



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:05 am BST

PDB ID : 2HHH
Title : Crystal structure of kasugamycin bound to the 30S ribosomal subunit
Authors : Schlutzen, F.
Deposited on : 2006-06-28
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

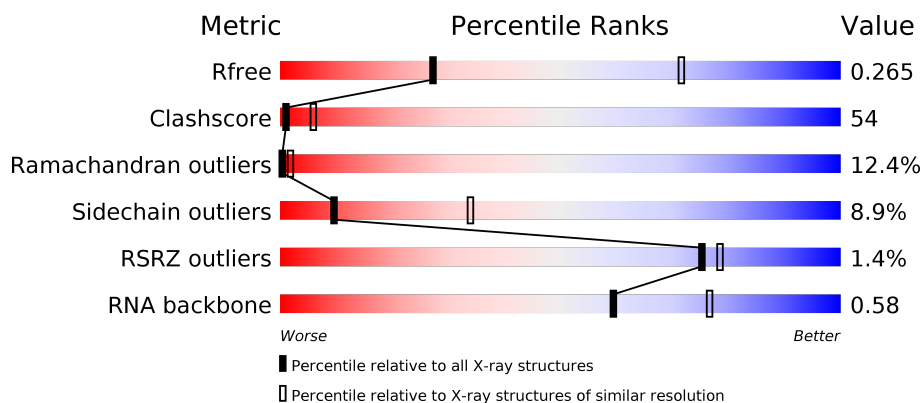
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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 | 1558 (3.42-3.30) |
| Clashscore | 141614 | 1627 (3.42-3.30) |
| Ramachandran outliers | 138981 | 1599 (3.42-3.30) |
| Sidechain outliers | 138945 | 1598 (3.42-3.30) |
| RSRZ outliers | 127900 | 1507 (3.42-3.30) |
| RNA backbone | 3102 | 1023 (3.80-2.92) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 1522 | <div> <div>15%</div> <div>60%</div> <div>19%</div> <div>5%</div> </div> |
| 2 | B | 256 | <div> <div>5%</div> <div>16%</div> <div>55%</div> <div>17%</div> <div>9%</div> </div> |
| 3 | C | 239 | <div> <div>14%</div> <div>54%</div> <div>16%</div> <div>14%</div> </div> |
| 4 | D | 209 | <div> <div>19%</div> <div>64%</div> <div>15%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5 | E | 162 | |
| 6 | F | 101 | |
| 7 | G | 156 | |
| 8 | H | 138 | |
| 9 | I | 128 | |
| 10 | J | 105 | |
| 11 | K | 129 | |
| 12 | L | 135 | |
| 13 | M | 126 | |
| 14 | N | 61 | |
| 15 | O | 89 | |
| 16 | P | 88 | |
| 17 | Q | 105 | |
| 18 | R | 88 | |
| 19 | S | 93 | |
| 20 | T | 106 | |
| 21 | U | 27 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22 | KSG | A | 1524 | - | - | - | X |

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 51632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1505 | Total | C | N | O | P | 44 | 0 | 0 |
| | | | 32349 | 14399 | 5994 | 10452 | 1504 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| I | 58 | ARG | HIS | CONFLICT | UNP P80374 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | J | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 794 | 499 | 156 | 138 | 1 | | | |

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| L | 2 | VAL | - | INSERTION | UNP P17293 |
| L | 3 | ALA | - | INSERTION | UNP P17293 |
| L | 4 | LEU | - | INSERTION | UNP P17293 |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

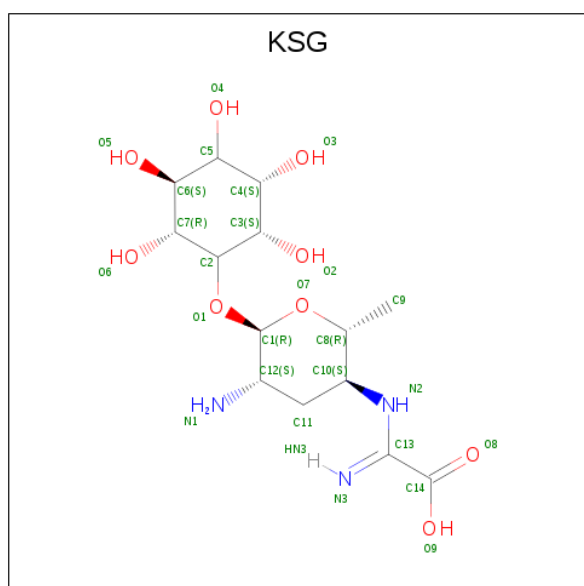
- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 22 is (1S,2R,3S,4R,5S,6S)-2,3,4,5,6-PENTAHYDROXYCYCLOHEXYL 2-AMINO-4-{{CARBOXY(IMINO)METHYL}AMINO}-2,3,4,6-TETRADEOXY-ALPHA-D-ARABINO-HEXOPYRANOSIDE (three-letter code: KSG) (formula: $C_{14}H_{25}N_3O_9$).

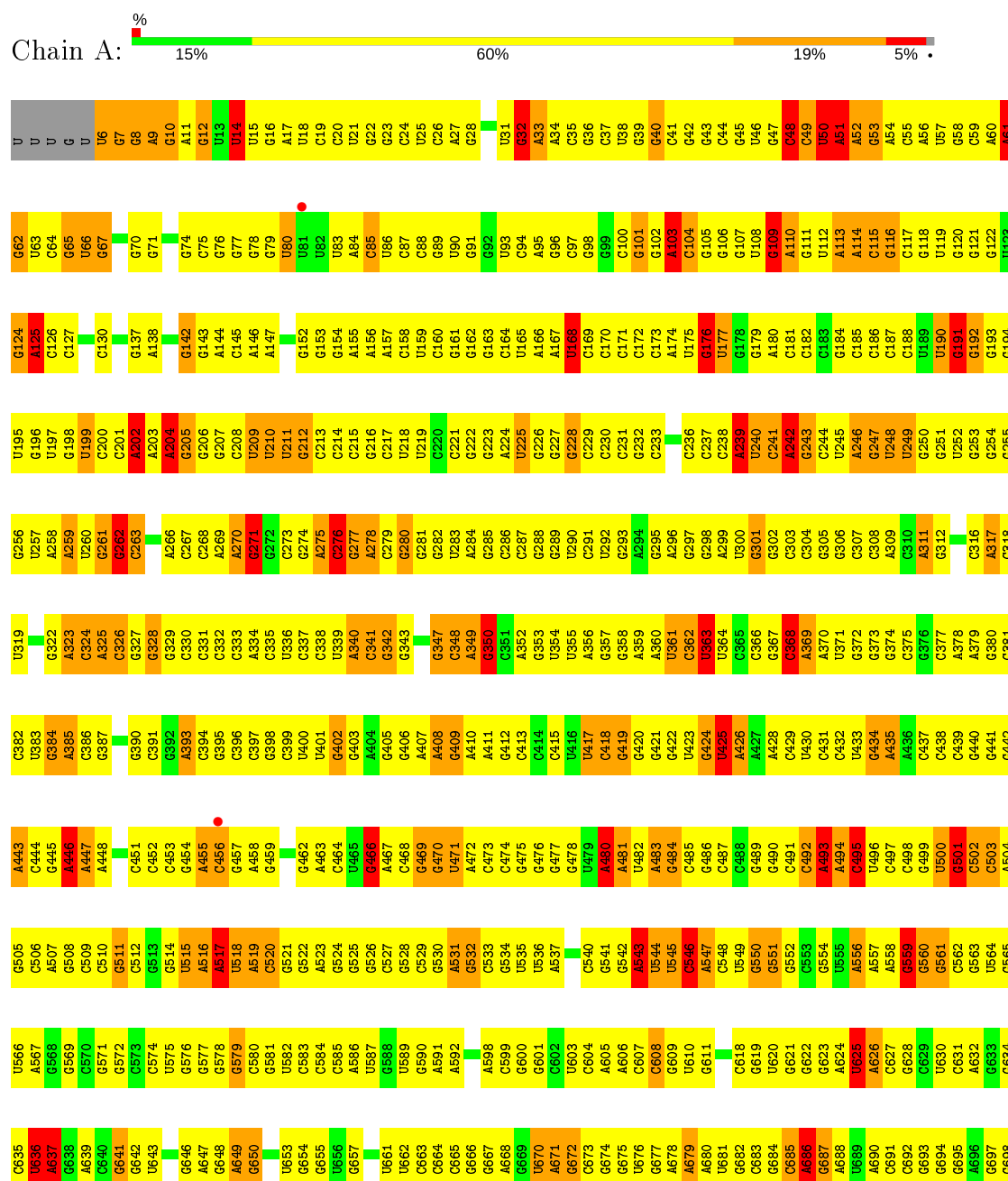


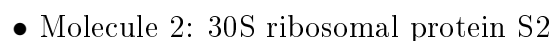
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 22 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 26 | 14 | 3 | 9 | | |
| 22 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 26 | 14 | 3 | 9 | | |

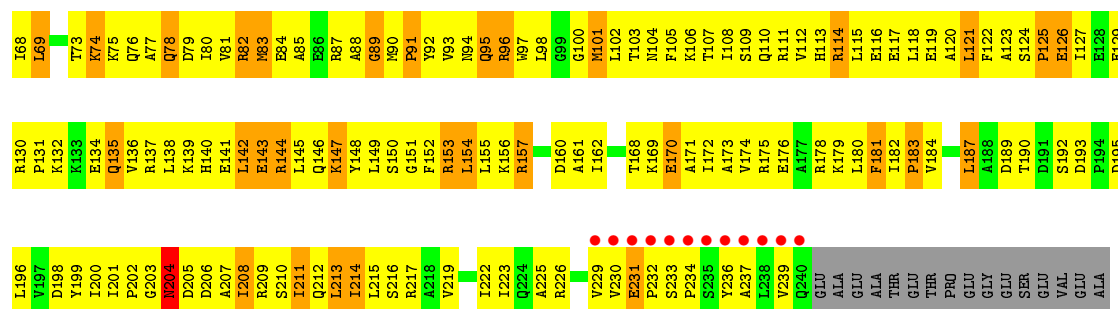
3 Residue-property plots

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

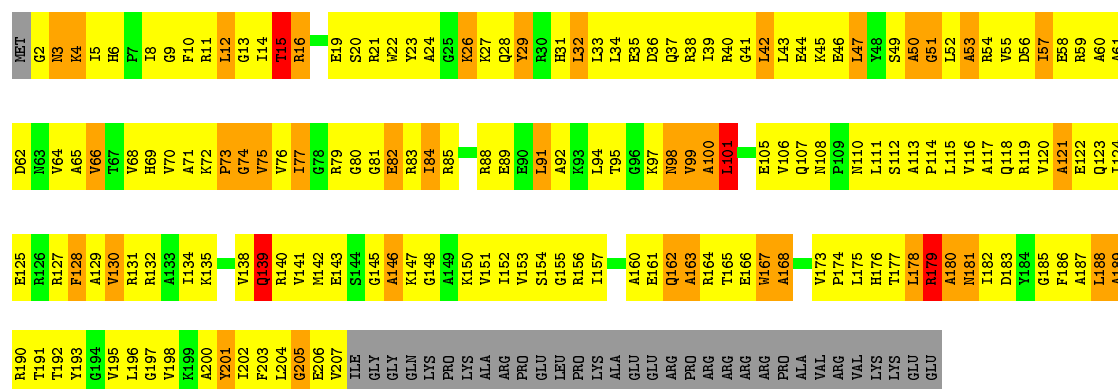
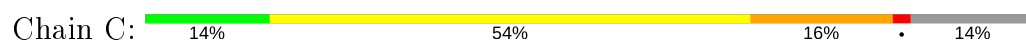
• Molecule 1: 16S ribosomal RNA



