2 | C | 49 | C | N1-C2-O2 | 6.63 | 122.88 | 118.90 |
| 2 | C | 50 | G | P-O5'-C5' | -6.58 | 110.38 | 120.90 |
| 2 | C | 39 | A | N7-C8-N9 | 6.53 | 117.06 | 113.80 |
| 2 | C | 37 | U | N1-C1'-C2' | 6.49 | 122.44 | 114.00 |
| 2 | D | 75 | C | P-O3'-C3' | -6.49 | 111.91 | 119.70 |
| 2 | D | 61 | U | N1-C1'-C2' | 6.48 | 122.43 | 114.00 |
| 2 | D | 37 | U | N1-C1'-C2' | 6.46 | 122.40 | 114.00 |
| 2 | C | 50 | G | N9-C1'-C2' | -6.38 | 104.98 | 112.00 |
| 2 | D | 30 | C | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 2 | D | 36 | A | O4'-C1'-N9 | 6.33 | 113.27 | 108.20 |
| 2 | C | 19 | G | P-O5'-C5' | -6.31 | 110.81 | 120.90 |
| 2 | C | 30 | C | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 2 | C | 19 | G | C3'-C2'-C1' | 6.25 | 106.50 | 101.50 |
| 2 | C | 18 | G | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 2 | D | 39 | A | N1-C6-N6 | 6.07 | 122.24 | 118.60 |
| 2 | C | 39 | A | O4'-C1'-N9 | 6.03 | 113.03 | 108.20 |
| 2 | D | 13 | C | O4'-C1'-N1 | -5.98 | 103.42 | 108.20 |
| 2 | D | 49 | C | O3'-P-O5' | -5.95 | 92.70 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | C | 63 | C | C3'-C2'-C1' | 5.91 | 106.23 | 101.50 |
| 2 | D | 10 | G | N9-C1'-C2' | -5.84 | 105.57 | 112.00 |
| 2 | D | 62 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 2 | C | 8 | U | C2-N1-C1' | 5.80 | 124.67 | 117.70 |
| 2 | C | 62 | C | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 2 | C | 67 | A | P-O3'-C3' | -5.78 | 112.77 | 119.70 |
| 2 | D | 40 | C | O4'-C1'-N1 | -5.76 | 103.59 | 108.20 |
| 2 | D | 63 | C | P-O3'-C3' | -5.70 | 112.86 | 119.70 |
| 2 | D | 63 | C | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 2 | C | 2 | G | N1-C6-O6 | 5.70 | 123.32 | 119.90 |
| 2 | D | 49 | C | C3'-C2'-C1' | 5.68 | 106.05 | 101.50 |
| 2 | D | 19 | G | P-O5'-C5' | -5.66 | 111.85 | 120.90 |
| 2 | C | 35 | C | N1-C1'-C2' | -5.65 | 105.79 | 112.00 |
| 2 | C | 49 | C | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 2 | D | 10 | G | P-O3'-C3' | -5.63 | 112.95 | 119.70 |
| 2 | C | 49 | C | O3'-P-O5' | -5.62 | 93.32 | 104.00 |
| 2 | D | 37 | U | N1-C2-N3 | -5.56 | 111.56 | 114.90 |
| 2 | D | 49 | C | N3-C2-O2 | -5.56 | 118.01 | 121.90 |
| 2 | C | 63 | C | P-O3'-C3' | -5.55 | 113.04 | 119.70 |
| 2 | D | 19 | G | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 2 | D | 35 | C | P-O3'-C3' | -5.54 | 113.05 | 119.70 |
| 2 | D | 39 | A | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 2 | D | 39 | A | N7-C8-N9 | 5.52 | 116.56 | 113.80 |
| 2 | C | 71 | U | P-O5'-C5' | -5.51 | 112.08 | 120.90 |
| 2 | C | 35 | C | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 2 | D | 42 | G | P-O3'-C3' | -5.46 | 113.15 | 119.70 |
| 2 | C | 39 | A | N1-C6-N6 | 5.43 | 121.86 | 118.60 |
| 2 | D | 35 | C | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 2 | D | 18 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 2 | D | 71 | U | P-O5'-C5' | -5.38 | 112.30 | 120.90 |
| 2 | C | 39 | A | C5-N7-C8 | -5.35 | 101.22 | 103.90 |
| 1 | A | 47 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 2 | C | 8 | U | C3'-C2'-C1' | 5.34 | 105.78 | 101.50 |
| 2 | C | 10 | G | N9-C1'-C2' | -5.33 | 106.13 | 112.00 |
| 2 | D | 39 | A | C8-N9-C4 | -5.31 | 103.68 | 105.80 |
| 2 | D | 35 | C | N1-C1'-C2' | -5.30 | 106.17 | 112.00 |
| 2 | D | 39 | A | C6-C5-N7 | -5.30 | 128.59 | 132.30 |
| 2 | C | 35 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 2 | C | 22 | A | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 2 | C | 13 | C | P-O3'-C3' | 5.26 | 126.01 | 119.70 |
| 2 | D | 67 | A | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 2 | D | 8 | U | C2-N1-C1' | 5.22 | 123.96 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 50 | G | N9-C1'-C2' | -5.20 | 106.28 | 112.00 |
| 2 | D | 50 | G | P-O3'-C3' | -5.19 | 113.47 | 119.70 |
| 2 | C | 39 | A | C6-C5-N7 | -5.18 | 128.68 | 132.30 |
| 2 | D | 2 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 2 | C | 27 | A | N1-C6-N6 | 5.16 | 121.69 | 118.60 |
| 2 | D | 17 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 2 | C | 35 | C | C2-N1-C1' | 5.15 | 124.46 | 118.80 |
| 2 | C | 16 | U | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 2 | D | 48 | C | C4'-C3'-C2' | 5.12 | 107.72 | 102.60 |
| 2 | C | 50 | G | P-O3'-C3' | -5.10 | 113.58 | 119.70 |
| 2 | D | 22 | A | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 2 | C | 36 | A | C2-N3-C4 | 5.06 | 113.13 | 110.60 |
| 1 | B | 47 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 2 | D | 2 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 2 | C | 10 | G | P-O3'-C3' | -5.04 | 113.66 | 119.70 |
| 2 | C | 52 | A | C8-N9-C4 | 5.04 | 107.81 | 105.80 |
| 2 | D | 13 | C | P-O3'-C3' | 5.01 | 125.72 | 119.70 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3724 | 0 | 3752 | 514 | 0 |
| 1 | B | 3724 | 0 | 3752 | 528 | 0 |
| 2 | C | 1638 | 0 | 831 | 152 | 1 |
| 2 | D | 1638 | 0 | 831 | 155 | 1 |
| All | All | 10724 | 0 | 9166 | 1239 | 1 |

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 62.

All (1239) 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:B:144:SER:HA | 2:D:39:A:H5' | 1.19 | 1.18 |
| 2:C:49:C:H2' | 2:C:49:C:O2 | 1.37 | 1.18 |
| 2:D:49:C:H2' | 2:D:49:C:O2 | 1.40 | 1.13 |
| 1:B:42:ARG:HD3 | 1:B:47:LEU:HB3 | 1.32 | 1.10 |
| 1:A:42:ARG:HD3 | 1:A:47:LEU:HB3 | 1.31 | 1.09 |
| 1:A:145:THR:HG22 | 1:A:149:TYR:HB2 | 1.38 | 1.05 |
| 1:B:417:ARG:HH11 | 1:B:417:ARG:N | 1.57 | 1.03 |
| 1:A:417:ARG:N | 1:A:417:ARG:HH11 | 1.57 | 1.03 |
| 1:B:145:THR:HG22 | 1:B:149:TYR:HB2 | 1.39 | 1.03 |
| 1:A:364:PRO:HG2 | 1:A:374:VAL:HG21 | 1.37 | 1.02 |
| 1:B:144:SER:CA | 2:D:39:A:H5' | 1.90 | 1.02 |
| 1:B:364:PRO:HG2 | 1:B:374:VAL:HG21 | 1.42 | 1.02 |
| 1:A:1:MET:N | 1:A:4:LYS:HB2 | 1.76 | 1.01 |
| 1:A:437:PRO:HB3 | 1:A:459:TYR:CD1 | 1.98 | 0.99 |
| 1:B:1:MET:N | 1:B:4:LYS:HB2 | 1.78 | 0.99 |
| 1:A:42:ARG:CD | 1:A:47:LEU:HB3 | 1.93 | 0.98 |
| 1:A:235:LEU:HD11 | 1:B:235:LEU:HD11 | 1.46 | 0.97 |
| 1:B:42:ARG:CD | 1:B:47:LEU:HB3 | 1.94 | 0.97 |
| 2:C:19:G:O2' | 2:C:20:U:H5" | 1.66 | 0.96 |
| 1:B:417:ARG:HH11 | 1:B:417:ARG:H | 0.97 | 0.95 |
| 2:D:19:G:O2' | 2:D:20:U:H5" | 1.66 | 0.94 |
| 1:A:25:VAL:HG13 | 1:A:31:SER:HB2 | 1.50 | 0.93 |
| 1:A:417:ARG:H | 1:A:417:ARG:NH1 | 1.67 | 0.93 |
| 1:B:46:LYS:O | 1:B:46:LYS:HG2 | 1.69 | 0.93 |
| 1:A:241:ASP:HB3 | 1:A:245:LYS:NZ | 1.83 | 0.93 |
| 1:A:417:ARG:HH11 | 1:A:417:ARG:H | 0.96 | 0.92 |
| 1:B:289:THR:HG23 | 2:D:39:A:C8 | 2.04 | 0.92 |
| 1:A:46:LYS:O | 1:A:46:LYS:HG2 | 1.68 | 0.92 |
| 1:B:5:VAL:O | 1:B:9:ILE:HG12 | 1.70 | 0.92 |
| 1:B:241:ASP:HB3 | 1:B:245:LYS:NZ | 1.84 | 0.91 |
| 1:B:127:HIS:CD2 | 1:B:165:ARG:HH11 | 1.88 | 0.91 |
| 1:B:417:ARG:H | 1:B:417:ARG:NH1 | 1.67 | 0.91 |
| 1:B:25:VAL:HG13 | 1:B:31:SER:HB2 | 1.52 | 0.91 |
| 1:A:5:VAL:O | 1:A:9:ILE:HG12 | 1.69 | 0.90 |
| 1:B:437:PRO:HB3 | 1:B:459:TYR:CD1 | 2.07 | 0.89 |
| 1:B:289:THR:H | 2:D:39:A:C2' | 1.85 | 0.88 |
| 1:B:15:LEU:HD22 | 1:B:164:ILE:HG23 | 1.54 | 0.88 |
| 1:B:114:LEU:O | 1:B:118:HIS:HB2 | 1.73 | 0.87 |
| 1:B:185:SER:HB2 | 1:B:186:PRO:HD2 | 1.56 | 0.87 |
| 1:A:115:MET:HE1 | 1:A:160:GLY:H | 1.36 | 0.87 |
| 1:A:127:HIS:CD2 | 1:A:165:ARG:HH11 | 1.92 | 0.87 |
| 2:C:60:G:C2' | 2:C:61:U:H5' | 2.05 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:104:ARG:HG3 | 2:C:36:A:C2 | 2.10 | 0.86 |
| 1:B:139:ARG:NH1 | 2:D:36:A:C8 | 2.44 | 0.86 |
| 1:A:185:SER:HB2 | 1:A:186:PRO:HD2 | 1.57 | 0.86 |
| 1:A:114:LEU:O | 1:A:118:HIS:HB2 | 1.75 | 0.85 |
| 1:B:271:ARG:HH11 | 1:B:271:ARG:CG | 1.89 | 0.85 |
| 1:A:42:ARG:HH11 | 1:A:48:GLN:N | 1.75 | 0.85 |
| 1:A:15:LEU:HD22 | 1:A:164:ILE:HG23 | 1.59 | 0.85 |
| 1:B:42:ARG:HH11 | 1:B:48:GLN:N | 1.75 | 0.84 |
| 1:A:210:LEU:HD12 | 1:B:141:VAL:HG11 | 1.57 | 0.84 |
| 1:A:145:THR:CG2 | 1:A:149:TYR:HB2 | 2.07 | 0.84 |
| 1:A:165:ARG:NH2 | 2:C:37:U:OP1 | 2.10 | 0.84 |
| 1:A:241:ASP:HB3 | 1:A:245:LYS:HZ2 | 1.43 | 0.83 |
| 1:B:115:MET:HE1 | 1:B:160:GLY:H | 1.43 | 0.83 |
| 1:A:144:SER:HA | 2:C:39:A:H5' | 1.59 | 0.83 |
| 1:A:86:ILE:CG2 | 1:A:88:VAL:HG22 | 2.08 | 0.83 |
| 2:C:49:C:O2 | 2:C:49:C:C2' | 2.25 | 0.82 |
| 2:D:60:G:C2' | 2:D:61:U:H5' | 2.08 | 0.82 |
| 1:B:145:THR:CG2 | 1:B:149:TYR:HB2 | 2.09 | 0.81 |
| 1:B:373:PHE:CD1 | 1:B:435:TRP:HB2 | 2.15 | 0.81 |
| 1:A:271:ARG:CG | 1:A:271:ARG:HH11 | 1.92 | 0.81 |
| 1:A:9:ILE:HA | 1:A:15:LEU:HD12 | 1.62 | 0.81 |
| 1:B:35:LEU:HD11 | 1:B:51:ALA:HB2 | 1.63 | 0.80 |
| 1:A:338:TRP:C | 1:A:339:PHE:HD2 | 1.83 | 0.80 |
| 1:A:35:LEU:HD11 | 1:A:51:ALA:HB2 | 1.62 | 0.80 |
| 1:B:338:TRP:C | 1:B:339:PHE:HD2 | 1.84 | 0.80 |
| 2:C:22:A:C6 | 2:C:49:C:C5 | 2.69 | 0.80 |
| 1:B:55:ASP:OD2 | 1:B:63:SER:HB2 | 1.82 | 0.80 |
| 1:B:107:ARG:HG3 | 1:B:111:PHE:HE1 | 1.47 | 0.80 |
| 1:A:1:MET:H1 | 1:A:4:LYS:HB2 | 1.47 | 0.80 |
| 1:A:57:MET:HE2 | 1:A:59:ARG:HB2 | 1.63 | 0.80 |
| 1:A:373:PHE:CD1 | 1:A:435:TRP:HB2 | 2.17 | 0.79 |
| 1:B:214:ASN:OD1 | 2:C:41:C:H4' | 1.82 | 0.79 |
| 1:A:46:LYS:O | 1:A:47:LEU:HD13 | 1.82 | 0.79 |
| 1:B:46:LYS:O | 1:B:47:LEU:HD13 | 1.83 | 0.79 |
| 1:B:1:MET:H2 | 1:B:4:LYS:HB2 | 1.46 | 0.79 |
| 1:B:13:GLN:HG3 | 1:B:14:LEU:H | 1.48 | 0.79 |
| 2:D:49:C:O2 | 2:D:49:C:C2' | 2.29 | 0.79 |
| 1:A:327:THR:HG23 | 1:A:329:ASP:HB3 | 1.65 | 0.79 |
| 1:B:128:HIS:HD2 | 1:B:130:ASP:HB2 | 1.49 | 0.78 |
| 1:B:408:GLU:O | 1:B:412:GLU:HG3 | 1.83 | 0.78 |
| 2:C:10:G:O2' | 2:C:11:C:H5' | 1.83 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:13:GLN:HG3 | 1:A:14:LEU:H | 1.47 | 0.78 |
| 1:A:364:PRO:HG2 | 1:A:374:VAL:CG2 | 2.12 | 0.78 |
| 1:B:289:THR:H | 2:D:39:A:H2' | 1.49 | 0.78 |
| 1:A:128:HIS:HD2 | 1:A:130:ASP:HB2 | 1.48 | 0.78 |
| 1:B:139:ARG:NH1 | 2:D:36:A:H8 | 1.81 | 0.77 |
| 1:B:311:LEU:HB3 | 1:B:312:PRO:HD2 | 1.64 | 0.77 |
| 1:B:363:TYR:CE1 | 1:B:448:ASN:HA | 2.19 | 0.77 |
| 1:B:86:ILE:CG2 | 1:B:88:VAL:HG22 | 2.14 | 0.77 |
| 1:A:145:THR:HG22 | 1:A:149:TYR:CB | 2.13 | 0.77 |
| 1:A:104:ARG:NH2 | 2:C:36:A:N6 | 2.33 | 0.76 |