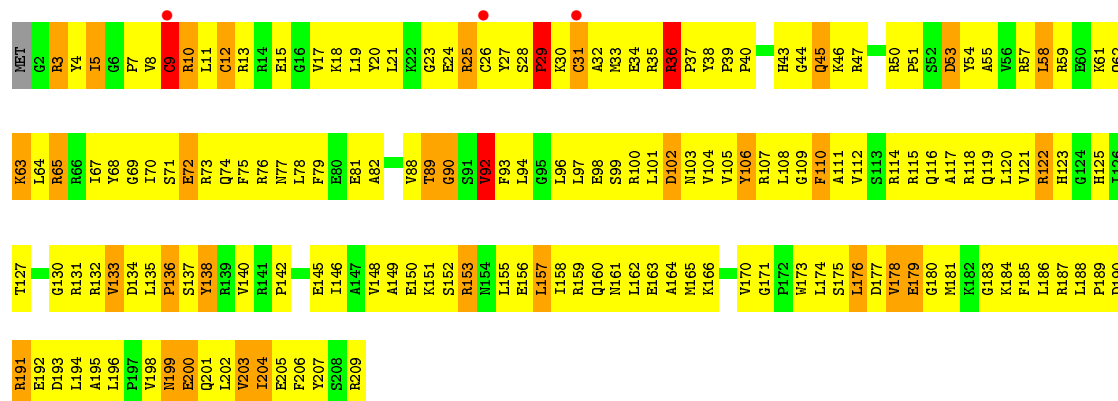




- Molecule 3: 30S ribosomal protein S3

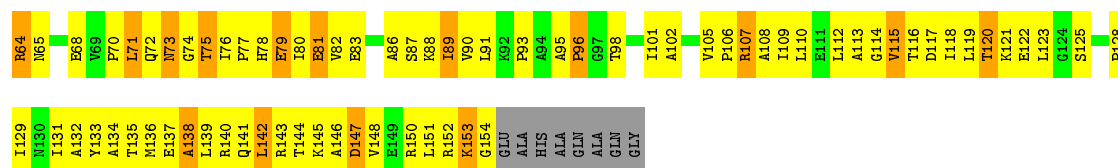


- Molecule 4: 30S ribosomal protein S4

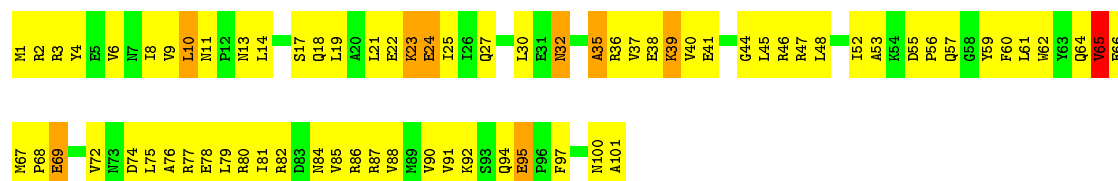


- Molecule 5: 30S ribosomal protein S5

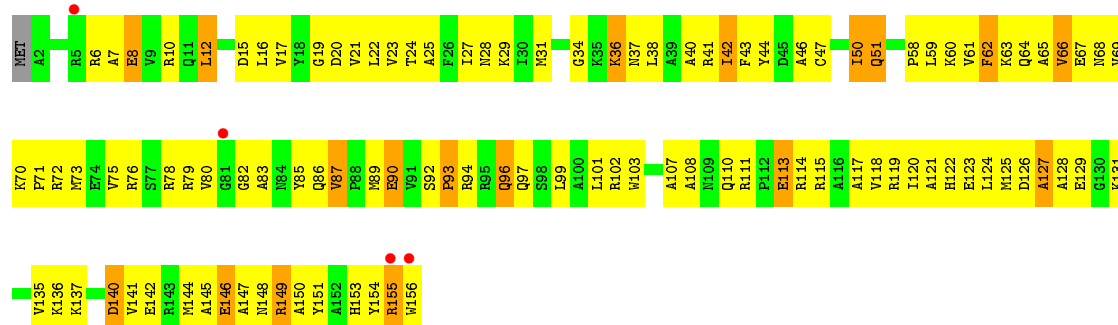




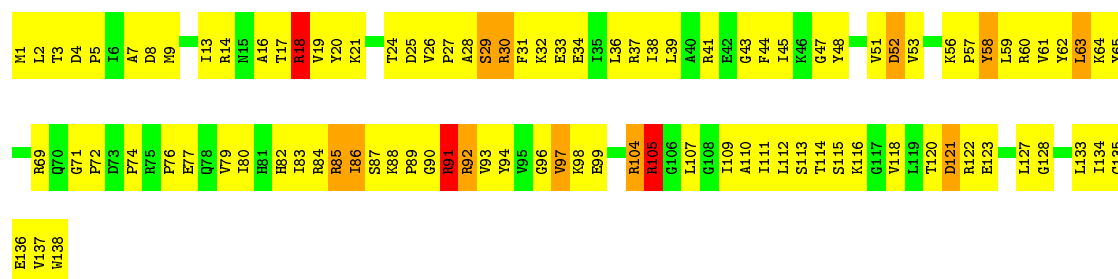
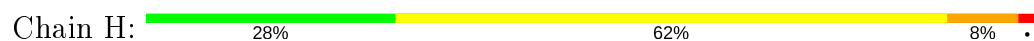
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

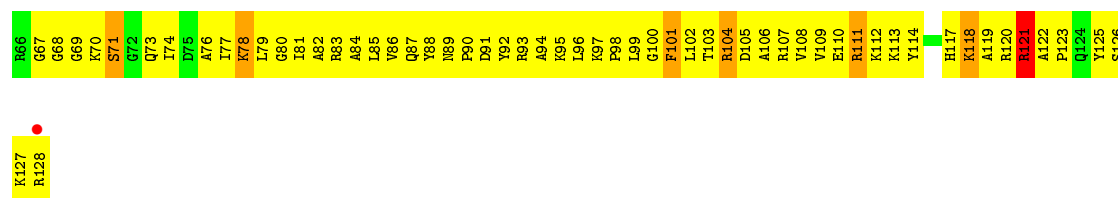


• Molecule 8: 30S ribosomal protein S8

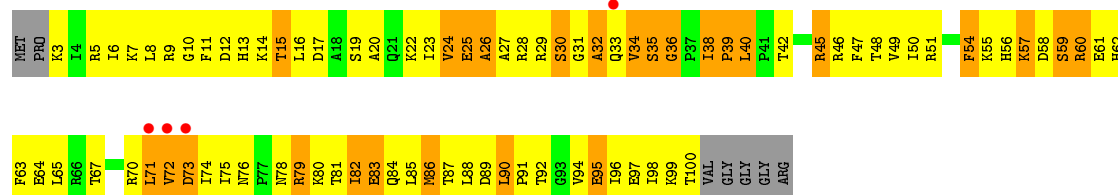
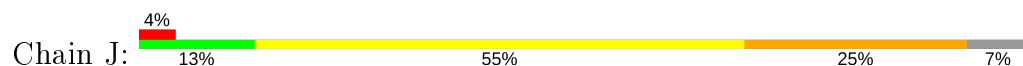


• Molecule 9: 30S ribosomal protein S9

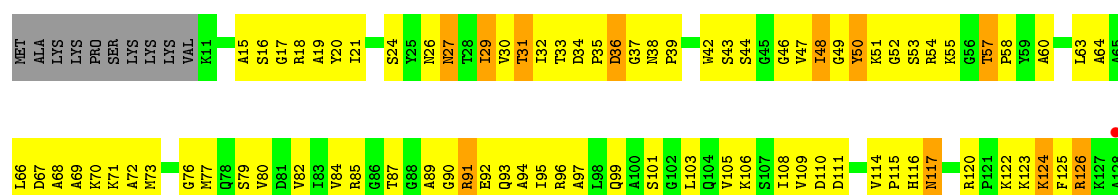




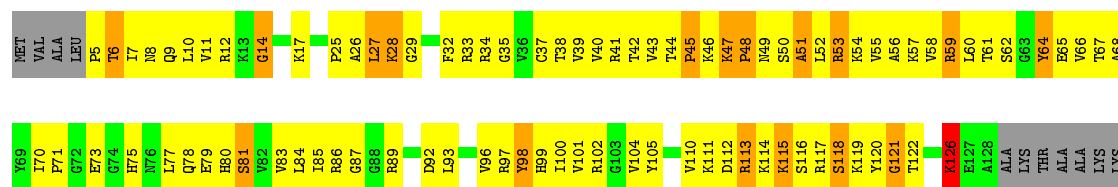
- Molecule 10: 30S ribosomal protein S10



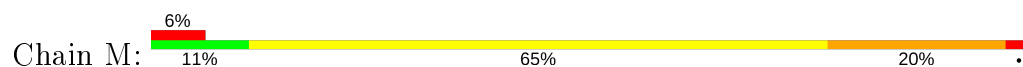
- Molecule 11: 30S ribosomal protein S11

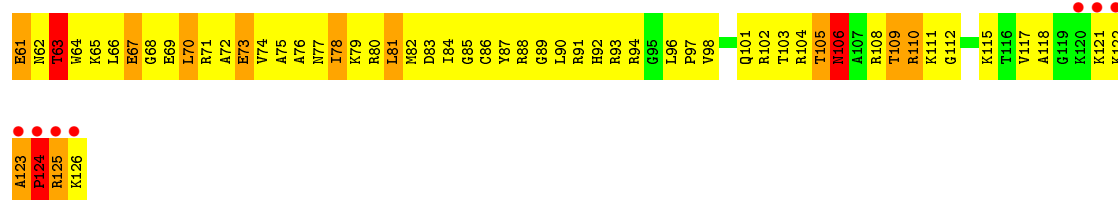


- Molecule 12: 30S ribosomal protein S12

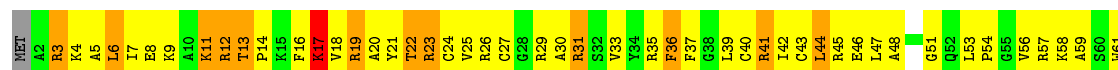
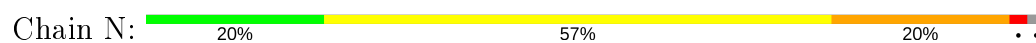


- Molecule 13: 30S ribosomal protein S13

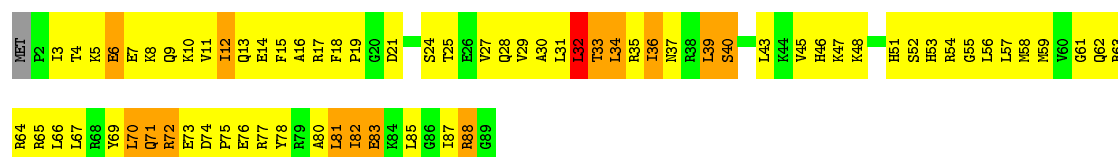




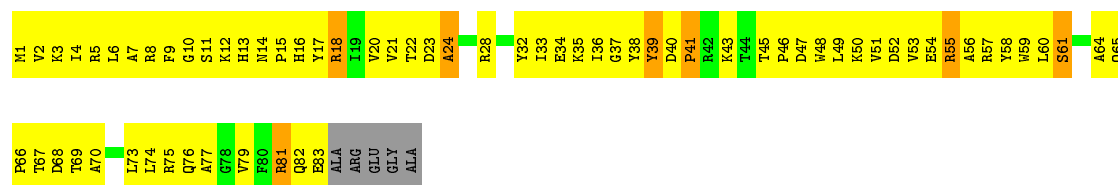
• Molecule 14: 30S ribosomal protein S14



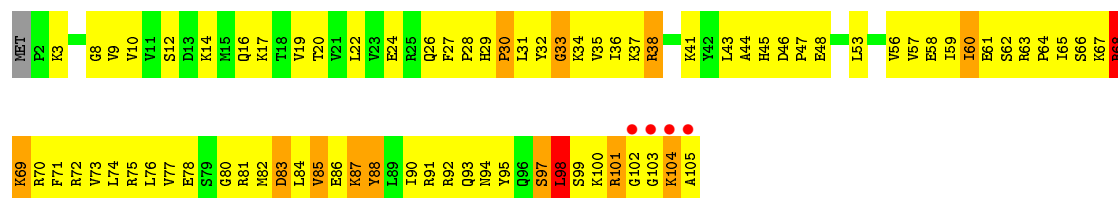
• Molecule 15: 30S ribosomal protein S15



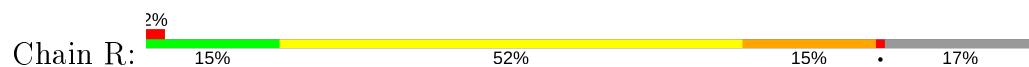
• Molecule 16: 30S ribosomal protein S16

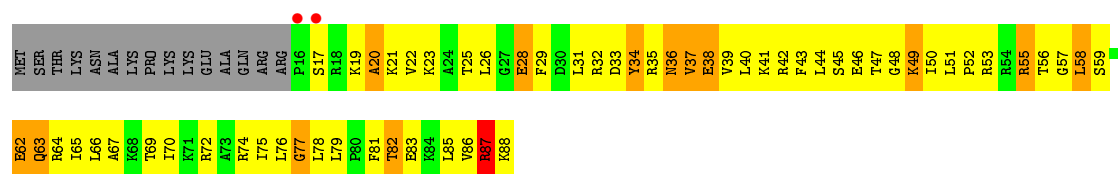


• Molecule 17: 30S ribosomal protein S17

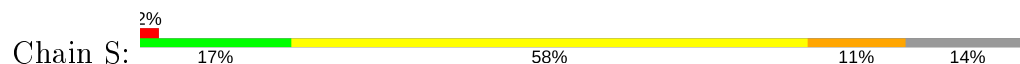


• Molecule 18: 30S ribosomal protein S18

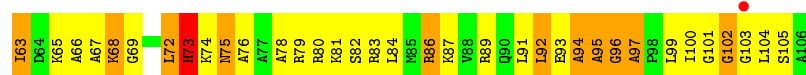
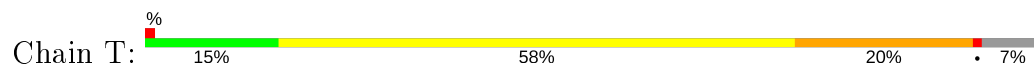




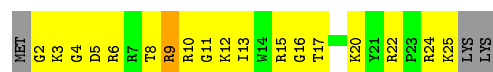
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein Thx



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 410.44Å 410.44Å 172.65Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.74 – 3.35 29.74 – 3.30 | Depositor EDS |
| % Data completeness (in resolution range) | 98.4 (29.74-3.35) 97.0 (29.74-3.30) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.55 (at 3.31Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.265 , 0.289 0.242 , 0.265 | Depositor DCC |
| R_{free} test set | 10101 reflections (4.76%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 56.5 | Xtriage |
| Anisotropy | 0.534 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.16 , 19.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 51632 | wwPDB-VP |
| Average B, all atoms (Å ²) | 38.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KSG

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 | 0.76 | 3/36212 (0.0%) | 0.84 | 69/56520 (0.1%) |
| 2 | B | 0.58 | 0/1935 | 0.77 | 1/2609 (0.0%) |
| 3 | C | 0.56 | 0/1636 | 0.74 | 0/2205 |
| 4 | D | 0.64 | 1/1733 (0.1%) | 0.79 | 2/2318 (0.1%) |
| 5 | E | 0.76 | 0/1162 | 0.94 | 1/1564 (0.1%) |
| 6 | F | 0.50 | 0/856 | 0.69 | 0/1154 |
| 7 | G | 0.48 | 0/1276 | 0.68 | 0/1709 |
| 8 | H | 0.69 | 0/1136 | 0.86 | 0/1527 |
| 9 | I | 0.51 | 0/1029 | 0.74 | 1/1378 (0.1%) |
| 10 | J | 0.46 | 0/807 | 0.74 | 0/1085 |
| 11 | K | 0.53 | 0/900 | 0.76 | 0/1213 |
| 12 | L | 0.59 | 0/986 | 0.82 | 0/1320 |
| 13 | M | 0.48 | 0/1008 | 0.75 | 0/1347 |
| 14 | N | 0.59 | 0/501 | 0.84 | 0/664 |
| 15 | O | 0.58 | 0/745 | 0.77 | 0/992 |
| 16 | P | 0.59 | 0/716 | 0.81 | 0/963 |
| 17 | Q | 0.65 | 0/870 | 0.85 | 0/1159 |
| 18 | R | 0.50 | 0/603 | 0.74 | 0/799 |
| 19 | S | 0.43 | 0/661 | 0.70 | 0/890 |
| 20 | T | 0.52 | 0/764 | 0.76 | 0/1006 |
| 21 | U | 0.55 | 0/212 | 0.76 | 0/277 |
| All | All | 0.70 | 4/55748 (0.0%) | 0.82 | 74/82699 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 86 |
| 8 | H | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All | 0 | 87 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 702 | G | C5-C6 | -6.16 | 1.36 | 1.42 |
| 4 | D | 12 | CYS | CB-SG | 6.00 | 1.92 | 1.82 |
| 1 | A | 1067 | G | C5-C6 | -5.41 | 1.36 | 1.42 |
| 1 | A | 1317 | C | N1-C2 | 5.04 | 1.45 | 1.40 |

All (74) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 637 | A | N9-C1'-C2' | 9.39 | 126.21 | 114.00 |
| 1 | A | 242 | A | N9-C1'-C2' | 9.14 | 125.89 | 114.00 |
| 1 | A | 802 | G | N9-C1'-C2' | 9.02 | 125.72 | 114.00 |
| 1 | A | 938 | U | N1-C1'-C2' | 8.16 | 124.61 | 114.00 |
| 1 | A | 48 | C | N1-C1'-C2' | 7.85 | 124.20 | 114.00 |
| 4 | D | 12 | CYS | CA-CB-SG | 7.43 | 127.38 | 114.00 |
| 1 | A | 262 | G | C2'-C3'-O3' | 7.18 | 125.30 | 109.50 |
| 1 | A | 949 | G | N9-C1'-C2' | 7.02 | 123.13 | 114.00 |
| 1 | A | 176 | G | C2'-C3'-O3' | 6.80 | 124.58 | 113.70 |
| 1 | A | 311 | A | N9-C1'-C2' | 6.66 | 122.66 | 114.00 |
| 1 | A | 1304 | C | N1-C1'-C2' | 6.63 | 122.62 | 114.00 |
| 1 | A | 168 | U | N1-C1'-C2' | 6.54 | 122.50 | 114.00 |
| 1 | A | 850 | A | O4'-C1'-N9 | 6.52 | 113.42 | 108.20 |
| 1 | A | 954 | G | N9-C1'-C2' | 6.50 | 122.44 | 114.00 |
| 1 | A | 705 | G | N9-C1'-C2' | 6.47 | 122.41 | 114.00 |
| 1 | A | 425 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 1 | A | 32 | G | N9-C1'-C2' | 6.34 | 122.24 | 114.00 |
| 1 | A | 543 | A | N9-C1'-C2' | 6.26 | 122.14 | 114.00 |
| 1 | A | 368 | C | C2'-C3'-O3' | 6.19 | 123.61 | 113.70 |
| 1 | A | 1483 | G | C2'-C3'-O3' | 6.18 | 123.59 | 113.70 |
| 1 | A | 1482 | G | OP2-P-O3' | 6.16 | 118.74 | 105.20 |
| 1 | A | 361 | U | N1-C1'-C2' | 6.13 | 121.97 | 114.00 |
| 1 | A | 912 | C | C1'-O4'-C4' | -6.04 | 105.07 | 109.90 |
| 1 | A | 949 | G | O4'-C1'-N9 | 6.01 | 113.00 | 108.20 |
| 2 | B | 187 | LEU | N-CA-C | -5.99 | 94.84 | 111.00 |
| 1 | A | 912 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 1 | A | 1507 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 1 | A | 262 | G | O4'-C1'-N9 | -5.92 | 103.47 | 108.20 |
| 9 | I | 6 | GLY | N-CA-C | -5.91 | 98.31 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1477 | A | O5'-P-OP1 | -5.90 | 100.39 | 105.70 |
| 1 | A | 1480 | A | N9-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 1 | A | 480 | A | N9-C1'-C2' | 5.84 | 121.59 | 114.00 |
| 1 | A | 862 | U | N1-C1'-C2' | 5.66 | 121.36 | 114.00 |
| 1 | A | 1091 | G | C4'-C3'-C2' | -5.65 | 96.95 | 102.60 |
| 1 | A | 1262 | A | C1'-O4'-C4' | -5.64 | 105.39 | 109.90 |
| 5 | E | 81 | GLU | N-CA-C | -5.56 | 95.99 | 111.00 |
| 1 | A | 204 | A | N9-C1'-C2' | 5.55 | 121.22 | 114.00 |
| 1 | A | 103 | A | N9-C1'-C2' | 5.55 | 121.21 | 114.00 |
| 1 | A | 109 | G | OP2-P-O3' | 5.53 | 117.36 | 105.20 |
| 1 | A | 125 | A | N9-C1'-C2' | 5.53 | 121.19 | 114.00 |
| 1 | A | 1050 | A | N9-C1'-C2' | 5.46 | 121.10 | 114.00 |
| 1 | A | 849 | U | N1-C1'-C2' | 5.45 | 121.09 | 114.00 |
| 1 | A | 938 | U | C2'-C3'-O3' | 5.45 | 122.42 | 113.70 |
| 1 | A | 239 | A | N9-C1'-C2' | 5.44 | 121.07 | 114.00 |
| 1 | A | 1262 | A | N9-C1'-C2' | 5.42 | 121.05 | 114.00 |
| 1 | A | 625 | U | N1-C1'-C2' | 5.42 | 121.04 | 114.00 |
| 1 | A | 949 | G | C1'-O4'-C4' | -5.37 | 105.61 | 109.90 |
| 1 | A | 168 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 1 | A | 1077 | G | N9-C1'-C2' | 5.33 | 120.93 | 114.00 |
| 1 | A | 493 | A | C2'-C3'-O3' | 5.30 | 122.18 | 113.70 |
| 1 | A | 543 | A | OP2-P-O3' | 5.28 | 116.82 | 105.20 |
| 1 | A | 1262 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 1 | A | 446 | A | N9-C1'-C2' | 5.25 | 120.82 | 114.00 |
| 1 | A | 1318 | C | N1-C1'-C2' | 5.24 | 120.81 | 114.00 |
| 1 | A | 301 | G | N9-C1'-C2' | 5.23 | 120.80 | 114.00 |
| 1 | A | 109 | G | N9-C1'-C2' | 5.21 | 120.77 | 114.00 |
| 1 | A | 191 | G | N9-C1'-C2' | 5.21 | 120.77 | 114.00 |
| 1 | A | 262 | G | C5'-C4'-C3' | -5.20 | 107.68 | 116.00 |
| 1 | A | 546 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 1 | A | 1134 | A | N9-C1'-C2' | 5.18 | 120.73 | 114.00 |
| 1 | A | 868 | G | OP2-P-O3' | 5.17 | 116.58 | 105.20 |
| 1 | A | 803 | A | OP2-P-O3' | 5.16 | 116.56 | 105.20 |
| 1 | A | 736 | G | N9-C1'-C2' | 5.16 | 120.71 | 114.00 |
| 1 | A | 1122 | G | N9-C1'-C2' | 5.15 | 120.69 | 114.00 |
| 1 | A | 954 | G | C1'-O4'-C4' | -5.14 | 105.79 | 109.90 |
| 1 | A | 495 | C | C1'-O4'-C4' | -5.12 | 105.81 | 109.90 |
| 1 | A | 777 | U | N1-C1'-C2' | 5.11 | 120.64 | 114.00 |
| 4 | D | 166 | LYS | N-CA-C | -5.10 | 97.22 | 111.00 |
| 1 | A | 501 | G | N9-C1'-C2' | 5.10 | 120.62 | 114.00 |
| 1 | A | 1363 | U | C2'-C3'-O3' | 5.09 | 121.85 | 113.70 |
| 1 | A | 686 | A | N9-C1'-C2' | 5.08 | 120.60 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 1 | A | 51 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 1 | A | 1280 | C | N1-C1'-C2' | 5.05 | 120.57 | 114.00 |
| 1 | A | 1480 | A | O4'-C1'-N9 | 5.03 | 112.23 | 108.20 |

There are no chirality outliers.