| 1:B:334:GLU:O | 1:B:335:LYS:HG3 | 1.85 | 0.76 |
| 1:B:373:PHE:CE1 | 1:B:435:TRP:HB2 | 2.20 | 0.76 |
| 1:A:55:ASP:OD2 | 1:A:63:SER:HB2 | 1.84 | 0.76 |
| 2:D:8:U:C6 | 2:D:15:G:O6 | 2.38 | 0.76 |
| 1:A:149:TYR:HE2 | 1:A:228:MET:HG3 | 1.50 | 0.76 |
| 1:A:408:GLU:O | 1:A:412:GLU:HG3 | 1.85 | 0.76 |
| 2:C:8:U:C6 | 2:C:15:G:O6 | 2.38 | 0.76 |
| 1:B:139:ARG:NH1 | 2:D:36:A:H1' | 1.99 | 0.76 |
| 2:D:36:A:H3' | 2:D:36:A:N3 | 2.01 | 0.76 |
| 1:A:363:TYR:CE1 | 1:A:448:ASN:HA | 2.21 | 0.75 |
| 1:A:14:LEU:HD13 | 1:A:162:TYR:HE1 | 1.50 | 0.75 |
| 2:D:60:G:H2' | 2:D:61:U:H5' | 1.68 | 0.75 |
| 1:B:57:MET:HE2 | 1:B:59:ARG:HB2 | 1.69 | 0.75 |
| 1:B:42:ARG:HD2 | 1:B:49:VAL:HG22 | 1.70 | 0.74 |
| 2:D:22:A:C6 | 2:D:49:C:C5 | 2.74 | 0.74 |
| 1:A:373:PHE:CE1 | 1:A:435:TRP:HB2 | 2.21 | 0.74 |
| 1:B:9:ILE:HA | 1:B:15:LEU:HD12 | 1.67 | 0.74 |
| 1:B:327:THR:HG23 | 1:B:329:ASP:HB3 | 1.69 | 0.74 |
| 1:B:144:SER:HA | 2:D:39:A:C5' | 2.10 | 0.74 |
| 1:A:224:TYR:OH | 1:B:224:TYR:OH | 2.06 | 0.74 |
| 1:B:149:TYR:HE2 | 1:B:228:MET:HG3 | 1.52 | 0.74 |
| 1:A:327:THR:CG2 | 1:A:329:ASP:HB3 | 2.18 | 0.74 |
| 1:B:241:ASP:HB3 | 1:B:245:LYS:HZ2 | 1.50 | 0.74 |
| 1:B:289:THR:OG1 | 2:D:39:A:H2' | 1.88 | 0.74 |
| 2:C:60:G:H2' | 2:C:61:U:H5' | 1.69 | 0.74 |
| 1:A:311:LEU:HB3 | 1:A:312:PRO:HD2 | 1.67 | 0.73 |
| 1:B:14:LEU:HD13 | 1:B:162:TYR:HE1 | 1.53 | 0.73 |
| 1:B:364:PRO:HG2 | 1:B:374:VAL:CG2 | 2.18 | 0.73 |
| 1:A:107:ARG:HG3 | 1:A:111:PHE:HE1 | 1.54 | 0.73 |
| 1:A:288:LEU:O | 1:A:291:VAL:HG22 | 1.89 | 0.73 |
| 1:A:423:TRP:NE1 | 1:A:439:LEU:HD12 | 2.04 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:311:LEU:CB | 1:B:312:PRO:HD2 | 2.18 | 0.73 |
| 2:C:48:C:OP1 | 2:C:48:C:H6 | 1.72 | 0.72 |
| 1:A:104:ARG:NH1 | 2:C:34:U:H2' | 2.05 | 0.72 |
| 2:D:62:C:HO2' | 2:D:63:C:H6 | 1.35 | 0.72 |
| 2:D:18:G:H2' | 2:D:58:G:N2 | 2.04 | 0.72 |
| 2:C:65:A:H2' | 2:C:66:C:H6 | 1.54 | 0.72 |
| 1:A:311:LEU:CB | 1:A:312:PRO:HD2 | 2.20 | 0.71 |
| 1:B:134:GLU:O | 1:B:138:MET:HB2 | 1.90 | 0.71 |
| 1:A:289:THR:HG23 | 2:C:39:A:H2' | 1.72 | 0.71 |
| 1:B:198:THR:HG21 | 2:D:33:C:O2' | 1.91 | 0.71 |
| 1:B:104:ARG:CZ | 2:D:36:A:N6 | 2.53 | 0.71 |
| 1:B:460:GLN:HG2 | 1:B:461:ALA:N | 2.05 | 0.71 |
| 1:B:407:LYS:O | 1:B:411:ILE:HG13 | 1.90 | 0.71 |
| 2:C:39:A:H4' | 2:C:39:A:OP1 | 1.89 | 0.71 |
| 1:A:193:GLU:O | 1:A:194:LYS:HB2 | 1.91 | 0.71 |
| 2:C:64:U:H2' | 2:C:65:A:C8 | 2.26 | 0.71 |
| 1:A:86:ILE:HG23 | 1:A:88:VAL:HG22 | 1.72 | 0.71 |
| 1:B:133:VAL:O | 1:B:137:LEU:HD12 | 1.91 | 0.70 |
| 1:B:145:THR:HG22 | 1:B:149:TYR:CB | 2.17 | 0.70 |
| 1:A:341:LEU:N | 1:A:384:LEU:O | 2.23 | 0.70 |
| 1:A:59:ARG:HA | 1:A:63:SER:HB3 | 1.73 | 0.70 |
| 1:A:261:PHE:O | 1:A:264:LEU:HB2 | 1.91 | 0.70 |
| 1:B:59:ARG:HA | 1:B:63:SER:HB3 | 1.72 | 0.70 |
| 1:B:149:TYR:CD1 | 1:B:149:TYR:C | 2.65 | 0.70 |
| 1:B:271:ARG:HH11 | 1:B:271:ARG:HG3 | 1.56 | 0.70 |
| 2:D:39:A:H4' | 2:D:39:A:OP1 | 1.91 | 0.70 |
| 1:B:289:THR:HG23 | 2:D:39:A:N9 | 2.06 | 0.70 |
| 2:D:18:G:H2' | 2:D:58:G:HG22 | 1.56 | 0.70 |
| 1:B:327:THR:CG2 | 1:B:329:ASP:HB3 | 2.22 | 0.70 |
| 2:C:44:C:H2' | 2:C:45:C:H6 | 1.57 | 0.70 |
| 1:B:14:LEU:HB2 | 1:B:155:LYS:HE3 | 1.73 | 0.70 |
| 2:D:10:G:O2' | 2:D:11:C:H5' | 1.92 | 0.70 |
| 1:B:193:GLU:O | 1:B:194:LYS:HB2 | 1.91 | 0.70 |
| 1:A:165:ARG:NH2 | 2:C:37:U:P | 2.64 | 0.69 |
| 1:B:288:LEU:O | 1:B:291:VAL:HG22 | 1.92 | 0.69 |
| 2:D:64:U:H2' | 2:D:65:A:C8 | 2.26 | 0.69 |
| 1:B:86:ILE:HG23 | 1:B:88:VAL:HG22 | 1.72 | 0.69 |
| 1:A:145:THR:HA | 1:A:149:TYR:HB2 | 1.75 | 0.69 |
| 1:B:341:LEU:N | 1:B:384:LEU:O | 2.25 | 0.69 |
| 1:A:171:SER:HB3 | 1:A:174:GLU:HG3 | 1.74 | 0.69 |
| 1:B:171:SER:HB3 | 1:B:174:GLU:HG3 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:48:C:H6 | 2:D:48:C:OP1 | 1.74 | 0.69 |
| 1:A:20:ALA:HB1 | 1:A:120:ALA:HA | 1.73 | 0.69 |
| 2:C:35:C:OP2 | 2:C:35:C:C4' | 2.41 | 0.69 |
| 1:A:149:TYR:OH | 1:A:224:TYR:CE2 | 2.44 | 0.69 |
| 1:A:288:LEU:HB2 | 1:A:291:VAL:HG22 | 1.75 | 0.69 |
| 1:A:14:LEU:HB2 | 1:A:155:LYS:HE3 | 1.74 | 0.68 |
| 1:A:134:GLU:O | 1:A:138:MET:HB2 | 1.93 | 0.68 |
| 1:A:281:TYR:OH | 1:A:315:LEU:HD12 | 1.92 | 0.68 |
| 2:D:35:C:C4' | 2:D:35:C:OP2 | 2.40 | 0.68 |
| 1:B:423:TRP:NE1 | 1:B:439:LEU:HD12 | 2.07 | 0.68 |
| 1:A:417:ARG:HA | 1:A:420:ARG:HG3 | 1.75 | 0.68 |
| 1:B:67:MET:O | 1:B:70:VAL:HG22 | 1.93 | 0.68 |
| 1:B:100:GLN:O | 1:B:103:ALA:HB3 | 1.94 | 0.68 |
| 1:A:405:LYS:HE3 | 2:C:67:A:P | 2.33 | 0.68 |
| 2:D:63:C:O2' | 2:D:64:U:H5' | 1.94 | 0.68 |
| 1:A:104:ARG:HH12 | 2:C:34:U:H2' | 1.59 | 0.68 |
| 2:D:44:C:H2' | 2:D:45:C:H6 | 1.58 | 0.68 |
| 1:A:42:ARG:HD2 | 1:A:49:VAL:HG22 | 1.76 | 0.68 |
| 2:C:36:A:N3 | 2:C:36:A:H3' | 2.08 | 0.68 |
| 1:A:407:LYS:O | 1:A:411:ILE:HG13 | 1.93 | 0.68 |
| 1:B:33:ALA:O | 1:B:37:VAL:HG23 | 1.92 | 0.68 |
| 1:B:288:LEU:HA | 2:D:39:A:O2' | 1.93 | 0.68 |
| 1:A:144:SER:CA | 2:C:39:A:H5' | 2.24 | 0.68 |
| 1:A:104:ARG:NE | 2:C:36:A:C6 | 2.62 | 0.67 |
| 1:A:149:TYR:C | 1:A:149:TYR:CD1 | 2.66 | 0.67 |
| 1:A:287:THR:O | 1:A:292:HIS:HD2 | 1.75 | 0.67 |
| 1:A:333:GLY:O | 1:A:334:GLU:HB2 | 1.94 | 0.67 |
| 2:D:59:A:C5 | 2:D:62:C:C4 | 2.82 | 0.67 |
| 1:A:416:PRO:O | 1:A:420:ARG:HG2 | 1.94 | 0.67 |
| 1:A:460:GLN:HG2 | 1:A:461:ALA:N | 2.08 | 0.67 |
| 1:B:288:LEU:HB2 | 1:B:291:VAL:HG22 | 1.75 | 0.67 |
| 2:C:18:G:H2' | 2:C:58:G:N2 | 2.10 | 0.67 |
| 1:B:56:HIS:CD2 | 1:B:56:HIS:H | 2.13 | 0.67 |
| 2:C:51:U:H3' | 2:C:52:A:H8 | 1.58 | 0.67 |
| 1:B:333:GLY:O | 1:B:334:GLU:HB2 | 1.95 | 0.67 |
| 2:C:59:A:C5 | 2:C:62:C:C4 | 2.82 | 0.67 |
| 1:B:107:ARG:O | 1:B:111:PHE:HD1 | 1.78 | 0.67 |
| 2:D:43:U:H2' | 2:D:44:C:H6 | 1.60 | 0.67 |
| 1:A:100:GLN:O | 1:A:103:ALA:HB3 | 1.95 | 0.67 |
| 1:B:15:LEU:HD22 | 1:B:164:ILE:CG2 | 2.23 | 0.67 |
| 1:B:20:ALA:HB1 | 1:B:120:ALA:HA | 1.74 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:432:ARG:HD3 | 1:B:444:PHE:HE1 | 1.59 | 0.67 |
| 1:A:45:TRP:O | 1:A:47:LEU:HD22 | 1.95 | 0.67 |
| 1:B:208:PRO:O | 1:B:212:GLN:HG3 | 1.95 | 0.67 |
| 1:A:289:THR:HG23 | 2:C:39:A:C8 | 2.30 | 0.66 |
| 2:D:51:U:H3' | 2:D:52:A:H8 | 1.59 | 0.66 |
| 1:A:133:VAL:O | 1:A:137:LEU:HD12 | 1.96 | 0.66 |
| 1:B:104:ARG:NH2 | 2:D:36:A:N6 | 2.43 | 0.66 |
| 1:B:192:ASN:HD22 | 1:B:204:HIS:CE1 | 2.13 | 0.66 |
| 2:D:65:A:H2' | 2:D:66:C:HG6 | 1.60 | 0.66 |
| 1:A:8:PHE:CG | 1:A:169:ALA:HB2 | 2.31 | 0.66 |
| 1:A:56:HIS:H | 1:A:56:HIS:CD2 | 2.14 | 0.66 |
| 1:B:127:HIS:HD2 | 1:B:165:ARG:HD3 | 1.61 | 0.66 |
| 1:B:261:PHE:O | 1:B:264:LEU:HB2 | 1.95 | 0.66 |
| 2:C:64:U:H2' | 2:C:65:A:HG8 | 1.61 | 0.66 |
| 1:A:289:THR:H | 2:C:39:A:C2' | 2.07 | 0.66 |
| 1:A:149:TYR:CE2 | 1:A:228:MET:HG3 | 2.32 | 0.65 |
| 1:B:145:THR:HA | 1:B:149:TYR:HB2 | 1.77 | 0.65 |
| 1:B:185:SER:HB2 | 1:B:186:PRO:CD | 2.25 | 0.65 |
| 1:A:185:SER:CB | 1:A:186:PRO:HD2 | 2.27 | 0.65 |
| 1:A:185:SER:HB2 | 1:A:186:PRO:CD | 2.26 | 0.65 |
| 1:A:271:ARG:HH11 | 1:A:271:ARG:HG2 | 1.61 | 0.65 |
| 1:A:334:GLU:O | 1:A:335:LYS:HG3 | 1.95 | 0.65 |
| 1:B:25:VAL:HG13 | 1:B:31:SER:CB | 2.26 | 0.65 |
| 1:A:67:MET:O | 1:A:70:VAL:HG22 | 1.96 | 0.65 |
| 1:A:194:LYS:C | 1:A:196:ASP:H | 1.99 | 0.65 |
| 1:B:185:SER:CB | 1:B:186:PRO:HD2 | 2.25 | 0.65 |
| 1:A:104:ARG:CZ | 2:C:36:A:N6 | 2.60 | 0.65 |
| 1:B:194:LYS:C | 1:B:196:ASP:H | 1.99 | 0.65 |
| 1:B:353:TYR:HD2 | 1:B:459:TYR:HH | 1.44 | 0.65 |
| 1:A:192:ASN:HD22 | 1:A:204:HIS:CE1 | 2.14 | 0.65 |
| 1:B:13:GLN:O | 1:B:15:LEU:N | 2.30 | 0.65 |
| 2:D:64:U:H2' | 2:D:65:A:H8 | 1.61 | 0.65 |
| 2:C:22:A:C6 | 2:C:49:C:C6 | 2.85 | 0.64 |
| 2:C:44:C:H2' | 2:C:45:C:C6 | 2.33 | 0.64 |
| 1:B:149:TYR:CE2 | 1:B:228:MET:HG3 | 2.33 | 0.64 |
| 2:C:63:C:O2' | 2:C:64:U:HG5' | 1.98 | 0.64 |
| 1:A:13:GLN:O | 1:A:15:LEU:N | 2.30 | 0.64 |
| 1:A:195:ASP:OD1 | 1:A:204:HIS:HD2 | 1.81 | 0.64 |
| 1:A:21:VAL:HG11 | 1:A:38:PHE:HE2 | 1.63 | 0.64 |
| 1:A:127:HIS:HD2 | 1:A:165:ARG:HD3 | 1.62 | 0.64 |
| 1:B:241:ASP:HB3 | 1:B:245:LYS:HZ1 | 1.60 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:107:ARG:NH2 | 2:C:35:C:O2' | 2.30 | 0.63 |
| 1:A:456:LEU:CD1 | 1:A:458:GLN:HG2 | 2.28 | 0.63 |
| 1:A:33:ALA:O | 1:A:37:VAL:HG23 | 1.98 | 0.63 |
| 1:A:141:VAL:HG11 | 1:B:210:LEU:HD12 | 1.79 | 0.63 |
| 1:B:289:THR:CB | 2:D:39:A:H2' | 2.29 | 0.63 |
| 2:C:22:A:N6 | 2:C:47:G:H1' | 2.13 | 0.63 |
| 1:B:258:ILE:HG12 | 1:B:322:ASP:O | 1.98 | 0.63 |
| 2:C:18:G:H2' | 2:C:58:G:H22 | 1.62 | 0.63 |
| 1:A:115:MET:HE1 | 1:A:160:GLY:N | 2.11 | 0.63 |
| 2:D:13:C:H2' | 2:D:14:A:H5' | 1.80 | 0.63 |
| 1:A:145:THR:HA | 1:A:149:TYR:CB | 2.28 | 0.63 |
| 1:A:432:ARG:HD3 | 1:A:444:PHE:HE1 | 1.63 | 0.63 |
| 1:B:274:GLN:HA | 2:D:39:A:N6 | 2.13 | 0.63 |
| 1:B:220:ARG:CZ | 1:B:220:ARG:HA | 2.28 | 0.63 |
| 2:D:44:C:H2' | 2:D:45:C:C6 | 2.33 | 0.63 |
| 1:A:156:ARG:NH1 | 2:C:37:U:H5' | 2.14 | 0.63 |
| 1:B:139:ARG:HH12 | 2:D:36:A:C1' | 2.11 | 0.63 |
| 1:A:411:ILE:HG12 | 1:A:420:ARG:NH2 | 2.13 | 0.63 |
| 1:A:104:ARG:CZ | 2:C:36:A:C6 | 2.82 | 0.62 |
| 1:B:89:PRO:O | 1:B:93:ARG:HG3 | 1.97 | 0.62 |
| 1:B:417:ARG:HA | 1:B:420:ARG:HG3 | 1.79 | 0.62 |
| 2:C:12:U:H2' | 2:C:12:U:O2 | 1.98 | 0.62 |
| 1:A:107:ARG:O | 1:A:111:PHE:HD1 | 1.81 | 0.62 |
| 1:A:139:ARG:NH1 | 2:C:36:A:H1' | 2.14 | 0.62 |
| 1:A:271:ARG:HH11 | 1:A:271:ARG:HG3 | 1.64 | 0.62 |
| 2:C:62:C:HO2' | 2:C:63:C:H6 | 1.47 | 0.62 |
| 1:A:14:LEU:HD13 | 1:A:162:TYR:CE1 | 2.34 | 0.62 |
| 2:C:49:C:N3 | 2:C:60:G:O4' | 2.32 | 0.62 |
| 2:D:75:C:H2' | 2:D:76:C:O4' | 1.99 | 0.62 |
| 2:C:59:A:C5 | 2:C:62:C:N4 | 2.67 | 0.62 |
| 1:A:42:ARG:NH1 | 1:A:48:GLN:N | 2.47 | 0.62 |
| 1:B:281:TYR:OH | 1:B:315:LEU:HD12 | 2.00 | 0.62 |
| 1:B:287:THR:O | 1:B:292:HIS:HD2 | 1.82 | 0.62 |
| 2:C:43:U:H2' | 2:C:44:C:H6 | 1.62 | 0.62 |
| 1:A:25:VAL:HG13 | 1:A:31:SER:CB | 2.27 | 0.62 |
| 1:B:42:ARG:NH1 | 1:B:48:GLN:N | 2.47 | 0.62 |
| 1:B:289:THR:O | 1:B:290:SER:C | 2.38 | 0.62 |
| 2:C:19:G:N2 | 2:C:58:G:H1' | 2.13 | 0.62 |
| 2:D:12:U:O2 | 2:D:12:U:H2' | 1.99 | 0.62 |
| 2:D:22:A:N6 | 2:D:47:G:H1' | 2.15 | 0.62 |
| 1:B:21:VAL:HG11 | 1:B:38:PHE:HE2 | 1.65 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:165:ARG:NH2 | 2:D:37:U:OP1 | 2.33 | 0.62 |