All (87) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 101 | G | Sidechain |
| 1 | A | 1032 | U | Sidechain |
| 1 | A | 1038 | A | Sidechain |
| 1 | A | 1050 | A | Sidechain |
| 1 | A | 1056 | U | Sidechain |
| 1 | A | 1060 | G | Sidechain |
| 1 | A | 109 | G | Sidechain |
| 1 | A | 1091 | G | Sidechain |
| 1 | A | 112 | U | Sidechain |
| 1 | A | 1122 | G | Sidechain |
| 1 | A | 1163 | G | Sidechain |
| 1 | A | 1187 | U | Sidechain |
| 1 | A | 12 | G | Sidechain |
| 1 | A | 1202 | G | Sidechain |
| 1 | A | 1213 | G | Sidechain |
| 1 | A | 1238 | A | Sidechain |
| 1 | A | 125 | A | Sidechain |
| 1 | A | 1263 | U | Sidechain |
| 1 | A | 1283 | U | Sidechain |
| 1 | A | 1304 | C | Sidechain |
| 1 | A | 1353 | G | Sidechain |
| 1 | A | 1355 | U | Sidechain |
| 1 | A | 1376 | U | Sidechain |
| 1 | A | 1381 | A | Sidechain |
| 1 | A | 14 | U | Sidechain |
| 1 | A | 1419 | U | Sidechain |
| 1 | A | 142 | G | Sidechain |
| 1 | A | 1475 | G | Sidechain |
| 1 | A | 1503 | G | Sidechain |
| 1 | A | 199 | U | Sidechain |
| 1 | A | 202 | A | Sidechain |
| 1 | A | 204 | A | Sidechain |
| 1 | A | 225 | U | Sidechain |
| 1 | A | 228 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 249 | U | Sidechain |
| 1 | A | 259 | A | Sidechain |
| 1 | A | 261 | G | Sidechain |
| 1 | A | 262 | G | Sidechain |
| 1 | A | 271 | G | Sidechain |
| 1 | A | 276 | C | Sidechain |
| 1 | A | 280 | G | Sidechain |
| 1 | A | 295 | G | Sidechain |
| 1 | A | 317 | A | Sidechain |
| 1 | A | 350 | G | Sidechain |
| 1 | A | 363 | U | Sidechain |
| 1 | A | 408 | A | Sidechain |
| 1 | A | 443 | A | Sidechain |
| 1 | A | 466 | G | Sidechain |
| 1 | A | 480 | A | Sidechain |
| 1 | A | 50 | U | Sidechain |
| 1 | A | 500 | U | Sidechain |
| 1 | A | 501 | G | Sidechain |
| 1 | A | 517 | A | Sidechain |
| 1 | A | 52 | A | Sidechain |
| 1 | A | 554 | G | Sidechain |
| 1 | A | 559 | G | Sidechain |
| 1 | A | 608 | C | Sidechain |
| 1 | A | 61 | A | Sidechain |
| 1 | A | 636 | U | Sidechain |
| 1 | A | 641 | G | Sidechain |
| 1 | A | 650 | G | Sidechain |
| 1 | A | 703 | C | Sidechain |
| 1 | A | 711 | G | Sidechain |
| 1 | A | 736 | G | Sidechain |
| 1 | A | 747 | G | Sidechain |
| 1 | A | 750 | A | Sidechain |
| 1 | A | 777 | U | Sidechain |
| 1 | A | 796 | C | Sidechain |
| 1 | A | 803 | A | Sidechain |
| 1 | A | 811 | U | Sidechain |
| 1 | A | 819 | U | Sidechain |
| 1 | A | 820 | G | Sidechain |
| 1 | A | 842 | A | Sidechain |
| 1 | A | 846 | C | Sidechain |
| 1 | A | 847 | G | Sidechain |
| 1 | A | 848 | U | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 85 | C | Sidechain |
| 1 | A | 850 | A | Sidechain |
| 1 | A | 856 | G | Sidechain |
| 1 | A | 858 | C | Sidechain |
| 1 | A | 898 | U | Sidechain |
| 1 | A | 924 | A | Sidechain |
| 1 | A | 925 | G | Sidechain |
| 1 | A | 933 | U | Sidechain |
| 1 | A | 941 | G | Sidechain |
| 1 | A | 952 | A | Sidechain |
| 8 | H | 58 | TYR | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32349 | 0 | 16328 | 2022 | 0 |
| 2 | B | 1900 | 0 | 1951 | 273 | 0 |
| 3 | C | 1612 | 0 | 1677 | 302 | 0 |
| 4 | D | 1703 | 0 | 1767 | 271 | 0 |
| 5 | E | 1146 | 0 | 1207 | 206 | 0 |
| 6 | F | 843 | 0 | 857 | 101 | 0 |
| 7 | G | 1257 | 0 | 1296 | 158 | 0 |
| 8 | H | 1116 | 0 | 1177 | 132 | 0 |
| 9 | I | 1011 | 0 | 1043 | 181 | 0 |
| 10 | J | 794 | 0 | 840 | 144 | 0 |
| 11 | K | 885 | 0 | 904 | 116 | 0 |
| 12 | L | 970 | 0 | 1057 | 170 | 0 |
| 13 | M | 997 | 0 | 1072 | 185 | 0 |
| 14 | N | 492 | 0 | 533 | 93 | 0 |
| 15 | O | 734 | 0 | 771 | 101 | 0 |
| 16 | P | 700 | 0 | 720 | 102 | 0 |
| 17 | Q | 857 | 0 | 930 | 147 | 0 |
| 18 | R | 597 | 0 | 668 | 120 | 0 |
| 19 | S | 647 | 0 | 673 | 111 | 0 |
| 20 | T | 762 | 0 | 856 | 132 | 0 |
| 21 | U | 208 | 0 | 221 | 28 | 0 |
| 22 | A | 52 | 0 | 46 | 12 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 51632 | 0 | 36594 | 4702 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (4702) 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) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:89:PRO:HA | 8:H:92:ARG:NH1 | 1.49 | 1.27 |
| 12:L:41:ARG:HG2 | 12:L:42:THR:H | 1.05 | 1.13 |
| 3:C:156:ARG:H | 3:C:163:ALA:HA | 1.04 | 1.13 |
| 19:S:28:LYS:HG2 | 19:S:29:ARG:H | 1.07 | 1.12 |
| 10:J:45:ARG:HB3 | 10:J:45:ARG:HH11 | 1.15 | 1.11 |
| 3:C:91:LEU:HD21 | 3:C:99:VAL:HG13 | 1.17 | 1.09 |
| 12:L:28:LYS:HD2 | 12:L:33:ARG:HH22 | 1.00 | 1.08 |
| 1:A:239:A:H4' | 1:A:240:U:C5' | 1.84 | 1.08 |
| 1:A:1132:C:H2' | 1:A:1133:U:H6 | 1.12 | 1.07 |
| 1:A:181:C:O3' | 20:T:82:SER:HB3 | 1.54 | 1.06 |
| 1:A:917:G:H5'' | 7:G:102:ARG:HH22 | 1.17 | 1.05 |
| 5:E:139:LEU:HD22 | 5:E:142:LEU:HD11 | 1.33 | 1.05 |
| 5:E:18:ARG:HG2 | 5:E:19:MET:H | 0.98 | 1.05 |
| 2:B:68:ILE:H | 2:B:90:MET:HE3 | 1.20 | 1.04 |
| 1:A:239:A:H4' | 1:A:240:U:H5' | 1.38 | 1.03 |
| 1:A:1030:G:H5'' | 14:N:4:LYS:HD2 | 1.38 | 1.03 |
| 19:S:20:LEU:HA | 19:S:23:ASN:HD22 | 1.21 | 1.02 |
| 1:A:106:G:H21 | 1:A:350:G:H5' | 1.20 | 1.02 |
| 16:P:74:LEU:HB3 | 16:P:79:VAL:HG21 | 1.42 | 1.01 |
| 1:A:1207:A:H5' | 13:M:103:THR:OG1 | 1.61 | 1.01 |
| 9:I:26:VAL:HG22 | 9:I:61:ALA:HB3 | 1.39 | 1.01 |
| 1:A:917:G:H5'' | 7:G:102:ARG:NH2 | 1.75 | 1.01 |
| 7:G:113:GLU:HG2 | 7:G:119:ARG:HG2 | 1.43 | 1.01 |
| 8:H:87:SER:HA | 8:H:93:VAL:HG23 | 1.40 | 1.00 |
| 9:I:93:ARG:HD3 | 9:I:97:LYS:HE3 | 1.40 | 1.00 |
| 1:A:1432:A:H5'' | 1:A:1433:C:H5 | 1.25 | 0.99 |
| 1:A:1426:G:H5'' | 1:A:1427:A:H5' | 1.40 | 0.99 |
| 13:M:65:LYS:HE3 | 13:M:69:GLU:HG2 | 1.44 | 0.99 |
| 6:F:48:LEU:HD13 | 6:F:52:ILE:HG13 | 1.44 | 0.98 |
| 4:D:131:ARG:H | 4:D:131:ARG:HD2 | 1.28 | 0.98 |
| 14:N:41:ARG:HG2 | 14:N:41:ARG:HH11 | 1.27 | 0.98 |
| 4:D:140:VAL:HG11 | 4:D:146:ILE:HD11 | 1.42 | 0.98 |
| 3:C:94:LEU:HD23 | 3:C:95:THR:HG23 | 1.45 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1425:G:N2 | 1:A:1427:A:H3' | 1.78 | 0.97 |
| 1:A:1480:A:H2 | 1:A:1483:G:H1 | 1.03 | 0.97 |
| 5:E:18:ARG:HG2 | 5:E:19:MET:N | 1.78 | 0.97 |
| 12:L:41:ARG:HG2 | 12:L:42:THR:N | 1.80 | 0.97 |
| 1:A:563:G:H5' | 1:A:712:A:H1' | 1.46 | 0.97 |
| 9:I:28:VAL:HG22 | 9:I:63:ILE:HB | 1.45 | 0.97 |
| 1:A:1135:A:H5'' | 10:J:13:HIS:CD2 | 1.99 | 0.96 |
| 1:A:1132:C:H2' | 1:A:1133:U:C6 | 2.01 | 0.96 |
| 1:A:1331:A:H2' | 1:A:1332:A:H8 | 1.30 | 0.96 |
| 1:A:791:A:H2' | 1:A:792:C:H6 | 1.29 | 0.95 |
| 3:C:58:GLU:H | 3:C:65:ALA:HB3 | 1.28 | 0.95 |
| 12:L:28:LYS:HD2 | 12:L:33:ARG:NH2 | 1.81 | 0.95 |
| 3:C:195:VAL:O | 3:C:196:LEU:HD23 | 1.65 | 0.94 |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:HG13 | 1.48 | 0.94 |
| 5:E:79:GLU:HG3 | 5:E:93:PRO:HD2 | 1.50 | 0.94 |
| 5:E:80:ILE:HD11 | 5:E:91:LEU:HD12 | 1.48 | 0.94 |
| 1:A:1467:G:C2' | 1:A:1468:C:H5'' | 1.98 | 0.94 |
| 20:T:43:LEU:HD11 | 20:T:55:ILE:HD12 | 1.48 | 0.94 |
| 1:A:937:A:H3' | 1:A:938:U:H5'' | 1.48 | 0.94 |
| 6:F:30:LEU:HD23 | 6:F:75:LEU:HD21 | 1.50 | 0.94 |
| 1:A:1418:G:H2' | 1:A:1419:U:C6 | 2.03 | 0.93 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:HG21 | 1.48 | 0.93 |
| 1:A:1467:G:H2' | 1:A:1468:C:H5'' | 1.47 | 0.93 |
| 1:A:531:A:H4' | 1:A:532:G:O5' | 1.68 | 0.93 |
| 5:E:89:ILE:HD13 | 5:E:90:VAL:N | 1.84 | 0.93 |
| 1:A:1325:G:H1' | 9:I:121:ARG:HH12 | 1.31 | 0.92 |
| 3:C:70:VAL:HG21 | 3:C:76:VAL:HG21 | 1.49 | 0.92 |
| 1:A:246:A:H4' | 1:A:247:G:O5' | 1.68 | 0.92 |
| 9:I:26:VAL:HB | 9:I:33:PHE:HB2 | 1.50 | 0.92 |
| 5:E:41:VAL:CG2 | 5:E:113:ALA:HA | 2.00 | 0.92 |
| 1:A:1282:G:HO2' | 1:A:1283:U:H6 | 1.13 | 0.91 |
| 9:I:108:VAL:HG12 | 9:I:109:VAL:H | 1.34 | 0.91 |
| 5:E:43:LEU:HD23 | 5:E:44:GLY:N | 1.85 | 0.91 |
| 3:C:91:LEU:HD21 | 3:C:99:VAL:CG1 | 1.99 | 0.91 |
| 1:A:347:G:H4' | 1:A:348:C:OP1 | 1.71 | 0.91 |
| 1:A:1425:G:H21 | 1:A:1427:A:H3' | 1.31 | 0.91 |
| 3:C:52:LEU:HD23 | 3:C:52:LEU:H | 1.35 | 0.91 |
| 1:A:1218:A:H4' | 1:A:1286:G:H4' | 1.52 | 0.91 |
| 1:A:945:C:H4' | 9:I:128:ARG:HG3 | 1.52 | 0.91 |
| 15:O:56:LEU:HA | 15:O:59:MET:HE2 | 1.52 | 0.91 |
| 1:A:1486:G:H2' | 1:A:1487:C:H6 | 1.36 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:13:LEU:HD12 | 20:T:13:LEU:H | 1.35 | 0.91 |
| 2:B:204:ASN:HD22 | 2:B:206:ASP:H | 1.19 | 0.90 |
| 1:A:1158:A:H2' | 1:A:1159:G:C8 | 2.06 | 0.90 |
| 1:A:858:C:H5'' | 12:L:12:ARG:HH21 | 1.37 | 0.90 |
| 2:B:209:ARG:HE | 2:B:239:VAL:CG1 | 1.84 | 0.90 |
| 3:C:3:ASN:HD22 | 3:C:3:ASN:N | 1.69 | 0.90 |
| 6:F:9:VAL:HB | 6:F:87:ARG:HB2 | 1.51 | 0.90 |
| 1:A:251:G:H1' | 17:Q:16:GLN:NE2 | 1.87 | 0.89 |
| 1:A:434:G:H4' | 1:A:435:A:OP1 | 1.69 | 0.89 |
| 3:C:26:LYS:HD3 | 3:C:26:LYS:H | 1.37 | 0.89 |
| 3:C:6:HIS:HD2 | 3:C:9:GLY:H | 1.16 | 0.89 |
| 4:D:104:VAL:HG12 | 4:D:108:LEU:HD11 | 1.53 | 0.89 |
| 1:A:1040:G:H5'' | 3:C:154:SER:HB2 | 1.53 | 0.89 |
| 12:L:67:THR:HG21 | 12:L:96:VAL:HG22 | 1.54 | 0.89 |
| 1:A:43:G:H2' | 1:A:44:C:C6 | 2.06 | 0.89 |
| 1:A:791:A:H2' | 1:A:792:C:C6 | 2.07 | 0.89 |
| 5:E:144:THR:HG22 | 5:E:145:LYS:N | 1.87 | 0.89 |
| 1:A:823:U:H5' | 1:A:824:C:H5 | 1.38 | 0.89 |
| 20:T:57:ARG:HE | 20:T:102:GLY:HA3 | 1.36 | 0.89 |
| 1:A:584:C:OP1 | 8:H:97:VAL:HG12 | 1.73 | 0.89 |
| 10:J:34:VAL:HG22 | 10:J:74:ILE:HG12 | 1.55 | 0.89 |
| 1:A:1287:G:HO2' | 1:A:1288:A:H8 | 0.93 | 0.88 |
| 1:A:1396:A:H2 | 1:A:1465:G:H22 | 1.10 | 0.88 |
| 11:K:54:ARG:O | 11:K:57:THR:HG22 | 1.73 | 0.88 |
| 8:H:83:ILE:HG13 | 8:H:137:VAL:HG22 | 1.56 | 0.88 |
| 1:A:1433:C:H4' | 1:A:1434:G:O5' | 1.71 | 0.88 |
| 4:D:70:ILE:HD11 | 4:D:100:ARG:NE | 1.87 | 0.88 |
| 10:J:12:ASP:HB3 | 10:J:15:THR:HB | 1.56 | 0.88 |
| 1:A:1120:C:H4' | 1:A:1121:G:C2 | 2.08 | 0.88 |
| 11:K:48:ILE:HD13 | 11:K:63:LEU:HB2 | 1.54 | 0.88 |
| 19:S:28:LYS:HG2 | 19:S:29:ARG:N | 1.89 | 0.88 |
| 1:A:804:U:H4' | 1:A:805:G:OP2 | 1.71 | 0.87 |
| 1:A:1328:A:H2' | 7:G:10:ARG:HH22 | 1.39 | 0.87 |
| 7:G:51:GLN:HG2 | 7:G:58:PRO:HD3 | 1.56 | 0.87 |
| 12:L:41:ARG:CG | 12:L:42:THR:H | 1.87 | 0.87 |
| 1:A:1140:A:H1' | 1:A:1163:G:N2 | 1.90 | 0.87 |
| 1:A:1269:A:H2 | 1:A:1335:G:H1' | 1.40 | 0.87 |
| 13:M:81:LEU:HA | 13:M:84:ILE:HG12 | 1.57 | 0.87 |
| 14:N:27:CYS:SG | 14:N:29:ARG:HB2 | 2.15 | 0.87 |
| 1:A:648:G:H22 | 1:A:725:G:H1 | 1.20 | 0.87 |
| 2:B:142:LEU:HD22 | 2:B:146:GLN:NE2 | 1.90 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:97:LYS:HE2 | 9:I:102:LEU:HD12 | 1.55 | 0.87 |
| 1:A:61:A:H4' | 1:A:62:G:O5' | 1.73 | 0.87 |
| 3:C:156:ARG:N | 3:C:163:ALA:HA | 1.88 | 0.87 |
| 1:A:367:G:O2' | 1:A:368:C:H5' | 1.75 | 0.87 |
| 3:C:14:ILE:HG22 | 3:C:15:THR:H | 1.39 | 0.87 |
| 1:A:1177:C:H3' | 1:A:1178:U:C5' | 2.05 | 0.86 |
| 4:D:28:SER:O | 4:D:30:LYS:N | 2.08 | 0.86 |
| 8:H:123:GLU:O | 8:H:127:LEU:HD23 | 1.76 | 0.86 |
| 1:A:106:G:N2 | 1:A:350:G:H5' | 1.90 | 0.86 |
| 3:C:84:ILE:O | 3:C:88:ARG:HB2 | 1.74 | 0.86 |
| 2:B:98:LEU:HB2 | 2:B:101:MET:SD | 2.14 | 0.86 |
| 13:M:6:GLY:O | 13:M:7:VAL:HG22 | 1.74 | 0.86 |
| 1:A:1288:A:N6 | 1:A:1313:G:H1' | 1.90 | 0.86 |
| 3:C:188:LEU:CD1 | 3:C:189:ALA:H | 1.88 | 0.86 |
| 1:A:1432:A:H5'' | 1:A:1433:C:C5 | 2.09 | 0.86 |
| 1:A:43:G:H2' | 1:A:44:C:H6 | 1.39 | 0.86 |
| 2:B:53:ARG:HA | 2:B:56:ARG:NH1 | 1.91 | 0.86 |
| 1:A:191:G:H4' | 1:A:192:G:OP2 | 1.76 | 0.86 |
| 3:C:188:LEU:HD12 | 3:C:189:ALA:H | 1.41 | 0.86 |
| 1:A:603:U:H3 | 4:D:135:LEU:HD21 | 1.39 | 0.85 |
| 1:A:722:C:OP2 | 6:F:92:LYS:HE3 | 1.75 | 0.85 |
| 10:J:90:LEU:H | 10:J:91:PRO:HD2 | 1.40 | 0.85 |
| 1:A:550:G:H4' | 1:A:551:G:OP1 | 1.73 | 0.85 |
| 1:A:661:U:H3 | 1:A:697:G:H22 | 1.20 | 0.85 |
| 1:A:900:G:H2' | 1:A:901:A:C8 | 2.10 | 0.85 |
| 4:D:125:HIS:HD1 | 4:D:152:SER:HG | 1.25 | 0.85 |
| 1:A:485:C:H2' | 1:A:486:G:H8 | 1.40 | 0.85 |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HD12 | 1.59 | 0.85 |
| 7:G:59:LEU:HD11 | 7:G:63:LYS:HE3 | 1.56 | 0.85 |
| 8:H:89:PRO:HA | 8:H:92:ARG:HH12 | 1.36 | 0.85 |
| 1:A:103:A:H2' | 1:A:322:G:H21 | 1.41 | 0.85 |
| 5:E:139:LEU:CD2 | 5:E:142:LEU:HD11 | 2.06 | 0.85 |
| 15:O:25:THR:HG21 | 15:O:70:LEU:HD23 | 1.56 | 0.85 |
| 4:D:150:GLU:H | 4:D:150:GLU:CD | 1.78 | 0.85 |
| 1:A:1207:A:H5' | 13:M:103:THR:HG1 | 1.37 | 0.85 |
| 1:A:1233:A:H2' | 1:A:1234:A:C8 | 2.12 | 0.84 |
| 1:A:1331:A:H2' | 1:A:1332:A:C8 | 2.13 | 0.84 |
| 1:A:1383:C:H4' | 1:A:1384:G:OP2 | 1.78 | 0.84 |
| 7:G:50:ILE:HD11 | 7:G:121:ALA:HA | 1.57 | 0.84 |
| 1:A:1099:C:H2' | 1:A:1100:G:H5' | 1.60 | 0.84 |
| 9:I:17:VAL:HG11 | 9:I:81:ILE:HA | 1.59 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1172:G:OP1 | 3:C:4:LYS:HA | 1.78 | 0.84 |
| 3:C:91:LEU:CD2 | 3:C:99:VAL:HG13 | 2.05 | 0.84 |
| 5:E:80:ILE:O | 5:E:80:ILE:HD12 | 1.78 | 0.83 |
| 8:H:53:VAL:HB | 8:H:58:TYR:CD1 | 2.12 | 0.83 |
| 9:I:65:VAL:HG21 | 9:I:73:GLN:HB3 | 1.58 | 0.83 |
| 3:C:64:VAL:HB | 3:C:99:VAL:HB | 1.58 | 0.83 |
| 13:M:81:LEU:HA | 13:M:84:ILE:CG1 | 2.08 | 0.83 |
| 1:A:1216:C:H5' | 1:A:1348:G:OP1 | 1.78 | 0.83 |
| 2:B:74:LYS:HZ1 | 2:B:206:ASP:HB2 | 1.44 | 0.83 |
| 17:Q:101:ARG:HE | 17:Q:101:ARG:HA | 1.42 | 0.83 |
| 1:A:1287:G:H5' | 21:U:4:GLY:HA3 | 1.59 | 0.83 |
| 7:G:37:ASN:ND2 | 9:I:41:VAL:HG23 | 1.94 | 0.83 |
| 13:M:62:ASN:O | 13:M:63:THR:HB | 1.76 | 0.83 |
| 4:D:151:LYS:HD2 | 4:D:151:LYS:H | 1.43 | 0.82 |
| 19:S:64:GLU:O | 19:S:67:VAL:HG23 | 1.80 | 0.82 |
| 5:E:89:ILE:HD13 | 5:E:89:ILE:C | 1.99 | 0.82 |
| 1:A:1282:G:O2' | 1:A:1283:U:H6 | 1.62 | 0.82 |
| 1:A:130:C:O2 | 16:P:1:MET:HB2 | 1.80 | 0.82 |
| 5:E:18:ARG:CG | 5:E:19:MET:H | 1.87 | 0.82 |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:H | 1.44 | 0.82 |
| 3:C:130:VAL:HG21 | 3:C:157:ILE:HG23 | 1.58 | 0.82 |
| 1:A:397:C:H2' | 1:A:398:G:H8 | 1.44 | 0.82 |
| 2:B:30:ARG:HG3 | 2:B:31:TYR:CD2 | 2.15 | 0.82 |
| 13:M:98:VAL:HG23 | 13:M:110:ARG:HH12 | 1.44 | 0.82 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.62 | 0.82 |
| 13:M:4:ILE:HG22 | 13:M:5:ALA:H | 1.45 | 0.82 |
| 1:A:182:C:N3 | 20:T:105:SER:HB3 | 1.95 | 0.82 |
| 1:A:970:U:H4' | 1:A:971:G:O5' | 1.79 | 0.82 |