| 1:B:320:SER:HA | 1:B:417:ARG:HH22 | 1.65 | 0.62 |
| 1:B:456:LEU:CD1 | 1:B:458:GLN:HG2 | 2.29 | 0.62 |
| 2:C:59:A:C6 | 2:C:62:C:C4 | 2.87 | 0.62 |
| 1:B:139:ARG:NH1 | 2:D:36:A:C1' | 2.64 | 0.61 |
| 2:C:75:C:H2' | 2:C:76:C:O4' | 2.00 | 0.61 |
| 2:D:59:A:C5 | 2:D:62:C:N4 | 2.68 | 0.61 |
| 1:A:29:PRO:HG3 | 1:A:187:ARG:O | 2.01 | 0.61 |
| 1:A:363:TYR:CD2 | 1:A:364:PRO:HD2 | 2.34 | 0.61 |
| 1:B:8:PHE:CG | 1:B:169:ALA:HB2 | 2.36 | 0.61 |
| 2:D:59:A:C6 | 2:D:62:C:C4 | 2.89 | 0.61 |
| 2:D:63:C:O2' | 2:D:64:U:C5' | 2.47 | 0.61 |
| 1:A:275:LEU:N | 1:A:275:LEU:HD23 | 2.16 | 0.61 |
| 1:A:317:VAL:C | 1:A:318:ILE:HD12 | 2.21 | 0.61 |
| 1:B:391:ARG:O | 2:D:68:A:OP1 | 2.19 | 0.61 |
| 2:C:19:G:H5' | 2:C:61:U:O4 | 2.01 | 0.61 |
| 2:D:8:U:H2' | 2:D:8:U:O2 | 2.01 | 0.61 |
| 1:B:41:LEU:HD13 | 1:B:44:GLU:CD | 2.21 | 0.61 |
| 1:B:416:PRO:O | 1:B:420:ARG:HG2 | 2.00 | 0.61 |
| 1:A:129:GLY:O | 1:A:133:VAL:HG23 | 2.01 | 0.61 |
| 1:A:208:PRO:O | 1:A:212:GLN:HG3 | 2.00 | 0.61 |
| 1:A:137:LEU:HD12 | 1:A:137:LEU:H | 1.65 | 0.61 |
| 1:A:425:ILE:CG2 | 1:A:433:ILE:HG23 | 2.30 | 0.61 |
| 1:B:199:ARG:CZ | 2:D:35:C:H5" | 2.31 | 0.61 |
| 1:B:343:VAL:HG23 | 1:B:357:SER:HB2 | 1.82 | 0.61 |
| 1:A:15:LEU:HD22 | 1:A:164:ILE:CG2 | 2.30 | 0.61 |
| 1:A:89:PRO:O | 1:A:93:ARG:HG3 | 1.99 | 0.61 |
| 1:A:269:GLN:NE2 | 1:A:297:LEU:HD21 | 2.16 | 0.61 |
| 1:B:197:TYR:HB2 | 1:B:200:ASN:OD1 | 1.99 | 0.61 |
| 1:B:397:LEU:O | 1:B:399:GLY:N | 2.33 | 0.61 |
| 2:C:63:C:O2' | 2:C:64:U:C5' | 2.49 | 0.61 |
| 1:B:29:PRO:HG3 | 1:B:187:ARG:O | 2.00 | 0.61 |
| 1:B:271:ARG:HH11 | 1:B:271:ARG:HG2 | 1.64 | 0.61 |
| 2:D:35:C:OP2 | 2:D:35:C:H4' | 2.01 | 0.61 |
| 1:B:278:LEU:HD12 | 1:B:278:LEU:O | 2.00 | 0.60 |
| 1:B:34:LEU:HA | 1:B:167:PHE:CE1 | 2.36 | 0.60 |
| 2:C:9:A:C2 | 2:C:46:G:C2 | 2.89 | 0.60 |
| 1:A:343:VAL:HG23 | 1:A:357:SER:HB2 | 1.82 | 0.60 |
| 1:B:14:LEU:CB | 1:B:155:LYS:HE3 | 2.31 | 0.60 |
| 1:B:152:ILE:CD1 | 2:D:36:A:H4' | 2.31 | 0.60 |
| 1:B:195:ASP:OD1 | 1:B:204:HIS:HD2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:19:G:N2 | 2:D:58:G:H1' | 2.16 | 0.60 |
| 2:D:22:A:C6 | 2:D:49:C:C6 | 2.88 | 0.60 |
| 1:A:3:ASP:HA | 1:A:6:ARG:HB3 | 1.83 | 0.60 |
| 1:B:165:ARG:NH2 | 2:D:37:U:P | 2.75 | 0.60 |
| 1:A:149:TYR:HE2 | 1:A:228:MET:CG | 2.15 | 0.60 |
| 1:B:149:TYR:CG | 1:B:150:ALA:N | 2.68 | 0.60 |
| 2:C:35:C:OP2 | 2:C:35:C:O4' | 2.20 | 0.60 |
| 1:A:310:ASP:O | 1:A:311:LEU:HD23 | 2.02 | 0.60 |
| 2:C:65:A:H2' | 2:C:66:C:C6 | 2.37 | 0.60 |
| 2:D:37:U:O2' | 2:D:38:A:P | 2.59 | 0.60 |
| 1:A:205:HIS:O | 1:A:209:LEU:HG | 2.01 | 0.59 |
| 1:A:278:LEU:HD12 | 1:A:278:LEU:O | 2.01 | 0.59 |
| 1:A:288:LEU:HB2 | 1:A:291:VAL:CG2 | 2.30 | 0.59 |
| 1:B:145:THR:HA | 1:B:149:TYR:CB | 2.32 | 0.59 |
| 2:C:13:C:H5" | 2:C:13:C:H6 | 1.65 | 0.59 |
| 1:B:288:LEU:HB2 | 1:B:291:VAL:CG2 | 2.32 | 0.59 |
| 1:B:291:VAL:CG2 | 1:B:292:HIS:N | 2.65 | 0.59 |
| 2:D:43:U:H2' | 2:D:44:C:C6 | 2.38 | 0.59 |
| 1:A:289:THR:O | 1:A:290:SER:C | 2.40 | 0.59 |
| 1:A:139:ARG:HH12 | 2:C:36:A:H1' | 1.67 | 0.59 |
| 1:B:3:ASP:HA | 1:B:6:ARG:HB3 | 1.84 | 0.59 |
| 1:B:137:LEU:HD12 | 1:B:137:LEU:H | 1.67 | 0.59 |
| 1:B:425:ILE:CG2 | 1:B:433:ILE:HG23 | 2.33 | 0.59 |
| 1:A:1:MET:HA | 1:A:5:VAL:HG12 | 1.85 | 0.59 |
| 1:B:289:THR:CG2 | 2:D:39:A:C8 | 2.84 | 0.59 |
| 1:A:291:VAL:CG2 | 1:A:292:HIS:N | 2.65 | 0.59 |
| 1:A:437:PRO:CB | 1:A:459:TYR:CD1 | 2.82 | 0.59 |
| 1:B:45:TRP:O | 1:B:47:LEU:HD22 | 2.01 | 0.59 |
| 1:B:127:HIS:CD2 | 1:B:165:ARG:NH1 | 2.67 | 0.59 |
| 2:D:9:A:C2 | 2:D:46:G:C2 | 2.91 | 0.59 |
| 2:D:19:G:H5' | 2:D:61:U:O4 | 2.03 | 0.59 |
| 1:B:353:TYR:HD2 | 1:B:459:TYR:CZ | 2.21 | 0.59 |
| 1:A:197:TYR:HB2 | 1:A:200:ASN:OD1 | 2.02 | 0.58 |
| 1:A:86:ILE:HG21 | 1:A:88:VAL:HG22 | 1.85 | 0.58 |
| 1:B:149:TYR:HE2 | 1:B:228:MET:CG | 2.14 | 0.58 |
| 1:A:214:ASN:OD1 | 2:D:41:C:H4' | 2.03 | 0.58 |
| 2:D:13:C:H5" | 2:D:13:C:H6 | 1.68 | 0.58 |
| 1:A:14:LEU:CB | 1:A:155:LYS:HE3 | 2.34 | 0.58 |
| 1:A:327:THR:HG23 | 1:A:329:ASP:CB | 2.31 | 0.58 |
| 1:B:310:ASP:O | 1:B:311:LEU:HD23 | 2.03 | 0.58 |
| 1:A:22:ILE:HD13 | 1:A:114:LEU:HB2 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:291:VAL:HG23 | 1:B:292:HIS:N | 2.18 | 0.58 |
| 2:D:62:C:O2' | 2:D:63:C:H6 | 1.86 | 0.58 |
| 2:C:49:C:N3 | 2:C:60:G:C1' | 2.66 | 0.58 |
| 1:A:41:LEU:HD13 | 1:A:44:GLU:CD | 2.23 | 0.58 |
| 1:A:274:GLN:HA | 2:C:39:A:N6 | 2.19 | 0.58 |
| 1:B:337:TYR:H | 1:B:388:THR:CG2 | 2.17 | 0.58 |
| 1:B:80:LEU:HD12 | 1:B:81:CYS:N | 2.19 | 0.58 |
| 1:B:372:TRP:HA | 1:B:457:LEU:O | 2.04 | 0.58 |
| 1:B:363:TYR:HE1 | 1:B:448:ASN:HA | 1.68 | 0.58 |
| 1:B:456:LEU:HD11 | 1:B:458:GLN:HG2 | 1.85 | 0.58 |
| 2:C:44:C:C2 | 2:C:45:C:C5 | 2.92 | 0.58 |
| 1:A:320:SER:HA | 1:A:417:ARG:HH22 | 1.68 | 0.57 |
| 1:B:14:LEU:HD13 | 1:B:162:TYR:CE1 | 2.37 | 0.57 |
| 1:B:247:MET:CE | 1:B:247:MET:HA | 2.34 | 0.57 |
| 2:D:20:U:OP1 | 2:D:21:U:H5 | 1.87 | 0.57 |
| 1:A:247:MET:HA | 1:A:247:MET:CE | 2.34 | 0.57 |
| 1:B:240:ALA:O | 1:B:243:LEU:HB3 | 2.04 | 0.57 |
| 1:A:387:ARG:NE | 1:A:390:ARG:HH21 | 2.03 | 0.57 |
| 1:A:404:LYS:HG2 | 1:A:405:LYS:N | 2.17 | 0.57 |
| 2:D:44:C:C2 | 2:D:45:C:C5 | 2.92 | 0.57 |
| 1:A:34:LEU:HA | 1:A:167:PHE:CE1 | 2.40 | 0.57 |
| 1:A:456:LEU:HD11 | 1:A:458:GLN:HG2 | 1.86 | 0.57 |
| 1:B:9:ILE:HD13 | 1:B:166:PRO:HB3 | 1.85 | 0.57 |
| 1:B:278:LEU:CD1 | 1:B:282:GLY:HA2 | 2.34 | 0.57 |
| 2:C:40:C:H2' | 2:C:41:C:H6 | 1.70 | 0.57 |
| 1:B:180:ARG:CB | 1:B:187:ARG:HE | 2.18 | 0.57 |
| 1:B:205:HIS:O | 1:B:209:LEU:HG | 2.04 | 0.57 |
| 1:A:180:ARG:CB | 1:A:187:ARG:HE | 2.18 | 0.57 |
| 1:A:337:TYR:H | 1:A:388:THR:CG2 | 2.18 | 0.57 |
| 1:B:460:GLN:HG2 | 1:B:461:ALA:H | 1.69 | 0.57 |
| 2:D:52:A:C2 | 2:D:53:G:C8 | 2.93 | 0.57 |
| 1:A:18:GLY:H | 1:A:46:LYS:NZ | 2.03 | 0.57 |
| 1:A:291:VAL:HG23 | 1:A:292:HIS:N | 2.20 | 0.57 |
| 1:B:327:THR:HG23 | 1:B:329:ASP:CB | 2.35 | 0.57 |
| 1:A:241:ASP:HB3 | 1:A:245:LYS:HZ1 | 1.65 | 0.57 |
| 1:A:278:LEU:CD1 | 1:A:282:GLY:HA2 | 2.35 | 0.57 |
| 1:A:315:LEU:HA | 1:A:328:PHE:HA | 1.87 | 0.57 |
| 1:A:378:ALA:O | 1:A:380:VAL:N | 2.37 | 0.57 |
| 1:B:12:HIS:O | 1:B:13:GLN:O | 2.21 | 0.57 |
| 1:A:400:THR:O | 1:A:402:GLY:N | 2.37 | 0.57 |
| 2:D:65:A:H2' | 2:D:66:C:C6 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:397:LEU:HD12 | 1:A:402:GLY:N | 2.19 | 0.56 |
| 1:A:20:ALA:CB | 1:A:120:ALA:HA | 2.35 | 0.56 |
| 1:A:337:TYR:CZ | 1:A:349:LEU:HD22 | 2.41 | 0.56 |
| 1:B:149:TYR:OH | 1:B:224:TYR:CZ | 2.57 | 0.56 |
| 2:C:17:U:O4' | 2:C:17:U:OP1 | 2.23 | 0.56 |
| 1:A:333:GLY:O | 1:A:334:GLU:CB | 2.52 | 0.56 |
| 1:A:460:GLN:HG2 | 1:A:461:ALA:H | 1.70 | 0.56 |
| 1:B:107:ARG:CG | 1:B:111:PHE:HE1 | 2.16 | 0.56 |
| 2:D:66:C:O2' | 2:D:67:A:H5' | 2.05 | 0.56 |
| 2:C:43:U:H2' | 2:C:44:C:C6 | 2.41 | 0.56 |
| 1:A:220:ARG:HA | 1:A:220:ARG:CZ | 2.36 | 0.56 |
| 1:A:338:TRP:O | 1:A:339:PHE:HD2 | 1.88 | 0.56 |
| 1:A:142:ARG:HE | 2:C:40:C:H1' | 1.70 | 0.56 |
| 1:B:42:ARG:HD2 | 1:B:49:VAL:CG2 | 2.35 | 0.56 |
| 1:B:261:PHE:C | 1:B:261:PHE:CD2 | 2.79 | 0.56 |
| 1:B:274:GLN:HG2 | 1:B:293:ILE:HD11 | 1.88 | 0.56 |
| 2:D:49:C:N3 | 2:D:60:G:C1' | 2.69 | 0.56 |
| 1:A:127:HIS:CD2 | 1:A:165:ARG:HD3 | 2.41 | 0.56 |
| 1:A:25:VAL:O | 1:A:53:HIS:CD2 | 2.59 | 0.56 |
| 1:B:42:ARG:CZ | 1:B:47:LEU:HG | 2.36 | 0.56 |
| 1:B:129:GLY:O | 1:B:133:VAL:HG23 | 2.06 | 0.56 |
| 1:B:338:TRP:O | 1:B:339:PHE:HD2 | 1.88 | 0.56 |
| 2:D:49:C:N3 | 2:D:60:G:O4' | 2.38 | 0.56 |
| 2:C:37:U:O2' | 2:C:38:A:P | 2.64 | 0.55 |
| 1:B:206:ILE:O | 1:B:210:LEU:HD23 | 2.06 | 0.55 |
| 1:B:275:LEU:N | 1:B:275:LEU:HD23 | 2.20 | 0.55 |
| 1:B:289:THR:N | 2:D:39:A:H2' | 2.21 | 0.55 |
| 1:B:333:GLY:O | 1:B:334:GLU:CB | 2.53 | 0.55 |
| 2:C:20:U:OP1 | 2:C:21:U:H5 | 1.88 | 0.55 |
| 1:A:289:THR:CG2 | 2:C:39:A:H2' | 2.36 | 0.55 |
| 1:B:127:HIS:HD2 | 1:B:165:ARG:HH11 | 1.45 | 0.55 |
| 1:B:337:TYR:H | 1:B:388:THR:HG23 | 1.72 | 0.55 |
| 1:B:223:GLN:O | 1:B:223:GLN:HG3 | 2.05 | 0.55 |
| 1:B:321:TYR:CE2 | 1:B:414:LYS:HB3 | 2.42 | 0.55 |
| 1:B:432:ARG:HD3 | 1:B:444:PHE:CE1 | 2.41 | 0.55 |
| 2:C:35:C:OP2 | 2:C:35:C:H4' | 2.06 | 0.55 |
| 1:B:45:TRP:O | 1:B:46:LYS:HB3 | 2.06 | 0.55 |
| 1:B:289:THR:N | 2:D:39:A:O2' | 2.35 | 0.55 |
| 1:B:311:LEU:HB3 | 1:B:312:PRO:CD | 2.36 | 0.55 |
| 1:B:317:VAL:C | 1:B:318:ILE:HD12 | 2.26 | 0.55 |
| 2:D:35:C:OP2 | 2:D:35:C:O4' | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:12:HIS:O | 1:A:13:GLN:O | 2.24 | 0.55 |
| 1:B:13:GLN:C | 1:B:15:LEU:H | 2.10 | 0.55 |
| 1:B:180:ARG:HB2 | 1:B:187:ARG:HE | 1.72 | 0.55 |
| 1:B:394:ARG:HG2 | 1:B:394:ARG:HH11 | 1.72 | 0.55 |
| 1:A:311:LEU:HD13 | 1:A:312:PRO:HD2 | 1.87 | 0.55 |
| 1:B:152:ILE:HD12 | 2:D:36:A:H4' | 1.88 | 0.55 |
| 1:A:206:ILE:O | 1:A:210:LEU:HD23 | 2.07 | 0.55 |
| 1:A:303:GLY:O | 1:A:305:PRO:HD3 | 2.07 | 0.55 |
| 1:B:22:ILE:HD13 | 1:B:114:LEU:HB2 | 1.88 | 0.55 |
| 1:A:353:TYR:HD2 | 1:A:459:TYR:CZ | 2.25 | 0.55 |
| 1:B:210:LEU:O | 1:B:213:GLU:N | 2.40 | 0.55 |
| 1:A:197:TYR:O | 1:A:200:ASN:N | 2.39 | 0.54 |
| 1:A:340:GLU:O | 1:A:342:PRO:HD3 | 2.07 | 0.54 |
| 1:A:404:LYS:HD3 | 1:A:409:ILE:HG12 | 1.89 | 0.54 |
| 1:A:8:PHE:CD2 | 1:A:169:ALA:HB2 | 2.42 | 0.54 |
| 1:A:9:ILE:HD13 | 1:A:166:PRO:HB3 | 1.88 | 0.54 |
| 1:A:13:GLN:C | 1:A:15:LEU:H | 2.10 | 0.54 |
| 2:C:8:U:H2' | 2:C:8:U:O2 | 2.06 | 0.54 |
| 2:C:52:A:C2 | 2:C:53:G:C8 | 2.95 | 0.54 |
| 1:A:24:GLY:HA2 | 1:A:52:ALA:O | 2.07 | 0.54 |
| 1:A:80:LEU:HD12 | 1:A:81:CYS:N | 2.23 | 0.54 |
| 1:A:102:ALA:HA | 1:A:105:ILE:CG1 | 2.38 | 0.54 |
| 1:A:336:GLY:HA2 | 1:A:388:THR:HG21 | 1.89 | 0.54 |
| 1:A:353:TYR:HD2 | 1:A:459:TYR:HH | 1.55 | 0.54 |
| 1:B:23:VAL:HG21 | 1:B:34:LEU:HD22 | 1.89 | 0.54 |
| 1:B:67:MET:O | 1:B:71:LYS:HG2 | 2.08 | 0.54 |
| 2:D:52:A:N3 | 2:D:53:G:C8 | 2.76 | 0.54 |
| 1:A:21:VAL:HG11 | 1:A:38:PHE:CE2 | 2.42 | 0.54 |
| 1:A:74:CYS:HB3 | 1:A:81:CYS:HB2 | 1.78 | 0.54 |
| 1:B:135:THR:OG1 | 1:B:152:ILE:HD11 | 2.08 | 0.54 |
| 1:B:337:TYR:CZ | 1:B:349:LEU:HD22 | 2.43 | 0.54 |