| 18:R:86:VAL:O | 18:R:87:ARG:HG2 | 1.79 | 0.82 |
| 1:A:515:U:H4' | 1:A:516:A:H5'' | 1.62 | 0.82 |
| 4:D:127:THR:HG23 | 4:D:130:GLY:O | 1.78 | 0.82 |
| 10:J:49:VAL:O | 10:J:60:ARG:HA | 1.79 | 0.82 |
| 1:A:1009:C:H2' | 1:A:1010:G:H8 | 1.45 | 0.81 |
| 1:A:823:U:H5' | 1:A:824:C:C5 | 2.14 | 0.81 |
| 1:A:947:A:H61 | 13:M:126:LYS:HB2 | 1.43 | 0.81 |
| 1:A:1238:A:H4' | 1:A:1239:U:H5' | 1.60 | 0.81 |
| 4:D:121:VAL:O | 4:D:134:ASP:HA | 1.80 | 0.81 |
| 1:A:641:G:O2' | 1:A:642:G:H5' | 1.79 | 0.81 |
| 6:F:3:ARG:HH21 | 6:F:64:GLN:HE22 | 1.28 | 0.81 |
| 17:Q:9:VAL:HG22 | 17:Q:56:VAL:HG22 | 1.60 | 0.81 |
| 1:A:670:U:O4 | 1:A:687:G:H1' | 1.80 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:68:ILE:N | 2:B:90:MET:HE3 | 1.95 | 0.81 |
| 5:E:12:LEU:HD12 | 5:E:31:LEU:HB2 | 1.62 | 0.81 |
| 7:G:59:LEU:O | 7:G:62:PHE:HB3 | 1.80 | 0.81 |
| 12:L:75:HIS:HA | 12:L:102:ARG:HH22 | 1.45 | 0.81 |
| 13:M:57:ARG:HG3 | 13:M:61:GLU:OE2 | 1.80 | 0.81 |
| 2:B:204:ASN:ND2 | 2:B:206:ASP:H | 1.78 | 0.81 |
| 10:J:3:LYS:HA | 10:J:75:ILE:HA | 1.63 | 0.81 |
| 1:A:1274:U:H5' | 9:I:38:GLN:NE2 | 1.96 | 0.81 |
| 1:A:442:G:H2' | 1:A:470:G:N2 | 1.96 | 0.81 |
| 1:A:424:G:H4' | 1:A:425:U:O5' | 1.78 | 0.81 |
| 11:K:77:MET:HE1 | 11:K:80:VAL:HG22 | 1.62 | 0.81 |
| 12:L:70:ILE:HD13 | 12:L:77:LEU:HD12 | 1.61 | 0.81 |
| 13:M:75:ALA:HA | 13:M:78:ILE:HD12 | 1.60 | 0.81 |
| 17:Q:67:LYS:O | 17:Q:68:ARG:HB3 | 1.80 | 0.81 |
| 18:R:47:THR:HB | 18:R:49:LYS:HE3 | 1.61 | 0.81 |
| 1:A:1280:C:C2 | 7:G:114:ARG:NH1 | 2.49 | 0.81 |
| 1:A:609:G:H2' | 1:A:610:U:C6 | 2.16 | 0.80 |
| 2:B:130:ARG:NH2 | 3:C:207:VAL:HG22 | 1.95 | 0.80 |
| 10:J:3:LYS:HG2 | 10:J:75:ILE:HG23 | 1.63 | 0.80 |
| 4:D:102:ASP:HB3 | 4:D:136:PRO:HA | 1.62 | 0.80 |
| 11:K:66:LEU:HB3 | 11:K:70:LYS:HE3 | 1.62 | 0.80 |
| 1:A:1124:C:H2' | 1:A:1125:G:H8 | 1.43 | 0.80 |
| 6:F:100:ASN:HD22 | 18:R:23:LYS:HG2 | 1.45 | 0.80 |
| 20:T:79:ARG:HE | 20:T:83:ARG:HH12 | 1.26 | 0.80 |
| 1:A:1305:G:H2' | 1:A:1306:A:C8 | 2.17 | 0.80 |
| 1:A:205:G:H2' | 1:A:206:G:H8 | 1.47 | 0.80 |
| 10:J:8:LEU:HB2 | 10:J:70:ARG:HB2 | 1.61 | 0.80 |
| 16:P:39:TYR:CD2 | 16:P:73:LEU:HD11 | 2.17 | 0.80 |
| 18:R:53:ARG:NH1 | 18:R:59:SER:HA | 1.95 | 0.80 |
| 13:M:79:LYS:O | 13:M:82:MET:HB3 | 1.82 | 0.80 |
| 3:C:32:LEU:HD21 | 3:C:59:ARG:HD2 | 1.64 | 0.80 |
| 4:D:109:GLY:O | 4:D:111:ALA:N | 2.14 | 0.80 |
| 1:A:401:U:H3' | 1:A:402:G:H5' | 1.63 | 0.80 |
| 12:L:39:VAL:O | 12:L:56:ALA:HA | 1.81 | 0.80 |
| 11:K:21:ILE:HB | 11:K:84:VAL:HG12 | 1.65 | 0.80 |
| 1:A:603:U:N3 | 4:D:135:LEU:HD21 | 1.96 | 0.79 |
| 3:C:47:LEU:H | 3:C:47:LEU:HD12 | 1.47 | 0.79 |
| 5:E:12:LEU:CD1 | 5:E:31:LEU:HB2 | 2.12 | 0.79 |
| 20:T:57:ARG:NE | 20:T:102:GLY:HA3 | 1.97 | 0.79 |
| 1:A:1177:C:H3' | 1:A:1178:U:H5' | 1.62 | 0.79 |
| 1:A:1287:G:H22 | 1:A:1313:G:H2' | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:954:G:OP2 | 1:A:1340:U:H1' | 1.81 | 0.79 |
| 1:A:385:A:H2' | 1:A:386:C:H5' | 1.64 | 0.79 |
| 3:C:155:GLY:O | 3:C:196:LEU:HD22 | 1.81 | 0.79 |
| 1:A:1274:U:P | 7:G:41:ARG:HH22 | 2.04 | 0.79 |
| 14:N:41:ARG:NH1 | 14:N:41:ARG:HG2 | 1.94 | 0.79 |
| 11:K:58:PRO:HB2 | 11:K:93:GLN:HG3 | 1.64 | 0.79 |
| 1:A:1080:C:H2' | 1:A:1081:C:C6 | 2.18 | 0.79 |
| 1:A:386:C:H2' | 1:A:387:G:C8 | 2.18 | 0.79 |
| 1:A:822:G:H2' | 1:A:823:U:H5'' | 1.62 | 0.79 |
| 1:A:1329:G:O2' | 1:A:1330:U:OP2 | 1.98 | 0.79 |
| 1:A:1462:C:H2' | 1:A:1463:U:H6 | 1.48 | 0.79 |
| 1:A:386:C:H2' | 1:A:387:G:H8 | 1.46 | 0.79 |
| 1:A:65:G:H4' | 1:A:66:U:H5'' | 1.64 | 0.79 |
| 6:F:22:GLU:OE1 | 6:F:82:ARG:HD3 | 1.83 | 0.79 |
| 13:M:65:LYS:HE3 | 13:M:69:GLU:CG | 2.12 | 0.79 |
| 7:G:75:VAL:HG21 | 7:G:144:MET:HB3 | 1.63 | 0.79 |
| 13:M:4:ILE:HG22 | 13:M:5:ALA:N | 1.98 | 0.79 |
| 1:A:252:U:H2' | 1:A:253:G:H8 | 1.48 | 0.78 |
| 7:G:145:ALA:C | 7:G:147:ALA:H | 1.85 | 0.78 |
| 1:A:323:A:H4' | 1:A:324:C:OP1 | 1.84 | 0.78 |
| 4:D:64:LEU:HD23 | 4:D:198:VAL:HG11 | 1.63 | 0.78 |
| 13:M:96:LEU:HB3 | 13:M:97:PRO:HD2 | 1.64 | 0.78 |
| 4:D:131:ARG:H | 4:D:131:ARG:CD | 1.95 | 0.78 |
| 5:E:71:LEU:HD11 | 5:E:114:GLY:HA3 | 1.63 | 0.78 |
| 10:J:30:SER:OG | 10:J:81:THR:HA | 1.84 | 0.78 |
| 13:M:117:VAL:HG12 | 13:M:118:ALA:H | 1.46 | 0.78 |
| 9:I:117:HIS:O | 9:I:118:LYS:HG3 | 1.83 | 0.78 |
| 1:A:684:G:O3' | 1:A:687:G:H5' | 1.83 | 0.78 |
| 14:N:14:PRO:C | 14:N:16:PHE:H | 1.85 | 0.78 |
| 1:A:25:U:H2' | 1:A:26:C:H6 | 1.49 | 0.78 |
| 5:E:144:THR:HG22 | 5:E:145:LYS:H | 1.43 | 0.78 |
| 11:K:91:ARG:HD3 | 18:R:88:LYS:HE2 | 1.64 | 0.78 |
| 13:M:52:GLU:HG2 | 13:M:55:ARG:HH21 | 1.49 | 0.78 |
| 1:A:1419:U:H2' | 1:A:1420:C:C6 | 2.19 | 0.78 |
| 1:A:94:C:H2' | 1:A:95:A:C8 | 2.19 | 0.78 |
| 3:C:155:GLY:HA3 | 3:C:163:ALA:HB1 | 1.65 | 0.78 |
| 1:A:1200:C:H2' | 1:A:1201:U:C6 | 2.18 | 0.78 |
| 1:A:802:G:H3' | 1:A:803:A:C5' | 2.14 | 0.78 |
| 8:H:7:ALA:HB2 | 8:H:85:ARG:HD2 | 1.66 | 0.78 |
| 9:I:125:TYR:CE1 | 9:I:128:ARG:HD2 | 2.19 | 0.78 |
| 9:I:9:ARG:HG2 | 9:I:14:VAL:HG22 | 1.66 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:824:C:H5' | 1:A:825:U:OP1 | 1.84 | 0.78 |
| 5:E:51:VAL:O | 5:E:55:VAL:HG23 | 1.84 | 0.78 |
| 16:P:9:PHE:CE2 | 16:P:18:ARG:HD2 | 2.19 | 0.78 |
| 1:A:1080:C:H2' | 1:A:1081:C:H6 | 1.46 | 0.78 |
| 5:E:144:THR:O | 5:E:148:VAL:HG23 | 1.84 | 0.78 |
| 8:H:86:ILE:HD11 | 8:H:136:GLU:HB2 | 1.66 | 0.77 |
| 13:M:108:ARG:NH1 | 13:M:111:LYS:HD2 | 1.97 | 0.77 |
| 1:A:850:A:H4' | 1:A:851:A:OP1 | 1.83 | 0.77 |
| 8:H:34:GLU:O | 8:H:37:ARG:HB3 | 1.84 | 0.77 |
| 9:I:19:LEU:O | 9:I:20:ARG:HG3 | 1.83 | 0.77 |
| 18:R:45:SER:C | 18:R:47:THR:H | 1.86 | 0.77 |
| 1:A:1047:G:H4' | 1:A:1048:U:C5' | 2.14 | 0.77 |
| 1:A:400:U:H2' | 1:A:401:U:C6 | 2.19 | 0.77 |
| 1:A:489:G:H5' | 1:A:518:U:H2' | 1.66 | 0.77 |
| 3:C:110:ASN:O | 3:C:111:LEU:HD23 | 1.83 | 0.77 |
| 13:M:78:ILE:O | 13:M:81:LEU:HD23 | 1.85 | 0.77 |
| 4:D:70:ILE:HD11 | 4:D:100:ARG:CD | 2.14 | 0.77 |
| 17:Q:12:SER:HB3 | 17:Q:20:THR:HB | 1.65 | 0.77 |
| 17:Q:67:LYS:HA | 17:Q:70:ARG:HH12 | 1.49 | 0.77 |
| 6:F:80:ARG:NH1 | 6:F:88:VAL:HB | 1.99 | 0.77 |
| 12:L:120:TYR:O | 12:L:122:THR:HG23 | 1.84 | 0.77 |
| 17:Q:9:VAL:HG21 | 17:Q:84:LEU:HD13 | 1.66 | 0.77 |
| 18:R:39:VAL:HG13 | 18:R:40:LEU:N | 1.99 | 0.77 |
| 13:M:98:VAL:HG23 | 13:M:110:ARG:NH1 | 1.98 | 0.77 |
| 18:R:47:THR:CB | 18:R:49:LYS:HE3 | 2.14 | 0.77 |
| 19:S:12:ASP:HB2 | 19:S:35:SER:OG | 1.84 | 0.77 |
| 1:A:1498:G:H2' | 1:A:1499:G:H8 | 1.48 | 0.77 |
| 1:A:190:U:O4 | 17:Q:62:SER:HB3 | 1.84 | 0.77 |
| 6:F:18:GLN:O | 6:F:21:LEU:HB3 | 1.85 | 0.77 |
| 12:L:115:LYS:O | 12:L:117:ARG:N | 2.16 | 0.77 |
| 19:S:25:LYS:HD2 | 19:S:25:LYS:H | 1.50 | 0.77 |
| 1:A:1142:U:H5' | 1:A:1143:G:OP1 | 1.85 | 0.77 |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:CD1 | 2.19 | 0.77 |
| 1:A:11:A:H2' | 1:A:12:G:H8 | 1.50 | 0.77 |
| 1:A:496:U:H2' | 1:A:497:C:C6 | 2.19 | 0.77 |
| 1:A:737:A:H4' | 1:A:738:C:O5' | 1.83 | 0.77 |
| 2:B:187:LEU:HD21 | 2:B:214:ILE:HG13 | 1.66 | 0.77 |
| 3:C:141:VAL:HG11 | 3:C:202:ILE:HG12 | 1.66 | 0.77 |
| 19:S:12:ASP:H | 19:S:38:SER:HB3 | 1.49 | 0.77 |
| 1:A:1014:G:H2' | 1:A:1015:G:H8 | 1.49 | 0.76 |
| 3:C:14:ILE:HG22 | 3:C:15:THR:N | 2.00 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:148:ASN:C | 7:G:150:ALA:H | 1.85 | 0.76 |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:HD13 | 1.67 | 0.76 |
| 14:N:27:CYS:SG | 14:N:29:ARG:CB | 2.73 | 0.76 |
| 18:R:17:SER:HA | 18:R:19:LYS:NZ | 2.00 | 0.76 |
| 1:A:425:U:H4' | 1:A:426:A:O5' | 1.84 | 0.76 |
| 1:A:474:C:H2' | 1:A:475:G:H8 | 1.49 | 0.76 |
| 7:G:93:PRO:HG2 | 7:G:94:ARG:H | 1.51 | 0.76 |
| 1:A:1009:C:H2' | 1:A:1010:G:C8 | 2.19 | 0.76 |
| 1:A:1352:C:H2' | 1:A:1353:G:C8 | 2.20 | 0.76 |
| 1:A:1419:U:H2' | 1:A:1420:C:H6 | 1.49 | 0.76 |
| 1:A:1468:C:H6 | 1:A:1468:C:H5' | 1.51 | 0.76 |
| 5:E:151:LEU:HD11 | 8:H:77:GLU:OE2 | 1.83 | 0.76 |
| 1:A:1107:G:H5' | 10:J:35:SER:O | 1.85 | 0.76 |
| 1:A:486:G:H4' | 1:A:534:G:H4' | 1.67 | 0.76 |
| 3:C:123:GLN:O | 3:C:128:PHE:HB2 | 1.85 | 0.76 |
| 9:I:7:THR:HG22 | 9:I:8:GLY:N | 2.01 | 0.76 |
| 1:A:1010:G:N2 | 1:A:1012:G:H3' | 2.00 | 0.76 |
| 1:A:1232:A:H4' | 9:I:68:GLY:H | 1.50 | 0.76 |
| 1:A:290:U:H2' | 1:A:291:C:H6 | 1.49 | 0.76 |
| 2:B:142:LEU:HD22 | 2:B:146:GLN:HE22 | 1.47 | 0.76 |
| 1:A:1269:A:C2 | 1:A:1335:G:H1' | 2.20 | 0.76 |
| 2:B:112:VAL:O | 2:B:115:LEU:HB3 | 1.85 | 0.76 |
| 6:F:46:ARG:HB2 | 6:F:60:PHE:HE1 | 1.51 | 0.76 |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:HG3 | 1.51 | 0.76 |
| 1:A:1429:C:H2' | 1:A:1430:C:H6 | 1.50 | 0.76 |
| 7:G:145:ALA:O | 7:G:147:ALA:N | 2.19 | 0.76 |
| 8:H:19:VAL:HG23 | 8:H:21:LYS:HG2 | 1.66 | 0.76 |
| 1:A:1108:U:H3 | 10:J:5:ARG:NH2 | 1.84 | 0.76 |
| 10:J:84:GLN:O | 10:J:88:LEU:HD12 | 1.86 | 0.76 |
| 1:A:333:C:H2' | 1:A:334:A:H8 | 1.51 | 0.75 |
| 2:B:53:ARG:HA | 2:B:56:ARG:CZ | 2.15 | 0.75 |
| 4:D:104:VAL:HG11 | 4:D:146:ILE:HD12 | 1.67 | 0.75 |
| 15:O:39:LEU:HD13 | 15:O:56:LEU:HB2 | 1.68 | 0.75 |
| 18:R:56:THR:HG21 | 18:R:63:GLN:OE1 | 1.87 | 0.75 |
| 7:G:37:ASN:HD21 | 9:I:41:VAL:H | 1.34 | 0.75 |
| 1:A:502:C:O2' | 12:L:50:SER:HB3 | 1.85 | 0.75 |
| 2:B:88:ALA:C | 2:B:90:MET:H | 1.90 | 0.75 |
| 18:R:87:ARG:HG2 | 18:R:87:ARG:HH11 | 1.48 | 0.75 |
| 1:A:721:A:H2' | 1:A:722:C:C6 | 2.22 | 0.75 |
| 1:A:858:C:H5'' | 12:L:12:ARG:NH2 | 2.01 | 0.75 |
| 20:T:10:LEU:O | 20:T:12:ALA:N | 2.19 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:84:GLU:HB3 | 2:B:219:VAL:HG21 | 1.68 | 0.75 |
| 1:A:775:G:H2' | 1:A:776:A:H5' | 1.68 | 0.75 |
| 18:R:26:LEU:HD13 | 18:R:42:ARG:HH12 | 1.49 | 0.75 |
| 1:A:646:G:H2' | 1:A:647:A:H8 | 1.52 | 0.75 |
| 2:B:100:GLY:N | 2:B:176:GLU:OE2 | 2.16 | 0.75 |
| 1:A:1329:G:H3' | 9:I:108:VAL:O | 1.87 | 0.75 |
| 1:A:938:U:O2' | 1:A:1205:C:H4' | 1.86 | 0.75 |
| 9:I:7:THR:HG22 | 9:I:8:GLY:H | 1.50 | 0.75 |
| 12:L:10:LEU:O | 12:L:14:GLY:N | 2.16 | 0.75 |
| 1:A:472:A:H2' | 1:A:473:C:O4' | 1.88 | 0.74 |
| 3:C:47:LEU:N | 3:C:47:LEU:HD12 | 2.02 | 0.74 |
| 7:G:85:TYR:HD1 | 7:G:154:TYR:HE1 | 1.31 | 0.74 |
| 11:K:69:ALA:O | 11:K:73:MET:HG2 | 1.86 | 0.74 |
| 19:S:62:ILE:HD12 | 19:S:66:MET:HG3 | 1.69 | 0.74 |
| 2:B:88:ALA:O | 2:B:90:MET:N | 2.20 | 0.74 |
| 4:D:8:VAL:O | 4:D:10:ARG:N | 2.19 | 0.74 |
| 6:F:3:ARG:HH21 | 6:F:64:GLN:NE2 | 1.84 | 0.74 |
| 2:B:139:LYS:O | 2:B:143:GLU:HG2 | 1.87 | 0.74 |
| 2:B:209:ARG:HE | 2:B:239:VAL:HG11 | 1.52 | 0.74 |
| 3:C:3:ASN:N | 3:C:3:ASN:ND2 | 2.30 | 0.74 |
| 7:G:37:ASN:HD21 | 9:I:41:VAL:HG23 | 1.51 | 0.74 |
| 18:R:55:ARG:HB3 | 18:R:55:ARG:HH11 | 1.51 | 0.74 |
| 1:A:1124:C:H2' | 1:A:1125:G:C8 | 2.22 | 0.74 |
| 1:A:1201:U:H2' | 1:A:1202:G:H8 | 1.52 | 0.74 |
| 4:D:24:GLU:O | 4:D:25:ARG:HB3 | 1.88 | 0.74 |
| 1:A:1044:G:N2 | 1:A:1179:G:H1' | 2.03 | 0.74 |
| 1:A:802:G:H3' | 1:A:803:A:H5' | 1.70 | 0.74 |
| 3:C:131:ARG:HG2 | 3:C:135:LYS:HE3 | 1.69 | 0.74 |
| 8:H:13:ILE:O | 8:H:17:THR:HG23 | 1.88 | 0.74 |
| 1:A:103:A:H2' | 1:A:322:G:N2 | 2.02 | 0.74 |
| 17:Q:60:ILE:HB | 17:Q:74:LEU:HD12 | 1.70 | 0.74 |
| 19:S:33:THR:HG22 | 19:S:35:SER:H | 1.51 | 0.74 |
| 1:A:224:A:H2' | 1:A:225:U:C6 | 2.22 | 0.74 |
| 5:E:82:VAL:HG21 | 5:E:138:ALA:HA | 1.70 | 0.74 |
| 7:G:42:ILE:HG22 | 7:G:120:ILE:HD12 | 1.69 | 0.74 |
| 1:A:676:U:O2 | 1:A:678:A:H5'' | 1.88 | 0.74 |
| 5:E:12:LEU:O | 5:E:12:LEU:HD13 | 1.88 | 0.74 |
| 20:T:46:GLU:HB3 | 20:T:48:LYS:NZ | 2.02 | 0.74 |
| 1:A:515:U:H5'' | 1:A:516:A:OP1 | 1.88 | 0.74 |
| 1:A:9:A:N6 | 4:D:209:ARG:HB2 | 2.02 | 0.74 |
| 12:L:89:ARG:HG2 | 12:L:97:ARG:HA | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:P:67:THR:HG22 | 16:P:68:ASP:N | 2.01 | 0.74 |
| 1:A:1238:A:H8 | 3:C:27:LYS:HZ1 | 1.36 | 0.73 |
| 1:A:1475:G:H2' | 1:A:1476:U:H6 | 1.53 | 0.73 |
| 12:L:71:PRO:O | 12:L:102:ARG:HD2 | 1.88 | 0.73 |
| 1:A:1467:G:C3' | 1:A:1468:C:H5'' | 2.17 | 0.73 |
| 18:R:64:ARG:O | 18:R:67:ALA:HB3 | 1.89 | 0.73 |
| 2:B:124:SER:HB2 | 2:B:125:PRO:HD2 | 1.69 | 0.73 |
| 1:A:95:A:O2' | 1:A:96:G:H5' | 1.88 | 0.73 |
| 14:N:23:ARG:HD3 | 14:N:30:ALA:HB2 | 1.69 | 0.73 |
| 1:A:984:A:H2' | 1:A:985:C:H5' | 1.70 | 0.73 |
| 2:B:187:LEU:CD2 | 2:B:214:ILE:HG13 | 2.17 | 0.73 |
| 10:J:30:SER:HB3 | 10:J:80:LYS:HG3 | 1.70 | 0.73 |
| 16:P:81:ARG:HG3 | 16:P:83:GLU:HG2 | 1.68 | 0.73 |
| 1:A:1084:A:H4' | 1:A:1085:A:O5' | 1.88 | 0.73 |
| 1:A:1250:A:H2' | 1:A:1251:A:C8 | 2.22 | 0.73 |
| 1:A:1238:A:N6 | 1:A:1260:U:H1' | 2.03 | 0.73 |
| 8:H:91:ARG:HG3 | 12:L:7:ILE:HG13 | 1.69 | 0.73 |
| 1:A:496:U:H2' | 1:A:497:C:H6 | 1.54 | 0.73 |
| 2:B:206:ASP:CG | 2:B:207:ALA:N | 2.42 | 0.73 |
| 18:R:53:ARG:HG2 | 18:R:63:GLN:HG2 | 1.71 | 0.73 |
| 1:A:446:A:H1' | 1:A:447:A:C8 | 2.23 | 0.73 |
| 5:E:72:GLN:OE1 | 5:E:77:PRO:HB3 | 1.89 | 0.73 |
| 8:H:86:ILE:HD12 | 8:H:133:LEU:CD2 | 2.19 | 0.73 |
| 9:I:121:ARG:HH11 | 9:I:121:ARG:HG2 | 1.54 | 0.73 |
| 18:R:44:LEU:HD22 | 18:R:48:GLY:O | 1.87 | 0.73 |
| 1:A:1050:A:O2' | 1:A:1051:G:H8 | 1.71 | 0.72 |
| 1:A:242:A:N6 | 1:A:277:G:H1' | 2.04 | 0.72 |
| 8:H:83:ILE:O | 8:H:83:ILE:HG23 | 1.89 | 0.72 |
| 8:H:36:LEU:HD13 | 8:H:61:VAL:HG22 | 1.71 | 0.72 |
| 9:I:47:LEU:C | 9:I:49:PRO:HD2 | 2.08 | 0.72 |
| 10:J:19:SER:OG | 10:J:91:PRO:HG3 | 1.89 | 0.72 |
| 19:S:42:PRO:HA | 19:S:45:VAL:HG23 | 1.70 | 0.72 |
| 1:A:1202:G:H2' | 1:A:1203:G:H8 | 1.55 | 0.72 |
| 1:A:331:C:H2' | 1:A:332:C:C6 | 2.24 | 0.72 |
| 1:A:932:G:N2 | 1:A:1209:A:H62 | 1.86 | 0.72 |
| 1:A:943:A:C2 | 1:A:947:A:C2 | 2.78 | 0.72 |
| 12:L:113:ARG:HB2 | 12:L:122:THR:HG21 | 1.71 | 0.72 |
| 1:A:1178:U:H5'' | 1:A:1179:G:H5' | 1.71 | 0.72 |
| 1:A:1483:G:H3' | 1:A:1483:G:C8 | 2.25 | 0.72 |
| 1:A:896:A:H2' | 1:A:897:A:C8 | 2.24 | 0.72 |
| 11:K:77:MET:CE | 11:K:80:VAL:HG22 | 2.19 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:M:15:VAL:HG23 | 13:M:43:THR:O | 1.89 | 0.72 |
| 1:A:1380:C:H4' | 1:A:1381:A:OP2 | 1.90 | 0.72 |
| 3:C:15:THR:O | 3:C:16:ARG:HB2 | 1.89 | 0.72 |
| 1:A:584:C:H4' | 8:H:128:GLY:O | 1.90 | 0.72 |