| 1:B:411:ILE:HG12 | 1:B:420:ARG:NH2 | 2.22 | 0.54 |
| 1:B:1:MET:C | 1:B:3:ASP:H | 2.11 | 0.54 |
| 1:B:25:VAL:CG1 | 1:B:31:SER:HB2 | 2.33 | 0.54 |
| 1:B:65:GLU:O | 1:B:69:PHE:HD1 | 1.90 | 0.54 |
| 1:B:87:ASP:CA | 1:B:89:PRO:HD2 | 2.38 | 0.54 |
| 1:B:209:LEU:HA | 1:B:212:GLN:NE2 | 2.23 | 0.54 |
| 2:C:13:C:H2' | 2:C:14:A:H5' | 1.89 | 0.54 |
| 2:D:13:C:C2' | 2:D:14:A:H5' | 2.38 | 0.54 |
| 1:A:149:TYR:CG | 1:A:150:ALA:N | 2.73 | 0.54 |
| 1:A:456:LEU:C | 1:A:457:LEU:HD22 | 2.28 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:128:HIS:O | 1:A:131:ASP:HB2 | 2.08 | 0.54 |
| 1:A:269:GLN:HE21 | 1:A:297:LEU:HD21 | 1.72 | 0.54 |
| 1:B:87:ASP:HA | 1:B:89:PRO:HD2 | 1.89 | 0.54 |
| 1:B:197:TYR:O | 1:B:200:ASN:N | 2.40 | 0.54 |
| 2:C:52:A:H2' | 2:C:53:G:H8 | 1.72 | 0.54 |
| 2:D:40:C:H2' | 2:D:41:C:H6 | 1.73 | 0.54 |
| 1:B:21:VAL:HG11 | 1:B:38:PHE:CE2 | 2.43 | 0.54 |
| 1:B:21:VAL:HG21 | 1:B:38:PHE:CE2 | 2.43 | 0.54 |
| 2:C:62:C:O2' | 2:C:63:C:H6 | 1.90 | 0.54 |
| 1:A:375:VAL:HG23 | 1:A:455:ILE:HB | 1.89 | 0.54 |
| 1:A:416:PRO:O | 1:A:419:GLU:HB2 | 2.08 | 0.54 |
| 1:A:42:ARG:NH1 | 1:A:48:GLN:H | 2.06 | 0.54 |
| 1:A:180:ARG:HB2 | 1:A:187:ARG:HE | 1.71 | 0.54 |
| 1:B:1:MET:HA | 1:B:5:VAL:HG12 | 1.89 | 0.54 |
| 1:B:410:PHE:HB3 | 1:B:420:ARG:HD2 | 1.89 | 0.54 |
| 1:B:456:LEU:C | 1:B:456:LEU:HD13 | 2.28 | 0.54 |
| 1:A:87:ASP:CA | 1:A:89:PRO:HD2 | 2.38 | 0.53 |
| 1:A:217:LEU:C | 1:A:219:GLU:H | 2.11 | 0.53 |
| 1:B:107:ARG:CG | 1:B:111:PHE:CE1 | 2.90 | 0.53 |
| 1:B:127:HIS:CD2 | 1:B:165:ARG:HD3 | 2.41 | 0.53 |
| 1:B:437:PRO:CB | 1:B:459:TYR:CD1 | 2.89 | 0.53 |
| 1:A:1:MET:H2 | 1:A:4:LYS:HB2 | 1.70 | 0.53 |
| 1:A:147:LYS:HA | 1:A:232:GLU:OE1 | 2.08 | 0.53 |
| 1:B:302:ARG:HB2 | 1:B:319:ARG:HH12 | 1.73 | 0.53 |
| 1:A:45:TRP:O | 1:A:46:LYS:HB3 | 2.08 | 0.53 |
| 1:A:100:GLN:OE1 | 2:C:35:C:H1' | 2.09 | 0.53 |
| 1:B:207:VAL:HB | 1:B:208:PRO:HD3 | 1.91 | 0.53 |
| 1:A:42:ARG:CZ | 1:A:47:LEU:HG | 2.38 | 0.53 |
| 1:A:311:LEU:HB3 | 1:A:312:PRO:CD | 2.38 | 0.53 |
| 1:B:248:GLU:HB2 | 1:B:255:ALA:HB3 | 1.90 | 0.53 |
| 1:B:407:LYS:HG2 | 1:B:411:ILE:HD11 | 1.90 | 0.53 |
| 2:C:52:A:N3 | 2:C:53:G:C8 | 2.76 | 0.53 |
| 2:D:17:U:O4' | 2:D:17:U:OP1 | 2.26 | 0.53 |
| 1:B:315:LEU:HA | 1:B:328:PHE:HA | 1.90 | 0.53 |
| 2:D:7:U:O2' | 2:D:8:U:OP1 | 2.26 | 0.53 |
| 1:A:19:ALA:C | 1:A:42:ARG:HH12 | 2.12 | 0.53 |
| 1:A:127:HIS:CD2 | 1:A:165:ARG:NH1 | 2.71 | 0.53 |
| 1:A:127:HIS:HD2 | 1:A:165:ARG:HH11 | 1.51 | 0.53 |
| 1:B:83:THR:HG22 | 1:B:84:ALA:N | 2.24 | 0.53 |
| 1:A:67:MET:O | 1:A:71:LYS:HG2 | 2.09 | 0.53 |
| 1:A:223:GLN:HG3 | 1:A:223:GLN:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:ARG:HB2 | 1:A:319:ARG:HH12 | 1.74 | 0.53 |
| 1:B:42:ARG:NH1 | 1:B:48:GLN:H | 2.07 | 0.53 |
| 1:B:115:MET:HE1 | 1:B:160:GLY:N | 2.18 | 0.53 |
| 2:C:18:G:N2 | 2:C:59:A:C4 | 2.76 | 0.53 |
| 1:A:69:PHE:CD2 | 1:A:72:ARG:HD2 | 2.43 | 0.53 |
| 1:A:258:ILE:HG12 | 1:A:322:ASP:O | 2.08 | 0.53 |
| 1:A:272:VAL:HG23 | 1:A:273:LEU:N | 2.24 | 0.53 |
| 1:B:363:TYR:CD2 | 1:B:364:PRO:HD2 | 2.44 | 0.53 |
| 1:B:397:LEU:O | 1:B:398:LYS:C | 2.47 | 0.53 |
| 1:B:8:PHE:CD2 | 1:B:169:ALA:HB2 | 2.44 | 0.53 |
| 1:B:102:ALA:HA | 1:B:105:ILE:CG1 | 2.38 | 0.53 |
| 2:C:37:U:O2' | 2:C:38:A:C8 | 2.59 | 0.53 |
| 2:D:7:U:H3' | 2:D:8:U:C5' | 2.38 | 0.53 |
| 1:A:87:ASP:HA | 1:A:89:PRO:HD2 | 1.90 | 0.52 |
| 1:A:386:VAL:HB | 1:A:426:VAL:HG22 | 1.90 | 0.52 |
| 1:B:289:THR:HG23 | 2:D:39:A:C4 | 2.44 | 0.52 |
| 1:B:299:LEU:O | 1:B:299:LEU:HD22 | 2.09 | 0.52 |
| 1:B:336:GLY:HA2 | 1:B:388:THR:HG21 | 1.90 | 0.52 |
| 1:A:417:ARG:HA | 1:A:420:ARG:CG | 2.39 | 0.52 |
| 1:A:107:ARG:CG | 1:A:111:PHE:HE1 | 2.21 | 0.52 |
| 1:A:115:MET:CE | 1:A:160:GLY:H | 2.17 | 0.52 |
| 1:A:296:ILE:HD12 | 1:A:317:VAL:HG11 | 1.91 | 0.52 |
| 1:B:20:ALA:CB | 1:B:120:ALA:HA | 2.38 | 0.52 |
| 1:B:69:PHE:CD2 | 1:B:72:ARG:HD2 | 2.45 | 0.52 |
| 1:B:87:ASP:C | 1:B:89:PRO:HD2 | 2.29 | 0.52 |
| 1:B:269:GLN:NE2 | 1:B:297:LEU:HD21 | 2.24 | 0.52 |
| 2:C:51:U:H3' | 2:C:52:A:C8 | 2.41 | 0.52 |
| 2:D:29:A:O2' | 2:D:30:C:H5' | 2.09 | 0.52 |
| 1:A:144:SER:O | 1:A:145:THR:C | 2.47 | 0.52 |
| 1:A:156:ARG:CZ | 2:C:37:U:H5' | 2.40 | 0.52 |
| 1:A:183:GLY:O | 1:A:184:LEU:HD13 | 2.08 | 0.52 |
| 1:B:25:VAL:O | 1:B:53:HIS:CD2 | 2.63 | 0.52 |
| 2:C:9:A:N6 | 2:C:47:G:C2 | 2.78 | 0.52 |
| 1:A:2:ILE:O | 1:A:6:ARG:HB2 | 2.10 | 0.52 |
| 1:A:9:ILE:CG2 | 1:A:15:LEU:HB2 | 2.39 | 0.52 |
| 1:A:25:VAL:CG1 | 1:A:31:SER:HB2 | 2.32 | 0.52 |
| 1:A:217:LEU:C | 1:A:219:GLU:N | 2.63 | 0.52 |
| 1:A:276:LEU:O | 1:A:279:ARG:HB3 | 2.10 | 0.52 |
| 1:A:372:TRP:HA | 1:A:457:LEU:O | 2.09 | 0.52 |
| 1:B:57:MET:HB2 | 1:B:87:ASP:HA | 1.91 | 0.52 |
| 1:B:149:TYR:OH | 1:B:224:TYR:CE2 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:337:TYR:HD2 | 1:B:337:TYR:O | 1.92 | 0.52 |
| 1:B:416:PRO:O | 1:B:419:GLU:HB2 | 2.10 | 0.52 |
| 1:A:65:GLU:O | 1:A:69:PHE:HD1 | 1.93 | 0.52 |
| 1:A:370:ASN:HA | 1:A:441:LYS:HE3 | 1.92 | 0.52 |
| 1:B:128:HIS:O | 1:B:131:ASP:HB2 | 2.10 | 0.52 |
| 1:B:400:THR:O | 1:B:402:GLY:N | 2.42 | 0.52 |
| 1:A:207:VAL:HB | 1:A:208:PRO:HD3 | 1.92 | 0.52 |
| 1:A:397:LEU:O | 1:A:398:LYS:C | 2.48 | 0.52 |
| 1:A:235:LEU:HD23 | 1:A:271:ARG:NH2 | 2.25 | 0.52 |
| 1:B:136:ILE:HD12 | 1:B:149:TYR:HE1 | 1.75 | 0.52 |
| 1:B:183:GLY:O | 1:B:184:LEU:HD13 | 2.10 | 0.52 |
| 1:B:397:LEU:HD12 | 1:B:402:GLY:N | 2.25 | 0.52 |
| 2:D:7:U:H3' | 2:D:8:U:H5' | 1.91 | 0.52 |
| 1:A:149:TYR:O | 1:A:151:GLY:N | 2.44 | 0.51 |
| 1:A:240:ALA:O | 1:A:243:LEU:HB3 | 2.09 | 0.51 |
| 1:A:248:GLU:HB2 | 1:A:255:ALA:HB3 | 1.91 | 0.51 |
| 1:A:289:THR:CB | 2:C:39:A:H2' | 2.40 | 0.51 |
| 1:A:299:LEU:O | 1:A:299:LEU:HD22 | 2.10 | 0.51 |
| 1:A:337:TYR:H | 1:A:388:THR:HG23 | 1.75 | 0.51 |
| 1:B:149:TYR:O | 1:B:151:GLY:N | 2.44 | 0.51 |
| 2:C:29:A:O2' | 2:C:30:C:H5' | 2.10 | 0.51 |
| 2:D:52:A:C2 | 2:D:53:G:C5 | 2.98 | 0.51 |
| 1:A:57:MET:HB2 | 1:A:87:ASP:HA | 1.92 | 0.51 |
| 1:A:88:VAL:O | 1:A:92:GLN:N | 2.42 | 0.51 |
| 1:A:356:ILE:HD11 | 1:A:460:GLN:OE1 | 2.10 | 0.51 |
| 1:A:357:SER:HA | 1:A:456:LEU:O | 2.10 | 0.51 |
| 1:A:104:ARG:HG3 | 2:C:36:A:N1 | 2.24 | 0.51 |
| 1:A:274:GLN:HG2 | 1:A:293:ILE:HD11 | 1.92 | 0.51 |
| 1:B:57:MET:O | 1:B:58:PHE:HB3 | 2.10 | 0.51 |
| 1:B:107:ARG:HG3 | 1:B:111:PHE:CE1 | 2.36 | 0.51 |
| 1:B:315:LEU:HD23 | 1:B:316:LYS:N | 2.25 | 0.51 |
| 1:B:353:TYR:HD2 | 1:B:459:TYR:OH | 1.92 | 0.51 |
| 1:A:315:LEU:HD23 | 1:A:316:LYS:N | 2.26 | 0.51 |
| 1:A:197:TYR:O | 1:A:198:THR:C | 2.48 | 0.51 |
| 1:B:103:ALA:HB1 | 1:B:107:ARG:HH21 | 1.75 | 0.51 |
| 2:C:15:G:H2' | 2:C:60:G:N2 | 2.25 | 0.51 |
| 2:D:37:U:O2' | 2:D:38:A:C8 | 2.61 | 0.51 |
| 1:A:1:MET:C | 1:A:3:ASP:H | 2.13 | 0.51 |
| 1:A:210:LEU:HD12 | 1:B:141:VAL:CG1 | 2.36 | 0.51 |
| 1:A:337:TYR:N | 1:A:388:THR:CG2 | 2.74 | 0.51 |
| 1:A:410:PHE:HB3 | 1:A:420:ARG:NE | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:417:ARG:HA | 1:B:420:ARG:CG | 2.40 | 0.51 |
| 2:C:9:A:C4 | 2:C:46:G:N2 | 2.79 | 0.51 |
| 1:A:45:TRP:C | 1:A:47:LEU:HD22 | 2.31 | 0.51 |
| 1:A:267:PRO:HG2 | 1:B:234:PHE:HB2 | 1.93 | 0.51 |
| 1:A:287:THR:O | 1:A:292:HIS:CD2 | 2.61 | 0.51 |
| 1:B:21:VAL:HB | 1:B:42:ARG:NH2 | 2.26 | 0.51 |
| 1:B:340:GLU:OE2 | 1:B:383:PRO:HG2 | 2.11 | 0.51 |
| 1:A:261:PHE:C | 1:A:261:PHE:CD2 | 2.84 | 0.51 |
| 1:B:338:TRP:C | 1:B:339:PHE:CD2 | 2.76 | 0.51 |
| 1:B:410:PHE:HB3 | 1:B:420:ARG:NE | 2.25 | 0.51 |
| 2:C:18:G:N3 | 2:C:59:A:C2 | 2.79 | 0.51 |
| 2:C:19:G:C5' | 2:C:61:U:O4 | 2.58 | 0.51 |
| 1:A:42:ARG:HD2 | 1:A:49:VAL:CG2 | 2.40 | 0.51 |
| 1:B:149:TYR:OH | 1:B:224:TYR:CD2 | 2.64 | 0.51 |
| 1:B:323:ARG:NH1 | 1:B:325:LEU:HD21 | 2.25 | 0.51 |
| 1:B:341:LEU:HB3 | 1:B:384:LEU:HB2 | 1.93 | 0.51 |
| 1:B:387:ARG:NE | 1:B:390:ARG:HH21 | 2.08 | 0.51 |
| 1:A:266:ARG:O | 1:A:267:PRO:C | 2.49 | 0.51 |
| 1:A:407:LYS:HG2 | 1:A:411:ILE:HD11 | 1.91 | 0.51 |
| 1:A:437:PRO:HB3 | 1:A:459:TYR:CG | 2.45 | 0.51 |
| 1:B:357:SER:HA | 1:B:456:LEU:O | 2.10 | 0.51 |
| 2:C:7:U:O2' | 2:C:8:U:OP1 | 2.29 | 0.51 |
| 2:C:22:A:C5 | 2:C:49:C:C5 | 2.98 | 0.51 |
| 1:A:235:LEU:HD11 | 1:B:235:LEU:CD1 | 2.32 | 0.50 |
| 1:B:456:LEU:HD13 | 1:B:457:LEU:N | 2.26 | 0.50 |
| 1:A:266:ARG:N | 1:A:267:PRO:HD2 | 2.26 | 0.50 |
| 1:A:287:THR:O | 1:A:288:LEU:C | 2.50 | 0.50 |
| 1:A:21:VAL:HB | 1:A:42:ARG:NH2 | 2.27 | 0.50 |
| 1:A:397:LEU:O | 1:A:399:GLY:N | 2.45 | 0.50 |
| 1:A:415:ILE:O | 1:A:420:ARG:HD3 | 2.12 | 0.50 |
| 1:B:220:ARG:HH11 | 1:B:220:ARG:HB3 | 1.77 | 0.50 |
| 2:C:7:U:H3' | 2:C:8:U:C5' | 2.42 | 0.50 |
| 1:A:21:VAL:HG21 | 1:A:38:PHE:CE2 | 2.46 | 0.50 |
| 1:A:107:ARG:CG | 1:A:111:PHE:CE1 | 2.95 | 0.50 |
| 1:A:321:TYR:CE2 | 1:A:414:LYS:HB3 | 2.46 | 0.50 |
| 1:A:340:GLU:OE2 | 1:A:383:PRO:HG2 | 2.11 | 0.50 |
| 1:A:363:TYR:HE1 | 1:A:448:ASN:HA | 1.72 | 0.50 |
| 1:B:2:ILE:O | 1:B:6:ARG:HB2 | 2.11 | 0.50 |
| 1:B:197:TYR:O | 1:B:198:THR:C | 2.48 | 0.50 |
| 1:B:404:LYS:HD3 | 1:B:409:ILE:HG12 | 1.92 | 0.50 |
| 2:C:25:G:C5 | 2:C:26:C:C5 | 2.99 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:49:C:N3 | 2:C:60:G:H1' | 2.26 | 0.50 |
| 2:D:52:A:H2' | 2:D:53:G:H8 | 1.76 | 0.50 |
| 1:A:233:GLN:O | 1:A:233:GLN:HG2 | 2.08 | 0.50 |
| 1:B:428:ASP:HB3 | 1:B:434:LEU:HD11 | 1.92 | 0.50 |
| 1:A:103:ALA:HB1 | 1:A:107:ARG:HH21 | 1.77 | 0.50 |
| 1:A:210:LEU:O | 1:A:213:GLU:N | 2.44 | 0.50 |
| 1:A:394:ARG:HG2 | 1:A:394:ARG:HH11 | 1.76 | 0.50 |
| 1:B:14:LEU:O | 1:B:122:TYR:CZ | 2.65 | 0.50 |
| 1:A:83:THR:HG22 | 1:A:84:ALA:N | 2.26 | 0.50 |
| 1:A:337:TYR:N | 1:A:388:THR:HG21 | 2.27 | 0.50 |
| 1:A:432:ARG:HD3 | 1:A:444:PHE:CE1 | 2.46 | 0.50 |
| 1:A:87:ASP:C | 1:A:89:PRO:HD2 | 2.31 | 0.50 |
| 1:A:209:LEU:HA | 1:A:212:GLN:NE2 | 2.27 | 0.50 |
| 1:A:448:ASN:O | 1:A:449:ARG:C | 2.50 | 0.50 |
| 1:B:57:MET:HE3 | 1:B:57:MET:HA | 1.93 | 0.50 |
| 1:B:104:ARG:CZ | 2:D:36:A:C6 | 2.95 | 0.50 |
| 1:B:356:ILE:HD11 | 1:B:460:GLN:OE1 | 2.12 | 0.50 |
| 2:D:51:U:H3' | 2:D:52:A:C8 | 2.44 | 0.50 |
| 1:A:217:LEU:O | 1:A:219:GLU:N | 2.45 | 0.50 |
| 1:A:289:THR:H | 2:C:39:A:H2' | 1.76 | 0.49 |
| 1:A:410:PHE:HB3 | 1:A:420:ARG:HD2 | 1.94 | 0.49 |
| 1:B:303:GLY:O | 1:B:305:PRO:HD3 | 2.11 | 0.49 |
| 1:A:102:ALA:HA | 1:A:105:ILE:HD11 | 1.94 | 0.49 |
| 1:A:315:LEU:HA | 1:A:328:PHE:CB | 2.42 | 0.49 |
| 1:B:19:ALA:C | 1:B:42:ARG:HH12 | 2.15 | 0.49 |
| 1:B:163:LEU:HD23 | 1:B:163:LEU:O | 2.12 | 0.49 |
| 1:B:410:PHE:HB3 | 1:B:420:ARG:CD | 2.42 | 0.49 |
| 1:B:415:ILE:HD11 | 1:B:439:LEU:HD21 | 1.94 | 0.49 |
| 2:D:15:G:H2' | 2:D:60:G:N2 | 2.27 | 0.49 |
| 2:D:49:C:N3 | 2:D:60:G:H1' | 2.26 | 0.49 |
| 1:A:57:MET:O | 1:A:58:PHE:HB3 | 2.12 | 0.49 |
| 1:B:347:LEU:O | 1:B:354:ALA:HB1 | 2.12 | 0.49 |
| 1:A:14:LEU:O | 1:A:122:TYR:CZ | 2.65 | 0.49 |
| 1:A:242:ALA:O | 1:A:243:LEU:C | 2.51 | 0.49 |
| 1:A:405:LYS:HE2 | 2:C:68:A:OP2 | 2.13 | 0.49 |
| 1:B:13:GLN:O | 1:B:15:LEU:HG | 2.13 | 0.49 |
| 1:B:217:LEU:O | 1:B:219:GLU:N | 2.46 | 0.49 |
| 1:B:217:LEU:C | 1:B:219:GLU:H | 2.15 | 0.49 |
| 2:C:19:G:HO2' | 2:C:20:U:H5" | 1.76 | 0.49 |
| 2:D:65:A:C5 | 2:D:66:C:C5 | 3.01 | 0.49 |
| 1:A:136:ILE:HD12 | 1:A:149:TYR:HE1 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:88:VAL:O | 1:B:92:GLN:N | 2.42 | 0.49 |
| 1:B:207:VAL:O | 1:B:210:LEU:HB2 | 2.11 | 0.49 |
| 1:B:278:LEU:HD12 | 1:B:278:LEU:C | 2.33 | 0.49 |
| 1:A:282:GLY:O | 1:A:283:GLY:C | 2.49 | 0.49 |
| 1:A:375:VAL:HB | 1:A:455:ILE:HD12 | 1.95 | 0.49 |
| 1:B:185:SER:CB | 1:B:186:PRO:CD | 2.85 | 0.49 |
| 1:B:284:VAL:O | 1:B:287:THR:HG22 | 2.12 | 0.49 |
| 1:A:251:HIS:HE1 | 1:A:323:ARG:HH21 | 1.61 | 0.49 |
| 1:A:341:LEU:HB3 | 1:A:384:LEU:HB2 | 1.95 | 0.49 |
| 1:A:428:ASP:HB3 | 1:A:434:LEU:HD11 | 1.95 | 0.49 |
| 1:A:434:LEU:O | 1:A:442:SER:HB3 | 2.13 | 0.49 |
| 1:B:251:HIS:HB2 | 1:B:253:ASP:O | 2.13 | 0.49 |
| 1:B:437:PRO:HB3 | 1:B:459:TYR:CG | 2.48 | 0.49 |
| 1:A:456:LEU:C | 1:A:456:LEU:HD13 | 2.33 | 0.49 |
| 1:B:144:SER:O | 1:B:145:THR:C | 2.49 | 0.49 |
| 1:B:185:SER:O | 1:B:186:PRO:C | 2.51 | 0.49 |
| 1:A:22:ILE:HD13 | 1:A:114:LEU:CB | 2.43 | 0.49 |
| 1:A:185:SER:CB | 1:A:186:PRO:CD | 2.86 | 0.49 |
| 1:B:113:GLU:O | 1:B:117:LYS:HB2 | 2.13 | 0.49 |
| 1:B:115:MET:HE2 | 1:B:159:HIS:HB3 | 1.93 | 0.49 |
| 2:C:39:A:OP1 | 2:C:39:A:C4' | 2.58 | 0.49 |
| 2:D:39:A:OP1 | 2:D:39:A:C4' | 2.59 | 0.49 |
| 1:A:42:ARG:HD3 | 1:A:47:LEU:CB | 2.23 | 0.49 |
| 1:B:247:MET:HA | 1:B:247:MET:HE2 | 1.95 | 0.49 |
| 1:A:142:ARG:NE | 2:C:40:C:H1' | 2.28 | 0.48 |
| 1:A:288:LEU:O | 1:A:289:THR:O | 2.31 | 0.48 |
| 1:B:13:GLN:CG | 1:B:14:LEU:H | 2.18 | 0.48 |
| 1:B:115:MET:CE | 1:B:160:GLY:H | 2.20 | 0.48 |
| 1:A:13:GLN:O | 1:A:15:LEU:HG | 2.12 | 0.48 |
| 1:A:105:ILE:HG13 | 1:A:106:CYS:N | 2.28 | 0.48 |
| 1:A:128:HIS:NE2 | 1:A:172:ARG:NH2 | 2.61 | 0.48 |
| 1:A:247:MET:HE2 | 1:A:256:LEU:HA | 1.95 | 0.48 |
| 1:A:287:THR:C | 1:A:292:HIS:HD2 | 2.15 | 0.48 |
| 1:A:323:ARG:NH1 | 1:A:325:LEU:HD21 | 2.29 | 0.48 |
| 1:B:21:VAL:HG21 | 1:B:38:PHE:HE2 | 1.76 | 0.48 |
| 1:B:128:HIS:NE2 | 1:B:172:ARG:NH2 | 2.61 | 0.48 |
| 1:B:403:THR:OG1 | 2:D:1:G:OP1 | 2.27 | 0.48 |
| 2:C:52:A:C2 | 2:C:53:G:C5 | 3.00 | 0.48 |
| 2:D:5:C:H2' | 2:D:6:U:H6 | 1.77 | 0.48 |
| 1:A:207:VAL:O | 1:A:210:LEU:HB2 | 2.13 | 0.48 |
| 1:B:348:PRO:HA | 1:B:354:ALA:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:67:A:H2' | 2:C:68:A:C8 | 2.48 | 0.48 |
| 1:B:217:LEU:C | 1:B:219:GLU:N | 2.67 | 0.48 |
| 1:B:264:LEU:HD23 | 1:B:265:PRO:HD3 | 1.94 | 0.48 |
| 1:B:340:GLU:O | 1:B:342:PRO:HD3 | 2.13 | 0.48 |
| 2:C:13:C:C2' | 2:C:14:A:H5' | 2.44 | 0.48 |
| 1:B:337:TYR:N | 1:B:388:THR:CG2 | 2.76 | 0.48 |
| 2:D:9:A:C4 | 2:D:46:G:N2 | 2.82 | 0.48 |
| 1:B:22:ILE:HD13 | 1:B:114:LEU:CB | 2.44 | 0.48 |
| 1:B:272:VAL:HG23 | 1:B:273:LEU:N | 2.28 | 0.48 |
| 1:B:375:VAL:HG23 | 1:B:455:ILE:HB | 1.95 | 0.48 |
| 2:C:59:A:N7 | 2:C:62:C:N4 | 2.61 | 0.48 |
| 1:A:18:GLY:N | 1:A:46:LYS:NZ | 2.60 | 0.48 |
| 1:A:288:LEU:O | 1:A:289:THR:C | 2.52 | 0.48 |
| 1:B:18:GLY:H | 1:B:46:LYS:NZ | 2.11 | 0.48 |
| 1:A:278:LEU:HD12 | 1:A:278:LEU:C | 2.34 | 0.48 |
| 1:B:287:THR:O | 1:B:288:LEU:C | 2.52 | 0.48 |
| 1:B:378:ALA:O | 1:B:380:VAL:N | 2.46 | 0.48 |
| 1:A:241:ASP:O | 1:A:242:ALA:C | 2.52 | 0.48 |
| 1:B:266:ARG:HG2 | 1:B:269:GLN:NE2 | 2.29 | 0.48 |
| 2:C:66:C:O2' | 2:C:67:A:H5' | 2.14 | 0.48 |
| 1:A:108:TYR:CE1 | 2:C:36:A:OP2 | 2.67 | 0.48 |
| 1:A:386:VAL:HA | 1:A:425:ILE:O | 2.13 | 0.48 |
| 1:B:202:PHE:CD2 | 1:B:206:ILE:HD12 | 2.48 | 0.48 |
| 1:B:448:ASN:O | 1:B:449:ARG:C | 2.51 | 0.48 |
| 1:A:9:ILE:HG23 | 1:A:15:LEU:HB2 | 1.96 | 0.47 |
| 1:A:251:HIS:CE1 | 1:A:323:ARG:HH21 | 2.32 | 0.47 |
| 1:A:284:VAL:HG23 | 1:A:287:THR:HB | 1.95 | 0.47 |
| 1:A:298:MET:HE2 | 1:A:298:MET:HB2 | 1.74 | 0.47 |
| 1:A:332:SER:HA | 1:A:333:GLY:HA3 | 1.53 | 0.47 |
| 1:A:387:ARG:NE | 1:A:390:ARG:NH2 | 2.62 | 0.47 |
| 1:B:24:GLY:HA2 | 1:B:52:ALA:O | 2.13 | 0.47 |
| 1:B:152:ILE:HG22 | 1:B:165:ARG:HD2 | 1.96 | 0.47 |
| 1:B:251:HIS:HE1 | 1:B:323:ARG:HH21 | 1.60 | 0.47 |
| 2:D:19:G:C5' | 2:D:61:U:O4 | 2.61 | 0.47 |
| 1:A:194:LYS:C | 1:A:196:ASP:N | 2.65 | 0.47 |
| 1:B:288:LEU:CA | 2:D:39:A:O2' | 2.60 | 0.47 |
| 1:B:382:LEU:HD23 | 1:B:382:LEU:N | 2.29 | 0.47 |
| 1:A:18:GLY:H | 1:A:46:LYS:CE | 2.27 | 0.47 |
| 1:A:115:MET:HE2 | 1:A:159:HIS:HB3 | 1.95 | 0.47 |
| 1:A:163:LEU:HD23 | 1:A:163:LEU:O | 2.14 | 0.47 |
| 1:B:9:ILE:CD1 | 1:B:166:PRO:HB3 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:70:VAL:CG2 | 1:B:71:LYS:N | 2.77 | 0.47 |
| 1:B:127:HIS:CE1 | 2:D:36:A:OP1 | 2.67 | 0.47 |
| 1:B:128:HIS:CD2 | 1:B:172:ARG:HB3 | 2.49 | 0.47 |
| 1:B:282:GLY:O | 1:B:283:GLY:C | 2.52 | 0.47 |
| 2:C:7:U:H3' | 2:C:8:U:H5' | 1.96 | 0.47 |
| 2:C:7:U:HO2' | 2:C:8:U:P | 2.37 | 0.47 |
| 2:D:68:A:O5' | 2:D:68:A:H8 | 1.97 | 0.47 |
| 1:A:353:TYR:HD2 | 1:A:459:TYR:OH | 1.97 | 0.47 |
| 1:A:382:LEU:N | 1:A:382:LEU:HD23 | 2.29 | 0.47 |
| 1:B:233:GLN:O | 1:B:233:GLN:HG2 | 2.09 | 0.47 |
| 2:C:65:A:C5 | 2:C:66:C:C5 | 3.02 | 0.47 |
| 2:D:9:A:N6 | 2:D:47:G:C2 | 2.82 | 0.47 |
| 1:A:149:TYR:OH | 1:A:224:TYR:CD2 | 2.65 | 0.47 |
| 1:A:269:GLN:O | 1:A:273:LEU:HG | 2.14 | 0.47 |
| 1:B:102:ALA:HA | 1:B:105:ILE:HD11 | 1.95 | 0.47 |
| 1:B:296:ILE:HD12 | 1:B:317:VAL:HG11 | 1.96 | 0.47 |
| 2:D:7:U:HO2' | 2:D:8:U:P | 2.38 | 0.47 |
| 1:A:22:ILE:HB | 1:A:123:VAL:HG22 | 1.96 | 0.47 |
| 1:A:106:CYS:O | 1:A:107:ARG:C | 2.53 | 0.47 |
| 1:A:185:SER:O | 1:A:186:PRO:C | 2.51 | 0.47 |
| 1:A:251:HIS:HB2 | 1:A:253:ASP:O | 2.15 | 0.47 |
| 1:A:337:TYR:CD1 | 1:A:350:PRO:HG2 | 2.50 | 0.47 |
| 1:A:366:LYS:HD3 | 1:A:372:TRP:CD1 | 2.50 | 0.47 |
| 1:B:21:VAL:HG12 | 1:B:49:VAL:HA | 1.97 | 0.47 |
| 1:B:41:LEU:HD13 | 1:B:44:GLU:OE1 | 2.15 | 0.47 |
| 1:B:50:ILE:HD13 | 1:B:118:HIS:CE1 | 2.50 | 0.47 |
| 1:B:59:ARG:HG2 | 1:B:60:GLY:H | 1.80 | 0.47 |
| 1:B:147:LYS:O | 1:B:150:ALA:HB2 | 2.14 | 0.47 |
| 1:B:269:GLN:O | 1:B:273:LEU:HG | 2.14 | 0.47 |
| 1:B:327:THR:O | 1:B:327:THR:HG22 | 2.15 | 0.47 |
| 2:C:9:A:C6 | 2:C:47:G:C2 | 3.03 | 0.47 |
| 2:D:25:G:C5 | 2:D:26:C:C5 | 3.03 | 0.47 |
| 1:A:23:VAL:HG21 | 1:A:34:LEU:HD22 | 1.97 | 0.47 |
| 1:B:55:ASP:OD1 | 1:B:63:SER:HA | 2.15 | 0.47 |
| 1:B:305:PRO:O | 1:B:319:ARG:HG2 | 2.14 | 0.47 |
| 1:A:128:HIS:CD2 | 1:A:172:ARG:HB3 | 2.50 | 0.47 |
| 1:A:327:THR:HG23 | 1:A:329:ASP:N | 2.30 | 0.47 |
| 1:B:102:ALA:O | 1:B:106:CYS:HB2 | 2.15 | 0.47 |
| 1:A:72:ARG:HE | 1:A:72:ARG:HB3 | 1.43 | 0.47 |
| 1:A:266:ARG:N | 1:A:267:PRO:CD | 2.77 | 0.47 |
| 1:A:289:THR:O | 1:A:292:HIS:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:13:GLN:C | 1:B:15:LEU:N | 2.68 | 0.47 |
| 1:B:88:VAL:N | 1:B:89:PRO:CD | 2.78 | 0.47 |
| 1:B:156:ARG:NH1 | 2:D:37:U:H5' | 2.30 | 0.47 |
| 1:B:404:LYS:HG2 | 1:B:405:LYS:N | 2.30 | 0.47 |
| 2:D:14:A:H2' | 2:D:15:G:O4' | 2.15 | 0.47 |
| 2:D:22:A:C5 | 2:D:49:C:C5 | 3.03 | 0.47 |
| 1:A:139:ARG:HH12 | 2:C:36:A:C1' | 2.28 | 0.46 |
| 1:A:457:LEU:HD22 | 1:A:457:LEU:N | 2.29 | 0.46 |
| 1:B:194:LYS:C | 1:B:196:ASP:N | 2.66 | 0.46 |
| 1:B:315:LEU:HA | 1:B:328:PHE:CB | 2.44 | 0.46 |
| 1:B:432:ARG:CD | 1:B:444:PHE:CE1 | 2.98 | 0.46 |
| 2:C:14:A:H2' | 2:C:15:G:O4' | 2.15 | 0.46 |
| 2:C:60:G:C3' | 2:C:61:U:H5' | 2.42 | 0.46 |
| 1:A:21:VAL:HG21 | 1:A:38:PHE:HE2 | 1.80 | 0.46 |
| 1:A:59:ARG:HG2 | 1:A:60:GLY:H | 1.80 | 0.46 |
| 1:A:88:VAL:N | 1:A:89:PRO:CD | 2.78 | 0.46 |
| 1:A:201:ARG:HD2 | 1:B:213:GLU:OE2 | 2.15 | 0.46 |
| 1:A:242:ALA:O | 1:A:246:VAL:HG23 | 2.15 | 0.46 |
| 1:A:347:LEU:O | 1:A:354:ALA:HB1 | 2.15 | 0.46 |
| 1:B:270:ARG:O | 1:B:273:LEU:HB2 | 2.15 | 0.46 |
| 2:C:75:C:O5' | 2:C:75:C:H6 | 1.98 | 0.46 |
| 1:A:285:PRO:HD2 | 1:A:286:PRO:HD3 | 1.97 | 0.46 |
| 1:A:373:PHE:CD1 | 1:A:435:TRP:CB | 2.95 | 0.46 |
| 1:B:337:TYR:N | 1:B:388:THR:HG21 | 2.31 | 0.46 |
| 1:A:115:MET:CE | 1:A:159:HIS:HB3 | 2.46 | 0.46 |
| 1:A:238:LEU:HD12 | 1:A:238:LEU:H | 1.80 | 0.46 |
| 1:A:247:MET:HA | 1:A:247:MET:HE2 | 1.97 | 0.46 |
| 1:A:410:PHE:HB3 | 1:A:420:ARG:CD | 2.46 | 0.46 |
| 1:B:279:ARG:HE | 1:B:279:ARG:HB2 | 1.48 | 0.46 |
| 1:A:70:VAL:CG2 | 1:A:71:LYS:N | 2.79 | 0.46 |
| 1:A:339:PHE:HD2 | 1:A:339:PHE:N | 2.14 | 0.46 |
| 1:B:242:ALA:O | 1:B:243:LEU:C | 2.53 | 0.46 |
| 2:D:18:G:N2 | 2:D:59:A:C4 | 2.83 | 0.46 |
| 2:D:20:U:O2' | 2:D:21:U:OP2 | 2.30 | 0.46 |
| 2:D:59:A:N7 | 2:D:62:C:N4 | 2.62 | 0.46 |
| 1:A:46:LYS:O | 1:A:47:LEU:CD1 | 2.58 | 0.46 |
| 1:A:104:ARG:HH21 | 2:C:36:A:N6 | 2.12 | 0.46 |
| 1:A:133:VAL:O | 1:A:134:GLU:C | 2.54 | 0.46 |
| 1:B:251:HIS:CE1 | 1:B:323:ARG:HH21 | 2.33 | 0.46 |
| 1:B:276:LEU:O | 1:B:279:ARG:HB3 | 2.16 | 0.46 |
| 1:B:45:TRP:C | 1:B:47:LEU:HD22 | 2.36 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:337:TYR:O | 1:B:388:THR:HG23 | 2.15 | 0.46 |
| 2:C:20:U:O2' | 2:C:21:U:P | 2.73 | 0.46 |
| 1:A:13:GLN:C | 1:A:15:LEU:N | 2.69 | 0.46 |
| 1:A:24:GLY:HA3 | 1:A:111:PHE:HE2 | 1.81 | 0.46 |
| 1:B:198:THR:HG23 | 1:B:201:ARG:NH2 | 2.30 | 0.46 |
| 1:B:266:ARG:N | 1:B:267:PRO:HD2 | 2.30 | 0.46 |
| 1:B:269:GLN:HE21 | 1:B:297:LEU:HD21 | 1.81 | 0.46 |
| 1:A:339:PHE:N | 1:A:339:PHE:CD2 | 2.83 | 0.46 |
| 1:B:107:ARG:O | 1:B:110:PHE:HB3 | 2.16 | 0.46 |
| 1:B:158:PHE:CD2 | 1:B:159:HIS:HB2 | 2.51 | 0.46 |
| 1:B:406:LEU:HA | 1:B:406:LEU:HD12 | 1.68 | 0.46 |
| 1:B:415:ILE:O | 1:B:420:ARG:HD3 | 2.16 | 0.46 |
| 1:A:382:LEU:CB | 1:A:383:PRO:HA | 2.46 | 0.46 |
| 1:B:105:ILE:HG13 | 1:B:106:CYS:N | 2.31 | 0.46 |
| 1:B:261:PHE:CZ | 1:B:269:GLN:HB3 | 2.51 | 0.46 |
| 1:B:426:VAL:O | 1:B:426:VAL:HG12 | 2.13 | 0.46 |
| 2:C:14:A:C2 | 2:C:15:G:H1' | 2.51 | 0.46 |
| 2:D:20:U:O2' | 2:D:21:U:P | 2.73 | 0.46 |
| 1:A:364:PRO:CG | 1:A:374:VAL:HG21 | 2.28 | 0.45 |
| 1:B:128:HIS:O | 1:B:131:ASP:N | 2.48 | 0.45 |
| 1:B:284:VAL:HG23 | 1:B:287:THR:HB | 1.97 | 0.45 |
| 2:D:46:G:H5" | 2:D:47:G:OP2 | 2.16 | 0.45 |
| 1:A:132:GLN:OE1 | 1:A:152:ILE:HG12 | 2.16 | 0.45 |
| 1:A:424:PRO:HG2 | 1:A:437:PRO:HG2 | 1.98 | 0.45 |
| 1:B:46:LYS:O | 1:B:47:LEU:CD1 | 2.58 | 0.45 |
| 1:B:288:LEU:O | 1:B:289:THR:C | 2.54 | 0.45 |
| 2:C:76:C:C5 | 2:C:77:A:N3 | 2.85 | 0.45 |
| 1:A:1:MET:C | 1:A:2:ILE:HG13 | 2.36 | 0.45 |
| 1:A:50:ILE:HD13 | 1:A:118:HIS:CE1 | 2.51 | 0.45 |
| 1:A:128:HIS:O | 1:A:131:ASP:N | 2.49 | 0.45 |
| 1:A:274:GLN:HG2 | 1:A:293:ILE:CD1 | 2.46 | 0.45 |
| 1:A:338:TRP:O | 1:A:339:PHE:CD2 | 2.67 | 0.45 |
| 1:B:274:GLN:HG2 | 1:B:293:ILE:CD1 | 2.46 | 0.45 |
| 1:B:370:ASN:HA | 1:B:441:LYS:HE3 | 1.97 | 0.45 |
| 1:B:403:THR:O | 2:D:1:G:C8 | 2.70 | 0.45 |
| 2:C:68:A:O5' | 2:C:68:A:H8 | 2.00 | 0.45 |
| 1:A:13:GLN:CG | 1:A:14:LEU:H | 2.18 | 0.45 |
| 1:A:264:LEU:HD23 | 1:A:265:PRO:HD3 | 1.97 | 0.45 |
| 1:B:9:ILE:CG2 | 1:B:15:LEU:HB2 | 2.45 | 0.45 |
| 1:B:373:PHE:CD1 | 1:B:435:TRP:CB | 2.93 | 0.45 |
| 1:A:147:LYS:O | 1:A:150:ALA:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:152:ILE:HG22 | 1:A:165:ARG:HD2 | 1.99 | 0.45 |
| 1:A:276:LEU:C | 1:A:276:LEU:HD13 | 2.37 | 0.45 |
| 1:B:22:ILE:HB | 1:B:123:VAL:HG22 | 1.99 | 0.45 |
| 1:B:239:ALA:O | 1:B:240:ALA:C | 2.54 | 0.45 |
| 1:B:337:TYR:C | 1:B:337:TYR:CD2 | 2.90 | 0.45 |
| 1:B:390:ARG:O | 1:B:392:GLY:N | 2.49 | 0.45 |
| 2:D:52:A:N1 | 2:D:53:G:C5 | 2.85 | 0.45 |
| 1:A:18:GLY:O | 1:A:46:LYS:HE3 | 2.17 | 0.45 |
| 1:A:201:ARG:NH1 | 1:B:213:GLU:OE2 | 2.49 | 0.45 |
| 1:A:338:TRP:HA | 1:A:387:ARG:HB3 | 1.99 | 0.45 |
| 1:B:158:PHE:HD1 | 1:B:163:LEU:HB2 | 1.81 | 0.45 |
| 1:B:327:THR:HG23 | 1:B:329:ASP:N | 2.32 | 0.45 |
| 2:D:3:A:H2' | 2:D:4:C:H6 | 1.82 | 0.45 |
| 1:A:42:ARG:NE | 1:A:47:LEU:HB3 | 2.31 | 0.45 |
| 1:B:18:GLY:H | 1:B:46:LYS:CE | 2.30 | 0.45 |
| 1:B:199:ARG:NH1 | 2:D:35:C:H5" | 2.32 | 0.45 |
| 1:A:256:LEU:HD11 | 1:A:261:PHE:HB2 | 1.98 | 0.45 |
| 1:A:270:ARG:NE | 1:B:230:GLU:OE2 | 2.50 | 0.45 |
| 1:A:338:TRP:C | 1:A:339:PHE:CD2 | 2.74 | 0.45 |
| 1:A:425:ILE:HG22 | 1:A:426:VAL:N | 2.31 | 0.45 |
| 1:A:432:ARG:CD | 1:A:444:PHE:CE1 | 2.99 | 0.45 |
| 1:B:337:TYR:CD1 | 1:B:350:PRO:HG2 | 2.52 | 0.45 |
| 1:A:152:ILE:CG2 | 1:A:165:ARG:HD2 | 2.47 | 0.45 |
| 1:A:400:THR:HB | 1:A:401:GLY:H | 1.51 | 0.45 |
| 1:B:41:LEU:HD13 | 1:B:44:GLU:OE2 | 2.17 | 0.45 |
| 1:B:198:THR:CG2 | 2:D:33:C:O2' | 2.62 | 0.45 |
| 1:B:241:ASP:O | 1:B:242:ALA:C | 2.55 | 0.45 |
| 1:B:434:LEU:O | 1:B:442:SER:HB3 | 2.16 | 0.45 |
| 2:D:13:C:H2' | 2:D:14:A:C5' | 2.47 | 0.45 |
| 1:A:250:GLN:C | 1:A:251:HIS:HD2 | 2.21 | 0.45 |
| 1:B:216:ARG:NH2 | 2:C:41:C:OP1 | 2.46 | 0.45 |
| 2:C:47:G:HO2' | 2:C:48:C:P | 2.40 | 0.45 |
| 2:D:9:A:C6 | 2:D:47:G:C2 | 3.05 | 0.45 |
| 2:D:18:G:N3 | 2:D:59:A:C2 | 2.84 | 0.45 |
| 1:A:165:ARG:HH22 | 2:C:37:U:P | 2.40 | 0.44 |
| 1:A:289:THR:HG23 | 2:C:39:A:N9 | 2.32 | 0.44 |
| 1:A:372:TRP:O | 1:A:441:LYS:HE2 | 2.17 | 0.44 |
| 1:B:285:PRO:HD2 | 1:B:286:PRO:HD3 | 1.99 | 0.44 |
| 1:B:386:VAL:HB | 1:B:426:VAL:HG22 | 1.99 | 0.44 |
| 1:A:239:ALA:O | 1:A:240:ALA:C | 2.54 | 0.44 |
| 1:A:337:TYR:O | 1:A:388:THR:HG23 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:18:GLY:N | 1:B:46:LYS:NZ | 2.66 | 0.44 |
| 1:B:235:LEU:HD23 | 1:B:271:ARG:NH2 | 2.32 | 0.44 |
| 2:C:22:A:N1 | 2:C:49:C:C6 | 2.84 | 0.44 |
| 1:B:375:VAL:HB | 1:B:455:ILE:HD12 | 1.99 | 0.44 |
| 1:B:390:ARG:N | 1:B:393:ASP:OD2 | 2.50 | 0.44 |
| 2:C:12:U:O2 | 2:C:12:U:C2' | 2.65 | 0.44 |
| 1:A:158:PHE:C | 1:A:158:PHE:CD2 | 2.91 | 0.44 |
| 1:A:220:ARG:HH11 | 1:A:220:ARG:HB3 | 1.83 | 0.44 |
| 1:A:417:ARG:O | 1:A:420:ARG:N | 2.51 | 0.44 |
| 1:B:311:LEU:HD13 | 1:B:312:PRO:HD2 | 2.00 | 0.44 |
| 1:B:338:TRP:O | 1:B:339:PHE:CD2 | 2.68 | 0.44 |
| 1:B:363:TYR:HD2 | 1:B:364:PRO:O | 2.00 | 0.44 |
| 1:B:394:ARG:HG2 | 1:B:394:ARG:NH1 | 2.33 | 0.44 |
| 2:C:5:C:H2' | 2:C:6:U:H6 | 1.83 | 0.44 |
| 2:D:18:G:C2' | 2:D:58:G:N2 | 2.78 | 0.44 |
| 1:B:42:ARG:NE | 1:B:47:LEU:HB3 | 2.31 | 0.44 |
| 1:B:266:ARG:N | 1:B:267:PRO:CD | 2.80 | 0.44 |
| 1:B:338:TRP:C | 1:B:338:TRP:CD1 | 2.90 | 0.44 |
| 1:B:382:LEU:CB | 1:B:383:PRO:HA | 2.48 | 0.44 |
| 2:C:34:U:H5" | 2:C:35:C:OP1 | 2.18 | 0.44 |
| 1:B:66:GLU:O | 1:B:70:VAL:HG13 | 2.18 | 0.44 |
| 1:B:337:TYR:HD2 | 1:B:337:TYR:C | 2.20 | 0.44 |
| 2:D:37:U:H2' | 2:D:37:U:O2 | 2.18 | 0.44 |
| 2:D:67:A:H2' | 2:D:68:A:C8 | 2.53 | 0.44 |
| 1:A:135:THR:OG1 | 1:A:152:ILE:HD11 | 2.18 | 0.44 |
| 1:A:184:LEU:HD12 | 1:A:184:LEU:HA | 1.72 | 0.44 |
| 1:A:280:LEU:HA | 1:A:280:LEU:HD23 | 1.69 | 0.44 |
| 1:A:305:PRO:O | 1:A:319:ARG:HG2 | 2.18 | 0.44 |
| 1:B:152:ILE:CG2 | 1:B:165:ARG:HD2 | 2.48 | 0.44 |
| 1:B:332:SER:HA | 1:B:333:GLY:HA3 | 1.56 | 0.44 |
| 1:A:57:MET:H | 1:A:89:PRO:HG2 | 1.83 | 0.44 |
| 1:A:390:ARG:N | 1:A:393:ASP:OD2 | 2.50 | 0.44 |
| 1:A:405:LYS:HE3 | 2:C:67:A:OP1 | 2.17 | 0.44 |
| 1:B:287:THR:C | 1:B:292:HIS:HD2 | 2.21 | 0.44 |
| 1:B:403:THR:O | 2:D:1:G:H8 | 2.01 | 0.44 |
| 1:A:41:LEU:HD13 | 1:A:44:GLU:OE1 | 2.17 | 0.44 |
| 1:A:257:SER:O | 1:A:260:PRO:HG2 | 2.18 | 0.44 |
| 1:A:337:TYR:HD1 | 1:A:350:PRO:HG2 | 1.82 | 0.44 |
| 1:A:382:LEU:HB3 | 1:A:383:PRO:HA | 1.99 | 0.44 |
| 1:B:24:GLY:HA3 | 1:B:111:PHE:HE2 | 1.82 | 0.44 |
| 1:B:86:ILE:HG21 | 1:B:88:VAL:HG22 | 1.95 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:266:ARG:O | 1:B:267:PRO:C | 2.56 | 0.44 |
| 1:B:396:VAL:O | 1:B:442:SER:HA | 2.17 | 0.44 |
| 2:D:3:A:H2' | 2:D:4:C:C6 | 2.53 | 0.44 |
| 2:D:76:C:C5 | 2:D:77:A:N3 | 2.86 | 0.44 |
| 1:B:3:ASP:OD1 | 1:B:4:LYS:N | 2.50 | 0.43 |
| 1:B:88:VAL:N | 1:B:89:PRO:HD2 | 2.33 | 0.43 |
| 1:B:220:ARG:HA | 1:B:220:ARG:NH1 | 2.32 | 0.43 |
| 2:D:34:U:H5" | 2:D:35:C:OP1 | 2.17 | 0.43 |
| 1:B:1:MET:C | 1:B:2:ILE:HG13 | 2.38 | 0.43 |
| 1:B:18:GLY:O | 1:B:46:LYS:HE3 | 2.18 | 0.43 |
| 1:B:68:GLU:HA | 1:B:71:LYS:HG3 | 2.00 | 0.43 |
| 1:B:72:ARG:HE | 1:B:72:ARG:HB3 | 1.45 | 0.43 |
| 1:B:133:VAL:O | 1:B:134:GLU:C | 2.56 | 0.43 |
| 1:B:158:PHE:CD2 | 1:B:158:PHE:C | 2.92 | 0.43 |
| 1:B:194:LYS:O | 1:B:196:ASP:N | 2.49 | 0.43 |
| 1:B:203:ARG:NH2 | 2:D:35:C:N4 | 2.66 | 0.43 |
| 1:B:261:PHE:HD2 | 1:B:262:LEU:N | 2.16 | 0.43 |
| 1:B:385:ARG:CZ | 1:B:429:ALA:HA | 2.48 | 0.43 |
| 1:A:83:THR:CG2 | 1:A:84:ALA:N | 2.82 | 0.43 |
| 1:A:289:THR:OG1 | 2:C:39:A:H2' | 2.18 | 0.43 |
| 1:B:276:LEU:CD1 | 1:B:280:LEU:HD12 | 2.48 | 0.43 |
| 1:B:373:PHE:C | 1:B:373:PHE:CD2 | 2.92 | 0.43 |
| 1:B:409:ILE:HG22 | 1:B:410:PHE:N | 2.32 | 0.43 |
| 1:B:456:LEU:C | 1:B:457:LEU:HD22 | 2.39 | 0.43 |
| 2:D:47:G:HO2' | 2:D:48:C:P | 2.42 | 0.43 |
| 1:A:326:PHE:N | 1:A:326:PHE:CD1 | 2.86 | 0.43 |
| 1:B:34:LEU:CA | 1:B:167:PHE:HE1 | 2.31 | 0.43 |
| 1:B:74:CYS:HB3 | 1:B:81:CYS:HB2 | 1.75 | 0.43 |
| 1:B:169:ALA:C | 1:B:170:VAL:HG13 | 2.39 | 0.43 |
| 1:B:242:ALA:O | 1:B:246:VAL:HG23 | 2.18 | 0.43 |
| 1:A:55:ASP:HB2 | 1:A:67:MET:HE3 | 1.99 | 0.43 |
| 1:B:70:VAL:HG23 | 1:B:71:LYS:N | 2.33 | 0.43 |
| 1:B:158:PHE:HD2 | 1:B:159:HIS:N | 2.17 | 0.43 |
| 1:B:250:GLN:C | 1:B:251:HIS:HD2 | 2.21 | 0.43 |
| 1:B:386:VAL:HA | 1:B:425:ILE:O | 2.18 | 0.43 |
| 1:A:104:ARG:NH1 | 2:C:34:U:C2' | 2.80 | 0.43 |
| 1:A:270:ARG:O | 1:A:273:LEU:HB2 | 2.19 | 0.43 |
| 1:A:396:VAL:O | 1:A:442:SER:HA | 2.19 | 0.43 |
| 1:A:415:ILE:HD11 | 1:A:439:LEU:HD21 | 2.00 | 0.43 |
| 2:C:46:G:H5" | 2:C:47:G:OP2 | 2.18 | 0.43 |
| 1:A:147:LYS:HB3 | 1:A:232:GLU:CD | 2.38 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:PHE:HD1 | 1:A:163:LEU:HB2 | 1.84 | 0.43 |
| 1:B:83:THR:CG2 | 1:B:84:ALA:N | 2.81 | 0.43 |
| 1:B:184:LEU:HD12 | 1:B:184:LEU:HA | 1.76 | 0.43 |
| 2:C:59:A:C6 | 2:C:62:C:C5 | 3.06 | 0.43 |
| 2:D:64:U:O2' | 2:D:65:A:H5' | 2.18 | 0.43 |
| 1:A:233:GLN:O | 1:A:236:GLU:HB2 | 2.18 | 0.43 |
| 1:B:52:ALA:HA | 1:B:82:GLU:O | 2.19 | 0.43 |
| 1:B:55:ASP:HB2 | 1:B:67:MET:HE3 | 2.00 | 0.43 |
| 1:B:128:HIS:HA | 1:B:167:PHE:O | 2.18 | 0.43 |
| 1:B:158:PHE:H | 1:B:162:TYR:HA | 1.83 | 0.43 |
| 1:B:276:LEU:HD13 | 1:B:280:LEU:HD12 | 2.00 | 0.43 |
| 1:B:288:LEU:O | 1:B:289:THR:O | 2.37 | 0.43 |
| 1:B:337:TYR:HD1 | 1:B:350:PRO:HG2 | 1.83 | 0.43 |
| 1:B:425:ILE:HG22 | 1:B:426:VAL:N | 2.33 | 0.43 |
| 2:C:25:G:C6 | 2:C:26:C:C4 | 3.07 | 0.43 |
| 2:C:37:U:H2' | 2:C:37:U:O2 | 2.19 | 0.43 |
| 1:A:88:VAL:N | 1:A:89:PRO:HD2 | 2.33 | 0.43 |
| 1:A:155:LYS:HA | 1:A:163:LEU:O | 2.19 | 0.43 |
| 1:A:156:ARG:NH1 | 2:C:37:U:C5' | 2.82 | 0.43 |
| 1:B:132:GLN:OE1 | 1:B:152:ILE:HG12 | 2.19 | 0.43 |
| 1:B:318:ILE:HD12 | 1:B:318:ILE:N | 2.34 | 0.43 |
| 1:A:18:GLY:H | 1:A:46:LYS:HE3 | 1.83 | 0.43 |
| 1:A:41:LEU:HD13 | 1:A:44:GLU:OE2 | 2.19 | 0.43 |
| 1:A:102:ALA:O | 1:A:106:CYS:HB2 | 2.18 | 0.43 |
| 1:A:198:THR:HG21 | 2:C:33:C:O2' | 2.19 | 0.43 |
| 1:A:326:PHE:N | 1:A:326:PHE:HD1 | 2.17 | 0.43 |
| 1:A:352:GLY:O | 1:A:353:TYR:HD1 | 2.02 | 0.43 |
| 1:A:456:LEU:HD13 | 1:A:457:LEU:N | 2.33 | 0.43 |
| 1:B:42:ARG:HH11 | 1:B:47:LEU:C | 2.22 | 0.43 |
| 1:B:261:PHE:CE2 | 1:B:269:GLN:HB3 | 2.54 | 0.43 |
| 1:B:289:THR:HG23 | 2:D:39:A:H2' | 2.01 | 0.43 |
| 2:C:11:C:H2' | 2:C:12:U:H6 | 1.84 | 0.43 |
| 2:D:14:A:C2 | 2:D:15:G:H1' | 2.53 | 0.43 |
| 2:D:48:C:OP1 | 2:D:48:C:C6 | 2.64 | 0.43 |
| 1:A:10:HIS:O | 1:A:11:ARG:C | 2.58 | 0.42 |
| 1:A:104:ARG:NE | 2:C:36:A:N1 | 2.66 | 0.42 |
| 1:A:338:TRP:C | 1:A:338:TRP:CD1 | 2.91 | 0.42 |
| 1:B:18:GLY:H | 1:B:46:LYS:HE3 | 1.84 | 0.42 |
| 1:B:133:VAL:HG12 | 1:B:137:LEU:HD11 | 2.00 | 0.42 |
| 1:B:147:LYS:HA | 1:B:232:GLU:OE1 | 2.19 | 0.42 |
| 1:B:208:PRO:O | 1:B:211:ARG:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:256:LEU:HD11 | 1:B:261:PHE:HB2 | 2.01 | 0.42 |
| 1:B:289:THR:HG22 | 1:B:293:ILE:HD12 | 2.00 | 0.42 |
| 2:D:75:C:H6 | 2:D:75:C:O5' | 2.02 | 0.42 |
| 1:A:9:ILE:CD1 | 1:A:166:PRO:HB3 | 2.49 | 0.42 |
| 1:A:104:ARG:NH2 | 2:C:36:A:H62 | 2.16 | 0.42 |
| 1:A:198:THR:HG23 | 1:A:201:ARG:NH2 | 2.34 | 0.42 |
| 1:A:304:ARG:HA | 1:A:305:PRO:HD3 | 1.62 | 0.42 |
| 1:B:42:ARG:HD3 | 1:B:47:LEU:CB | 2.24 | 0.42 |
| 1:B:57:MET:H | 1:B:89:PRO:HG2 | 1.84 | 0.42 |
| 1:B:299:LEU:HD21 | 1:B:307:GLY:HA3 | 2.00 | 0.42 |
| 1:B:352:GLY:O | 1:B:353:TYR:HD1 | 2.02 | 0.42 |
| 1:A:24:GLY:HA3 | 1:A:111:PHE:CE2 | 2.54 | 0.42 |
| 1:A:158:PHE:H | 1:A:162:TYR:HA | 1.85 | 0.42 |
| 1:A:318:ILE:HD12 | 1:A:318:ILE:N | 2.33 | 0.42 |
| 1:B:247:MET:HE2 | 1:B:256:LEU:HA | 2.00 | 0.42 |
| 1:B:339:PHE:CD2 | 1:B:339:PHE:N | 2.87 | 0.42 |
| 1:A:70:VAL:HG23 | 1:A:71:LYS:N | 2.34 | 0.42 |
| 1:A:79:ILE:O | 1:A:79:ILE:HG22 | 2.20 | 0.42 |
| 1:A:194:LYS:O | 1:A:196:ASP:N | 2.50 | 0.42 |
| 1:B:133:VAL:HG12 | 1:B:137:LEU:CD1 | 2.49 | 0.42 |
| 1:B:233:GLN:O | 1:B:236:GLU:HB2 | 2.19 | 0.42 |
| 1:A:58:PHE:HZ | 1:A:62:GLU:HG2 | 1.84 | 0.42 |
| 1:A:74:CYS:HB3 | 1:A:79:ILE:O | 2.19 | 0.42 |
| 1:A:97:LEU:HD12 | 1:A:101:GLU:HG2 | 2.01 | 0.42 |
| 1:A:405:LYS:NZ | 2:C:68:A:OP2 | 2.50 | 0.42 |
| 1:B:58:PHE:CZ | 1:B:62:GLU:HG2 | 2.54 | 0.42 |
| 1:B:276:LEU:HD13 | 1:B:276:LEU:C | 2.39 | 0.42 |
| 1:B:338:TRP:HA | 1:B:387:ARG:HB3 | 2.02 | 0.42 |
| 1:A:58:PHE:CZ | 1:A:62:GLU:HG2 | 2.54 | 0.42 |
| 1:A:363:TYR:HD2 | 1:A:364:PRO:O | 2.03 | 0.42 |
| 1:B:9:ILE:HG23 | 1:B:15:LEU:HB2 | 2.02 | 0.42 |
| 1:B:58:PHE:HZ | 1:B:62:GLU:HG2 | 1.85 | 0.42 |
| 1:B:152:ILE:HA | 1:B:153:PRO:HD3 | 1.81 | 0.42 |
| 1:B:168:LEU:HA | 1:B:168:LEU:HD12 | 1.80 | 0.42 |
| 1:B:327:THR:CG2 | 1:B:327:THR:O | 2.67 | 0.42 |
| 1:A:46:LYS:C | 1:A:47:LEU:HD13 | 2.40 | 0.42 |
| 1:A:276:LEU:CD1 | 1:A:280:LEU:HD12 | 2.49 | 0.42 |
| 1:A:396:VAL:HA | 1:A:402:GLY:O | 2.19 | 0.42 |
| 1:B:382:LEU:HB3 | 1:B:383:PRO:HA | 2.00 | 0.42 |
| 1:B:104:ARG:NE | 2:D:36:A:C6 | 2.87 | 0.42 |
| 1:B:372:TRP:O | 1:B:441:LYS:HE2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:387:ARG:NE | 1:B:390:ARG:NH2 | 2.67 | 0.42 |
| 1:B:403:THR:OG1 | 2:D:1:G:P | 2.78 | 0.42 |
| 2:C:22:A:N6 | 2:C:49:C:C6 | 2.87 | 0.42 |
| 1:A:17:GLU:HA | 1:A:46:LYS:HZ1 | 1.85 | 0.42 |
| 1:B:363:TYR:CD1 | 1:B:448:ASN:HA | 2.53 | 0.42 |
| 2:C:14:A:C8 | 2:C:23:G:N2 | 2.88 | 0.42 |
| 2:D:59:A:C8 | 2:D:62:C:N4 | 2.88 | 0.42 |
| 1:A:373:PHE:C | 1:A:373:PHE:CD2 | 2.93 | 0.42 |
| 1:B:299:LEU:O | 1:B:319:ARG:NH1 | 2.53 | 0.42 |
| 2:D:11:C:H2' | 2:D:12:U:H6 | 1.85 | 0.42 |
| 2:D:22:A:N6 | 2:D:49:C:C6 | 2.88 | 0.42 |
| 1:A:39:LEU:HD23 | 1:A:39:LEU:HA | 1.89 | 0.41 |
| 1:A:101:GLU:CD | 2:C:34:U:C6 | 2.93 | 0.41 |
| 1:B:25:VAL:HG22 | 1:B:31:SER:HB2 | 2.02 | 0.41 |
| 1:B:155:LYS:HA | 1:B:163:LEU:O | 2.20 | 0.41 |
| 2:C:26:C:H2' | 2:C:27:A:H8 | 1.85 | 0.41 |
| 1:A:66:GLU:O | 1:A:70:VAL:HG13 | 2.20 | 0.41 |
| 1:A:158:PHE:CD2 | 1:A:159:HIS:HB2 | 2.55 | 0.41 |
| 1:A:299:LEU:HD21 | 1:A:307:GLY:HA3 | 2.01 | 0.41 |
| 1:A:337:TYR:O | 1:A:337:TYR:HD2 | 2.03 | 0.41 |
| 1:B:41:LEU:HA | 1:B:44:GLU:HB3 | 2.03 | 0.41 |
| 1:B:80:LEU:HD12 | 1:B:81:CYS:H | 1.84 | 0.41 |
| 1:B:226:GLU:O | 1:B:227:MET:C | 2.58 | 0.41 |
| 1:B:273:LEU:O | 1:B:274:GLN:C | 2.57 | 0.41 |
| 2:D:59:A:C6 | 2:D:62:C:C5 | 3.09 | 0.41 |
| 1:B:34:LEU:O | 1:B:35:LEU:C | 2.58 | 0.41 |
| 1:B:121:GLY:O | 1:B:161:GLY:HA3 | 2.19 | 0.41 |
| 1:B:271:ARG:HG2 | 1:B:271:ARG:NH1 | 2.33 | 0.41 |
| 1:B:370:ASN:HB3 | 1:B:438:GLY:HA2 | 2.02 | 0.41 |
| 1:A:55:ASP:OD1 | 1:A:63:SER:HA | 2.20 | 0.41 |
| 1:A:107:ARG:O | 1:A:110:PHE:HB3 | 2.20 | 0.41 |
| 1:A:247:MET:CE | 1:A:256:LEU:HB2 | 2.51 | 0.41 |
| 1:A:348:PRO:HA | 1:A:354:ALA:HB2 | 2.02 | 0.41 |
| 1:A:394:ARG:HG2 | 1:A:394:ARG:NH1 | 2.35 | 0.41 |
| 2:D:40:C:O2' | 2:D:41:C:H5' | 2.20 | 0.41 |
| 1:A:1:MET:CA | 1:A:5:VAL:HG12 | 2.50 | 0.41 |
| 1:A:327:THR:HG22 | 1:A:327:THR:O | 2.19 | 0.41 |
| 1:B:39:LEU:HD23 | 1:B:39:LEU:HA | 1.93 | 0.41 |
| 1:B:128:HIS:NE2 | 1:B:172:ARG:CZ | 2.83 | 0.41 |
| 1:B:188:CYS:SG | 1:B:189:ASP:N | 2.94 | 0.41 |
| 1:B:200:ASN:O | 1:B:203:ARG:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:275:LEU:O | 1:B:276:LEU:C | 2.59 | 0.41 |
| 2:C:52:A:N1 | 2:C:53:G:C5 | 2.88 | 0.41 |
| 2:D:30:C:N3 | 2:D:31:G:N7 | 2.69 | 0.41 |
| 1:A:153:PRO:O | 1:A:154:VAL:C | 2.58 | 0.41 |
| 1:A:275:LEU:O | 1:A:276:LEU:C | 2.59 | 0.41 |
| 1:B:169:ALA:HB3 | 1:B:170:VAL:HG13 | 2.01 | 0.41 |
| 1:B:271:ARG:CG | 1:B:271:ARG:NH1 | 2.60 | 0.41 |
| 1:B:349:LEU:HA | 1:B:350:PRO:HD3 | 1.91 | 0.41 |
| 1:B:373:PHE:CD2 | 1:B:374:VAL:N | 2.89 | 0.41 |
| 2:C:51:U:C3' | 2:C:52:A:H8 | 2.29 | 0.41 |
| 1:A:276:LEU:HD13 | 1:A:280:LEU:HD12 | 2.01 | 0.41 |
| 2:C:59:A:C8 | 2:C:62:C:N4 | 2.89 | 0.41 |
| 1:A:171:SER:OG | 1:A:173:ALA:HB3 | 2.21 | 0.41 |
| 1:A:202:PHE:CD2 | 1:A:206:ILE:HD12 | 2.56 | 0.41 |
| 1:A:226:GLU:O | 1:A:227:MET:C | 2.59 | 0.41 |
| 1:A:271:ARG:HG2 | 1:A:271:ARG:NH1 | 2.32 | 0.41 |
| 1:B:61:ARG:HG2 | 1:B:62:GLU:OE1 | 2.20 | 0.41 |
| 1:B:289:THR:OG1 | 2:D:39:A:C2' | 2.64 | 0.41 |
| 2:C:48:C:OP1 | 2:C:48:C:C6 | 2.61 | 0.41 |
| 1:A:21:VAL:HG12 | 1:A:49:VAL:HA | 2.03 | 0.41 |
| 1:A:34:LEU:CA | 1:A:167:PHE:HE1 | 2.33 | 0.41 |
| 1:A:42:ARG:HH11 | 1:A:47:LEU:C | 2.22 | 0.41 |
| 1:A:68:GLU:HA | 1:A:71:LYS:HG3 | 2.02 | 0.41 |
| 1:A:104:ARG:NE | 2:C:36:A:N6 | 2.69 | 0.41 |
| 1:A:113:GLU:O | 1:A:117:LYS:HB2 | 2.21 | 0.41 |
| 1:A:209:LEU:HD11 | 1:B:209:LEU:HD11 | 2.02 | 0.41 |
| 1:A:247:MET:HE1 | 1:A:256:LEU:HB2 | 2.02 | 0.41 |
| 1:A:393:ASP:HB3 | 1:A:406:LEU:HD22 | 2.03 | 0.41 |
| 1:B:115:MET:CE | 1:B:159:HIS:HB3 | 2.49 | 0.41 |
| 1:B:243:LEU:O | 1:B:247:MET:HG2 | 2.21 | 0.41 |
| 1:B:274:GLN:CA | 2:D:39:A:H61 | 2.34 | 0.41 |
| 1:B:351:ASN:O | 1:B:353:TYR:N | 2.54 | 0.41 |
| 2:C:22:A:H62 | 2:C:47:G:H1' | 1.83 | 0.41 |
| 1:A:41:LEU:HA | 1:A:44:GLU:HB3 | 2.03 | 0.41 |
| 1:A:132:GLN:O | 1:A:133:VAL:C | 2.59 | 0.41 |
| 1:A:133:VAL:HG12 | 1:A:137:LEU:HD11 | 2.03 | 0.41 |
| 1:A:136:ILE:O | 1:A:140:LEU:N | 2.54 | 0.41 |
| 1:A:315:LEU:C | 1:A:315:LEU:CD2 | 2.88 | 0.41 |
| 1:A:405:LYS:CE | 2:C:68:A:OP2 | 2.69 | 0.41 |
| 1:B:104:ARG:HG3 | 2:D:36:A:C2 | 2.55 | 0.41 |
| 1:B:203:ARG:HH22 | 2:D:35:C:N4 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:337:TYR:CE2 | 1:B:388:THR:HG22 | 2.56 | 0.41 |
| 2:C:25:G:C4 | 2:C:26:C:C5 | 3.09 | 0.41 |
| 1:A:128:HIS:NE2 | 1:A:172:ARG:CZ | 2.84 | 0.40 |
| 1:A:238:LEU:O | 1:A:239:ALA:C | 2.59 | 0.40 |
| 1:A:265:PRO:HG2 | 1:A:268:LEU:HD12 | 2.03 | 0.40 |
| 1:A:328:PHE:N | 1:A:328:PHE:CD2 | 2.88 | 0.40 |
| 1:A:347:LEU:HD23 | 1:A:347:LEU:C | 2.42 | 0.40 |
| 1:B:18:GLY:N | 1:B:46:LYS:HZ2 | 2.19 | 0.40 |
| 1:B:136:ILE:HD12 | 1:B:149:TYR:CE1 | 2.55 | 0.40 |
| 1:B:139:ARG:HH11 | 2:D:36:A:H8 | 1.64 | 0.40 |
| 1:B:159:HIS:HB3 | 1:B:160:GLY:H | 1.59 | 0.40 |
| 1:B:234:PHE:O | 1:B:235:LEU:C | 2.59 | 0.40 |
| 1:B:393:ASP:HB3 | 1:B:406:LEU:HD22 | 2.02 | 0.40 |
| 2:C:40:C:O2' | 2:C:41:C:H5' | 2.21 | 0.40 |
| 2:D:30:C:C2 | 2:D:31:G:C8 | 3.09 | 0.40 |
| 1:A:296:ILE:CD1 | 1:A:317:VAL:HG11 | 2.51 | 0.40 |
| 1:A:415:ILE:HG22 | 1:A:419:GLU:HB2 | 2.03 | 0.40 |
| 1:B:10:HIS:O | 1:B:11:ARG:C | 2.60 | 0.40 |
| 1:B:27:GLY:O | 1:B:66:GLU:HG2 | 2.20 | 0.40 |
| 1:B:38:PHE:O | 1:B:39:LEU:C | 2.58 | 0.40 |
| 1:B:153:PRO:HD2 | 2:D:37:U:OP1 | 2.21 | 0.40 |
| 1:B:257:SER:O | 1:B:260:PRO:HG2 | 2.20 | 0.40 |
| 1:B:289:THR:CG2 | 2:D:39:A:H2' | 2.51 | 0.40 |
| 1:A:39:LEU:CD1 | 1:A:77:ARG:HD2 | 2.51 | 0.40 |
| 1:A:311:LEU:HD22 | 1:A:311:LEU:HA | 1.76 | 0.40 |
| 1:A:404:LYS:CD | 1:A:409:ILE:HG12 | 2.51 | 0.40 |
| 1:B:107:ARG:HG2 | 1:B:111:PHE:CE1 | 2.56 | 0.40 |
| 1:B:391:ARG:O | 2:D:68:A:P | 2.80 | 0.40 |
| 1:B:415:ILE:HG22 | 1:B:419:GLU:HB2 | 2.03 | 0.40 |
| 1:B:448:ASN:O | 1:B:450:GLY:N | 2.54 | 0.40 |
| 1:A:198:THR:O | 1:A:199:ARG:C | 2.60 | 0.40 |
| 1:A:285:PRO:HD2 | 1:A:286:PRO:CD | 2.52 | 0.40 |
| 1:A:289:THR:N | 2:C:39:A:O2' | 2.43 | 0.40 |
| 1:A:311:LEU:HB2 | 1:A:315:LEU:O | 2.22 | 0.40 |
| 1:A:385:ARG:CZ | 1:A:429:ALA:HA | 2.52 | 0.40 |
| 1:A:407:LYS:HE2 | 1:A:408:GLU:HG3 | 2.03 | 0.40 |
| 1:B:50:ILE:O | 1:B:50:ILE:HG22 | 2.21 | 0.40 |
| 1:B:148:GLY:O | 1:B:149:TYR:C | 2.59 | 0.40 |
| 1:B:298:MET:HE2 | 1:B:298:MET:HB2 | 1.69 | 0.40 |
| 2:D:51:U:C3' | 2:D:52:A:H8 | 2.31 | 0.40 |
| 1:A:9:ILE:HG22 | 1:A:15:LEU:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:102:ALA:HA | 1:A:105:ILE:HG12 | 2.03 | 0.40 |
| 1:A:200:ASN:O | 1:A:203:ARG:N | 2.55 | 0.40 |
| 1:A:284:VAL:O | 1:A:287:THR:HG22 | 2.22 | 0.40 |
| 1:A:432:ARG:CD | 1:A:444:PHE:HE1 | 2.32 | 0.40 |
| 1:B:97:LEU:HD12 | 1:B:101:GLU:HG2 | 2.03 | 0.40 |
| 1:B:198:THR:O | 1:B:199:ARG:C | 2.60 | 0.40 |
| 1:B:326:PHE:N | 1:B:326:PHE:CD1 | 2.90 | 0.40 |
| 2:D:54:G:N3 | 2:D:54:G:H2' | 2.37 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------|--------------------|--------------------------|-------------------|
| 2:C:77:A:N7 | 2:D:77:A:N7[4_545] | 2.00 | 0.20 |

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 |
|-----|-------|---------------|-----------|-----------|----------|-------------|
| 1 | A | 460/464 (99%) | 330 (72%) | 81 (18%) | 49 (11%) | 0 6 |
| 1 | B | 460/464 (99%) | 327 (71%) | 83 (18%) | 50 (11%) | 0 5 |
| All | All | 920/928 (99%) | 657 (71%) | 164 (18%) | 99 (11%) | 0 6 |

All (99) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 13 | GLN |
| 1 | A | 14 | LEU |
| 1 | A | 27 | GLY |
| 1 | A | 58 | PHE |
| 1 | A | 146 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 150 | ALA |
| 1 | A | 185 | SER |
| 1 | A | 187 | ARG |
| 1 | A | 194 | LYS |
| 1 | A | 289 | THR |
| 1 | A | 290 | SER |
| 1 | A | 302 | ARG |
| 1 | A | 329 | ASP |
| 1 | A | 334 | GLU |
| 1 | A | 379 | SER |
| 1 | A | 391 | ARG |
| 1 | A | 452 | ALA |
| 1 | B | 13 | GLN |
| 1 | B | 14 | LEU |
| 1 | B | 58 | PHE |
| 1 | B | 146 | SER |
| 1 | B | 150 | ALA |
| 1 | B | 154 | VAL |
| 1 | B | 185 | SER |
| 1 | B | 187 | ARG |
| 1 | B | 194 | LYS |
| 1 | B | 289 | THR |
| 1 | B | 290 | SER |
| 1 | B | 329 | ASP |
| 1 | B | 334 | GLU |
| 1 | B | 379 | SER |
| 1 | B | 391 | ARG |
| 1 | B | 452 | ALA |
| 1 | A | 19 | ALA |
| 1 | A | 133 | VAL |
| 1 | A | 154 | VAL |
| 1 | A | 281 | TYR |
| 1 | A | 283 | GLY |
| 1 | A | 288 | LEU |
| 1 | A | 378 | ALA |
| 1 | A | 401 | GLY |
| 1 | A | 442 | SER |
| 1 | B | 19 | ALA |
| 1 | B | 27 | GLY |
| 1 | B | 281 | TYR |
| 1 | B | 283 | GLY |
| 1 | B | 288 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 302 | ARG |
| 1 | B | 378 | ALA |
| 1 | B | 442 | SER |
| 1 | A | 2 | ILE |
| 1 | A | 195 | ASP |
| 1 | B | 2 | ILE |
| 1 | B | 103 | ALA |
| 1 | B | 133 | VAL |
| 1 | B | 195 | ASP |
| 1 | B | 401 | GLY |
| 1 | B | 449 | ARG |
| 1 | B | 451 | GLN |
| 1 | A | 46 | LYS |
| 1 | A | 103 | ALA |
| 1 | A | 184 | LEU |
| 1 | A | 234 | PHE |
| 1 | A | 350 | PRO |
| 1 | A | 398 | LYS |
| 1 | A | 437 | PRO |
| 1 | A | 449 | ARG |
| 1 | A | 451 | GLN |
| 1 | B | 34 | LEU |
| 1 | B | 46 | LYS |
| 1 | B | 82 | GLU |
| 1 | B | 184 | LEU |
| 1 | B | 211 | ARG |
| 1 | B | 350 | PRO |
| 1 | B | 398 | LYS |
| 1 | B | 437 | PRO |
| 1 | A | 34 | LEU |
| 1 | A | 82 | GLU |
| 1 | A | 88 | VAL |
| 1 | A | 134 | GLU |
| 1 | A | 183 | GLY |
| 1 | A | 193 | GLU |
| 1 | A | 211 | ARG |
| 1 | A | 249 | LYS |
| 1 | A | 285 | PRO |
| 1 | B | 88 | VAL |
| 1 | B | 157 | PRO |
| 1 | B | 193 | GLU |
| 1 | B | 218 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 234 | PHE |
| 1 | B | 249 | LYS |
| 1 | B | 285 | PRO |
| 1 | A | 157 | PRO |
| 1 | A | 186 | PRO |
| 1 | B | 134 | GLU |
| 1 | B | 183 | GLY |
| 1 | B | 186 | PRO |
| 1 | B | 264 | LEU |
| 1 | A | 264 | LEU |

5.3.2 Protein sidechains [\(i\)](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|-----------|-------------|
| 1 | A | 391/393 (100%) | 300 (77%) | 91 (23%) | 1 5 |
| 1 | B | 391/393 (100%) | 297 (76%) | 94 (24%) | 0 5 |
| All | All | 782/786 (100%) | 597 (76%) | 185 (24%) | 1 5 |

All (185) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 1 | MET |
| 1 | A | 2 | ILE |
| 1 | A | 5 | VAL |
| 1 | A | 11 | ARG |
| 1 | A | 21 | VAL |
| 1 | A | 37 | VAL |
| 1 | A | 38 | PHE |
| 1 | A | 42 | ARG |
| 1 | A | 45 | TRP |
| 1 | A | 47 | LEU |
| 1 | A | 48 | GLN |
| 1 | A | 56 | HIS |
| 1 | A | 57 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 58 | PHE |
| 1 | A | 79 | ILE |
| 1 | A | 80 | LEU |
| 1 | A | 86 | ILE |
| 1 | A | 94 | SER |
| 1 | A | 104 | ARG |
| 1 | A | 107 | ARG |
| 1 | A | 113 | GLU |
| 1 | A | 118 | HIS |
| 1 | A | 125 | VAL |
| 1 | A | 130 | ASP |
| 1 | A | 135 | THR |
| 1 | A | 140 | LEU |
| 1 | A | 142 | ARG |
| 1 | A | 145 | THR |
| 1 | A | 149 | TYR |
| 1 | A | 156 | ARG |
| 1 | A | 158 | PHE |
| 1 | A | 159 | HIS |
| 1 | A | 163 | LEU |
| 1 | A | 164 | ILE |
| 1 | A | 179 | CYS |
| 1 | A | 182 | MET |
| 1 | A | 184 | LEU |
| 1 | A | 188 | CYS |
| 1 | A | 189 | ASP |
| 1 | A | 191 | SER |
| 1 | A | 198 | THR |
| 1 | A | 220 | ARG |
| 1 | A | 223 | GLN |
| 1 | A | 233 | GLN |
| 1 | A | 246 | VAL |
| 1 | A | 249 | LYS |
| 1 | A | 252 | ARG |
| 1 | A | 262 | LEU |
| 1 | A | 271 | ARG |
| 1 | A | 275 | LEU |
| 1 | A | 277 | LEU |
| 1 | A | 278 | LEU |
| 1 | A | 279 | ARG |
| 1 | A | 281 | TYR |
| 1 | A | 284 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 288 | LEU |
| 1 | A | 289 | THR |
| 1 | A | 290 | SER |
| 1 | A | 293 | ILE |
| 1 | A | 297 | LEU |
| 1 | A | 298 | MET |
| 1 | A | 299 | LEU |
| 1 | A | 308 | MET |
| 1 | A | 311 | LEU |
| 1 | A | 315 | LEU |
| 1 | A | 319 | ARG |
| 1 | A | 327 | THR |
| 1 | A | 328 | PHE |
| 1 | A | 332 | SER |
| 1 | A | 337 | TYR |
| 1 | A | 338 | TRP |
| 1 | A | 361 | GLU |
| 1 | A | 366 | LYS |
| 1 | A | 374 | VAL |
| 1 | A | 375 | VAL |
| 1 | A | 382 | LEU |
| 1 | A | 385 | ARG |
| 1 | A | 386 | VAL |
| 1 | A | 394 | ARG |
| 1 | A | 396 | VAL |
| 1 | A | 397 | LEU |
| 1 | A | 403 | THR |
| 1 | A | 406 | LEU |
| 1 | A | 407 | LYS |
| 1 | A | 409 | ILE |
| 1 | A | 417 | ARG |
| 1 | A | 420 | ARG |
| 1 | A | 432 | ARG |
| 1 | A | 433 | ILE |
| 1 | A | 458 | GLN |
| 1 | A | 462 | MET |
| 1 | B | 1 | MET |
| 1 | B | 2 | ILE |
| 1 | B | 11 | ARG |
| 1 | B | 21 | VAL |
| 1 | B | 37 | VAL |
| 1 | B | 38 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 40 | SER |
| 1 | B | 42 | ARG |
| 1 | B | 45 | TRP |
| 1 | B | 47 | LEU |
| 1 | B | 48 | GLN |
| 1 | B | 56 | HIS |
| 1 | B | 57 | MET |
| 1 | B | 58 | PHE |
| 1 | B | 79 | ILE |
| 1 | B | 80 | LEU |
| 1 | B | 86 | ILE |
| 1 | B | 94 | SER |
| 1 | B | 104 | ARG |
| 1 | B | 107 | ARG |
| 1 | B | 113 | GLU |
| 1 | B | 118 | HIS |
| 1 | B | 125 | VAL |
| 1 | B | 130 | ASP |
| 1 | B | 135 | THR |
| 1 | B | 140 | LEU |
| 1 | B | 142 | ARG |
| 1 | B | 145 | THR |
| 1 | B | 149 | TYR |
| 1 | B | 156 | ARG |
| 1 | B | 158 | PHE |
| 1 | B | 159 | HIS |
| 1 | B | 163 | LEU |
| 1 | B | 164 | ILE |
| 1 | B | 165 | ARG |
| 1 | B | 179 | CYS |
| 1 | B | 182 | MET |
| 1 | B | 184 | LEU |
| 1 | B | 188 | CYS |
| 1 | B | 189 | ASP |
| 1 | B | 191 | SER |
| 1 | B | 198 | THR |
| 1 | B | 217 | LEU |
| 1 | B | 220 | ARG |
| 1 | B | 223 | GLN |
| 1 | B | 233 | GLN |
| 1 | B | 246 | VAL |
| 1 | B | 249 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 252 | ARG |
| 1 | B | 262 | LEU |
| 1 | B | 271 | ARG |
| 1 | B | 275 | LEU |
| 1 | B | 277 | LEU |
| 1 | B | 278 | LEU |
| 1 | B | 279 | ARG |
| 1 | B | 281 | TYR |
| 1 | B | 284 | VAL |
| 1 | B | 288 | LEU |
| 1 | B | 289 | THR |
| 1 | B | 290 | SER |
| 1 | B | 293 | ILE |
| 1 | B | 297 | LEU |
| 1 | B | 298 | MET |
| 1 | B | 299 | LEU |
| 1 | B | 308 | MET |
| 1 | B | 311 | LEU |
| 1 | B | 315 | LEU |
| 1 | B | 319 | ARG |
| 1 | B | 327 | THR |
| 1 | B | 328 | PHE |
| 1 | B | 332 | SER |
| 1 | B | 337 | TYR |
| 1 | B | 338 | TRP |
| 1 | B | 361 | GLU |
| 1 | B | 365 | ARG |
| 1 | B | 366 | LYS |
| 1 | B | 370 | ASN |
| 1 | B | 374 | VAL |
| 1 | B | 375 | VAL |
| 1 | B | 381 | SER |
| 1 | B | 382 | LEU |
| 1 | B | 385 | ARG |
| 1 | B | 386 | VAL |
| 1 | B | 394 | ARG |
| 1 | B | 397 | LEU |
| 1 | B | 403 | THR |
| 1 | B | 406 | LEU |
| 1 | B | 407 | LYS |
| 1 | B | 409 | ILE |
| 1 | B | 417 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 420 | ARG |
| 1 | B | 432 | ARG |
| 1 | B | 458 | GLN |
| 1 | B | 462 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 36 | HIS |
| 1 | A | 53 | HIS |
| 1 | A | 56 | HIS |
| 1 | A | 118 | HIS |
| 1 | A | 127 | HIS |
| 1 | A | 204 | HIS |
| 1 | A | 212 | GLN |
| 1 | A | 251 | HIS |
| 1 | A | 269 | GLN |
| 1 | A | 274 | GLN |
| 1 | A | 292 | HIS |
| 1 | A | 362 | HIS |
| 1 | B | 36 | HIS |
| 1 | B | 53 | HIS |
| 1 | B | 56 | HIS |
| 1 | B | 118 | HIS |
| 1 | B | 127 | HIS |
| 1 | B | 204 | HIS |
| 1 | B | 212 | GLN |
| 1 | B | 251 | HIS |
| 1 | B | 269 | GLN |
| 1 | B | 274 | GLN |
| 1 | B | 292 | HIS |
| 1 | B | 362 | HIS |

5.3.3 RNA [\(i\)](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 2 | C | 76/77 (98%) | 29 (38%) | 16 (21%) |
| 2 | D | 76/77 (98%) | 30 (39%) | 16 (21%) |
| All | All | 152/154 (98%) | 59 (38%) | 32 (21%) |

All (59) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 7 | U |
| 2 | C | 8 | U |
| 2 | C | 9 | A |
| 2 | C | 13 | C |
| 2 | C | 16 | U |
| 2 | C | 17 | U |
| 2 | C | 18 | G |
| 2 | C | 19 | G |
| 2 | C | 20 | U |
| 2 | C | 21 | U |
| 2 | C | 22 | A |
| 2 | C | 23 | G |
| 2 | C | 34 | U |
| 2 | C | 35 | C |
| 2 | C | 37 | U |
| 2 | C | 38 | A |
| 2 | C | 39 | A |
| 2 | C | 40 | C |
| 2 | C | 42 | G |
| 2 | C | 47 | G |
| 2 | C | 48 | C |
| 2 | C | 49 | C |
| 2 | C | 50 | G |
| 2 | C | 52 | A |
| 2 | C | 59 | A |
| 2 | C | 60 | G |
| 2 | C | 62 | C |
| 2 | C | 63 | C |
| 2 | C | 64 | U |
| 2 | D | 7 | U |
| 2 | D | 8 | U |
| 2 | D | 9 | A |
| 2 | D | 12 | U |
| 2 | D | 13 | C |
| 2 | D | 16 | U |
| 2 | D | 17 | U |
| 2 | D | 18 | G |
| 2 | D | 19 | G |
| 2 | D | 20 | U |
| 2 | D | 21 | U |
| 2 | D | 22 | A |
| 2 | D | 23 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 34 | U |
| 2 | D | 35 | C |
| 2 | D | 37 | U |
| 2 | D | 38 | A |
| 2 | D | 39 | A |
| 2 | D | 40 | C |
| 2 | D | 42 | G |
| 2 | D | 47 | G |
| 2 | D | 48 | C |
| 2 | D | 49 | C |
| 2 | D | 50 | G |
| 2 | D | 52 | A |
| 2 | D | 59 | A |
| 2 | D | 60 | G |
| 2 | D | 62 | C |
| 2 | D | 63 | C |
| 2 | D | 64 | U |

All (32) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 7 | U |
| 2 | C | 8 | U |
| 2 | C | 18 | G |
| 2 | C | 19 | G |
| 2 | C | 20 | U |
| 2 | C | 22 | A |
| 2 | C | 34 | U |
| 2 | C | 35 | C |
| 2 | C | 37 | U |
| 2 | C | 38 | A |
| 2 | C | 39 | A |
| 2 | C | 48 | C |
| 2 | C | 49 | C |
| 2 | C | 61 | U |
| 2 | C | 62 | C |
| 2 | C | 63 | C |
| 2 | D | 7 | U |
| 2 | D | 8 | U |
| 2 | D | 18 | G |
| 2 | D | 19 | G |
| 2 | D | 20 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 22 | A |
| 2 | D | 34 | U |
| 2 | D | 35 | C |
| 2 | D | 37 | U |
| 2 | D | 38 | A |
| 2 | D | 39 | A |
| 2 | D | 48 | C |
| 2 | D | 49 | C |
| 2 | D | 61 | U |
| 2 | D | 62 | C |
| 2 | D | 63 | C |

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides 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 [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1 | A | 462/464 (99%) | -0.46 | 2 (0%) 92 88 | 69, 145, 232, 272 | 0 |
| 1 | B | 462/464 (99%) | -0.41 | 2 (0%) 92 88 | 73, 145, 232, 271 | 0 |
| 2 | C | 77/77 (100%) | -0.52 | 0 100 100 | 122, 162, 239, 263 | 0 |
| 2 | D | 77/77 (100%) | -0.26 | 0 100 100 | 125, 168, 244, 264 | 0 |
| All | All | 1078/1082 (99%) | -0.43 | 4 (0%) 92 88 | 69, 149, 235, 272 | 0 |

All (4) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 97 | LEU | 3.3 |
| 1 | B | 98 | GLY | 2.8 |
| 1 | A | 97 | LEU | 2.6 |
| 1 | A | 98 | GLY | 2.5 |

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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.