| 11:K:109:VAL:HG13 | 18:R:85:LEU:O | 1.89 | 0.72 |
| 12:L:126:LYS:N | 12:L:126:LYS:HD2 | 2.04 | 0.72 |
| 17:Q:101:ARG:NE | 17:Q:101:ARG:HA | 2.04 | 0.72 |
| 17:Q:90:ILE:O | 17:Q:93:GLN:HB3 | 1.89 | 0.72 |
| 1:A:197:U:H3 | 20:T:105:SER:HG | 1.38 | 0.72 |
| 1:A:251:G:H1' | 17:Q:16:GLN:HE22 | 1.51 | 0.72 |
| 1:A:627:C:H2' | 1:A:628:G:H8 | 1.55 | 0.72 |
| 5:E:11:ILE:HG22 | 5:E:12:LEU:HD12 | 1.72 | 0.72 |
| 5:E:40:ARG:HG2 | 5:E:40:ARG:HH11 | 1.54 | 0.72 |
| 7:G:85:TYR:HD1 | 7:G:154:TYR:CE1 | 2.08 | 0.72 |
| 8:H:110:ALA:HB3 | 8:H:121:ASP:HB3 | 1.69 | 0.72 |
| 11:K:96:ARG:HA | 11:K:99:GLN:OE1 | 1.89 | 0.72 |
| 16:P:6:LEU:HD23 | 16:P:17:TYR:CG | 2.24 | 0.72 |
| 1:A:1045:U:H2' | 1:A:1046:C:C6 | 2.24 | 0.72 |
| 1:A:1216:C:H1' | 1:A:1347:U:O2 | 1.89 | 0.72 |
| 1:A:1347:U:O2' | 1:A:1348:G:OP1 | 2.08 | 0.72 |
| 1:A:1359:U:H2' | 1:A:1360:A:C8 | 2.25 | 0.72 |
| 1:A:575:U:H2' | 1:A:576:G:H8 | 1.55 | 0.72 |
| 1:A:888:C:H2' | 1:A:889:U:H6 | 1.55 | 0.72 |
| 6:F:48:LEU:HD13 | 6:F:52:ILE:CG1 | 2.20 | 0.72 |
| 10:J:49:VAL:HG12 | 10:J:50:ILE:O | 1.89 | 0.72 |
| 1:A:1069:U:H3 | 1:A:1082:G:H22 | 1.36 | 0.72 |
| 19:S:20:LEU:HA | 19:S:23:ASN:ND2 | 2.02 | 0.72 |
| 1:A:23:G:H2' | 1:A:24:C:C6 | 2.25 | 0.71 |
| 1:A:546:C:H41 | 1:A:862:U:H2' | 1.55 | 0.71 |
| 1:A:811:U:H2' | 1:A:848:U:O4 | 1.89 | 0.71 |
| 13:M:23:TYR:CE2 | 13:M:70:LEU:HB3 | 2.25 | 0.71 |
| 1:A:544:U:H4' | 1:A:545:U:H5'' | 1.72 | 0.71 |
| 2:B:23:ARG:C | 2:B:23:ARG:HH11 | 1.92 | 0.71 |
| 1:A:50:U:H1' | 12:L:28:LYS:HZ3 | 1.53 | 0.71 |
| 16:P:1:MET:O | 16:P:24:ALA:HB2 | 1.90 | 0.71 |
| 18:R:39:VAL:HG13 | 18:R:40:LEU:HD23 | 1.72 | 0.71 |
| 1:A:1113:A:OP2 | 1:A:1113:A:H3' | 1.89 | 0.71 |
| 1:A:1232:A:H4' | 9:I:68:GLY:N | 2.04 | 0.71 |
| 1:A:179:G:H2' | 1:A:180:A:H8 | 1.55 | 0.71 |
| 3:C:94:LEU:CD2 | 3:C:95:THR:HG23 | 2.19 | 0.71 |
| 7:G:15:ASP:OD2 | 7:G:23:VAL:HG11 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:100:GLY:O | 9:I:102:LEU:N | 2.24 | 0.71 |
| 9:I:3:GLN:HG3 | 9:I:20:ARG:HE | 1.54 | 0.71 |
| 18:R:26:LEU:HD13 | 18:R:42:ARG:NH1 | 2.05 | 0.71 |
| 1:A:1287:G:H22 | 1:A:1313:G:C2' | 2.03 | 0.71 |
| 1:A:543:A:H4' | 1:A:544:U:O5' | 1.91 | 0.71 |
| 1:A:1480:A:H5'' | 1:A:1481:A:OP2 | 1.89 | 0.71 |
| 3:C:56:ASP:O | 3:C:57:ILE:HG13 | 1.91 | 0.71 |
| 7:G:99:LEU:HD22 | 7:G:103:TRP:CZ2 | 2.25 | 0.71 |
| 7:G:70:LYS:HB3 | 7:G:96:GLN:OE1 | 1.90 | 0.71 |
| 12:L:47:LYS:CB | 12:L:48:PRO:HD3 | 2.20 | 0.71 |
| 13:M:52:GLU:HG2 | 13:M:55:ARG:NH2 | 2.05 | 0.71 |
| 1:A:1374:U:H2' | 1:A:1375:G:C8 | 2.25 | 0.71 |
| 1:A:438:C:H2' | 1:A:439:C:H6 | 1.56 | 0.71 |
| 11:K:34:ASP:O | 11:K:36:ASP:N | 2.23 | 0.71 |
| 14:N:14:PRO:HG3 | 14:N:17:LYS:HA | 1.73 | 0.71 |
| 16:P:22:THR:HA | 16:P:33:ILE:HG13 | 1.72 | 0.71 |
| 1:A:1208:C:H4' | 1:A:1209:A:OP1 | 1.91 | 0.71 |
| 1:A:366:C:O2' | 1:A:367:G:H5' | 1.91 | 0.71 |
| 5:E:9:LYS:HG3 | 5:E:112:LEU:HD11 | 1.72 | 0.71 |
| 18:R:36:ASN:O | 18:R:39:VAL:HG12 | 1.90 | 0.71 |
| 8:H:1:MET:HG2 | 8:H:2:LEU:N | 2.03 | 0.71 |
| 9:I:108:VAL:HG12 | 9:I:109:VAL:N | 2.03 | 0.71 |
| 1:A:1111:C:H5' | 9:I:16:ARG:NH2 | 2.05 | 0.71 |
| 12:L:55:VAL:CG1 | 12:L:67:THR:HG23 | 2.19 | 0.71 |
| 18:R:36:ASN:ND2 | 18:R:38:GLU:HG2 | 2.06 | 0.71 |
| 1:A:385:A:H2' | 1:A:386:C:C5' | 2.21 | 0.71 |
| 1:A:483:A:O2' | 1:A:484:G:C8 | 2.42 | 0.71 |
| 4:D:102:ASP:HB3 | 4:D:136:PRO:CA | 2.21 | 0.71 |
| 7:G:126:ASP:HA | 7:G:129:GLU:HB2 | 1.71 | 0.71 |
| 1:A:1230:A:H1' | 9:I:70:LYS:NZ | 2.06 | 0.70 |
| 1:A:1399:G:N2 | 1:A:1463:U:H1' | 2.05 | 0.70 |
| 1:A:673:C:P | 11:K:46:GLY:HA3 | 2.31 | 0.70 |
| 2:B:209:ARG:HE | 2:B:239:VAL:HG13 | 1.54 | 0.70 |
| 5:E:80:ILE:HD13 | 5:E:138:ALA:HB1 | 1.73 | 0.70 |
| 8:H:89:PRO:HA | 8:H:92:ARG:CZ | 2.19 | 0.70 |
| 19:S:40:ILE:HB | 19:S:67:VAL:O | 1.90 | 0.70 |
| 20:T:30:LYS:HB3 | 20:T:34:LYS:HE3 | 1.71 | 0.70 |
| 1:A:1222:U:H4' | 1:A:1223:G:OP2 | 1.89 | 0.70 |
| 1:A:244:C:O2' | 1:A:245:U:H5' | 1.91 | 0.70 |
| 1:A:454:G:H3' | 1:A:455:A:H5'' | 1.74 | 0.70 |
| 3:C:188:LEU:CD1 | 3:C:189:ALA:N | 2.55 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:73:MET:SD | 7:G:90:GLU:HA | 2.32 | 0.70 |
| 1:A:252:U:H2' | 1:A:253:G:C8 | 2.26 | 0.70 |
| 1:A:333:C:H2' | 1:A:334:A:C8 | 2.27 | 0.70 |
| 3:C:54:ARG:HB3 | 3:C:69:HIS:HD2 | 1.57 | 0.70 |
| 7:G:83:ALA:HB3 | 7:G:85:TYR:CE2 | 2.26 | 0.70 |
| 1:A:324:C:H4' | 1:A:325:A:O5' | 1.90 | 0.70 |
| 2:B:91:PRO:HB3 | 2:B:154:LEU:HB2 | 1.73 | 0.70 |
| 1:A:1184:G:C2 | 14:N:42:ILE:HG21 | 2.27 | 0.70 |
| 15:O:25:THR:CG2 | 15:O:70:LEU:HD23 | 2.21 | 0.70 |
| 1:A:1037:C:O2' | 1:A:1038:A:H5'' | 1.91 | 0.70 |
| 3:C:6:HIS:CD2 | 3:C:8:ILE:HB | 2.27 | 0.70 |
| 4:D:112:VAL:N | 4:D:116:GLN:OE1 | 2.19 | 0.70 |
| 5:E:144:THR:HG22 | 5:E:146:ALA:H | 1.57 | 0.70 |
| 17:Q:24:GLU:OE2 | 17:Q:37:LYS:HD3 | 1.91 | 0.70 |
| 1:A:1216:C:H2' | 1:A:1217:U:H6 | 1.57 | 0.70 |
| 1:A:1221:A:H62 | 1:A:1281:A:H62 | 1.39 | 0.70 |
| 1:A:1349:C:H2' | 1:A:1350:C:C6 | 2.26 | 0.70 |
| 8:H:111:ILE:O | 8:H:134:ILE:HD12 | 1.92 | 0.70 |
| 11:K:91:ARG:HD2 | 11:K:92:GLU:OE1 | 1.92 | 0.70 |
| 11:K:95:ILE:O | 11:K:99:GLN:HG3 | 1.91 | 0.70 |
| 12:L:55:VAL:HG11 | 12:L:67:THR:HG23 | 1.73 | 0.70 |
| 14:N:26:ARG:HH12 | 14:N:47:LEU:HG | 1.56 | 0.70 |
| 1:A:397:C:H2' | 1:A:398:G:C8 | 2.27 | 0.70 |
| 1:A:801:C:H1' | 1:A:803:A:H5' | 1.74 | 0.70 |
| 2:B:206:ASP:CG | 2:B:207:ALA:H | 1.95 | 0.70 |
| 15:O:31:LEU:HD12 | 15:O:31:LEU:H | 1.56 | 0.70 |
| 3:C:11:ARG:O | 3:C:14:ILE:N | 2.19 | 0.70 |
| 1:A:378:A:H2' | 1:A:379:A:C8 | 2.25 | 0.70 |
| 3:C:110:ASN:HD21 | 3:C:140:ARG:HB3 | 1.57 | 0.70 |
| 1:A:1440:G:H2' | 1:A:1441:C:C6 | 2.27 | 0.69 |
| 4:D:120:LEU:O | 4:D:125:HIS:HB2 | 1.92 | 0.69 |
| 9:I:8:GLY:HA2 | 9:I:79:LEU:HD12 | 1.72 | 0.69 |
| 10:J:16:LEU:HD23 | 10:J:94:VAL:HG22 | 1.73 | 0.69 |
| 1:A:823:U:C5' | 1:A:824:C:H5 | 2.04 | 0.69 |
| 8:H:20:TYR:HA | 8:H:65:TYR:CE2 | 2.27 | 0.69 |
| 15:O:17:ARG:NH1 | 15:O:77:ARG:NH1 | 2.39 | 0.69 |
| 1:A:380:G:H2' | 1:A:381:C:H6 | 1.57 | 0.69 |
| 12:L:67:THR:CG2 | 12:L:96:VAL:HG22 | 2.23 | 0.69 |
| 17:Q:68:ARG:O | 17:Q:69:LYS:HB2 | 1.93 | 0.69 |
| 4:D:192:GLU:OE1 | 4:D:192:GLU:N | 2.25 | 0.69 |
| 5:E:110:LEU:O | 5:E:113:ALA:HB3 | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:12:ASP:O | 10:J:15:THR:HG22 | 1.93 | 0.69 |
| 1:A:1350:C:H4' | 10:J:48:THR:HG21 | 1.73 | 0.69 |
| 20:T:79:ARG:HE | 20:T:83:ARG:NH1 | 1.91 | 0.69 |
| 1:A:419:G:N2 | 1:A:420:G:C8 | 2.61 | 0.69 |
| 20:T:54:LYS:HG3 | 20:T:100:ILE:HD13 | 1.74 | 0.69 |
| 1:A:1280:C:C5 | 7:G:114:ARG:HD3 | 2.28 | 0.69 |
| 10:J:32:ALA:HB2 | 10:J:76:ASN:HB2 | 1.74 | 0.69 |
| 1:A:1204:G:P | 19:S:77:THR:HG21 | 2.33 | 0.69 |
| 1:A:1507:G:H5'' | 1:A:1508:G:OP2 | 1.93 | 0.69 |
| 14:N:22:THR:HB | 14:N:33:VAL:HG21 | 1.74 | 0.69 |
| 1:A:749:G:H1 | 1:A:796:C:H2' | 1.58 | 0.69 |
| 5:E:109:ILE:HD12 | 5:E:135:THR:HG21 | 1.74 | 0.69 |
| 10:J:61:GLU:OE1 | 14:N:45:ARG:NH1 | 2.25 | 0.69 |
| 1:A:452:C:H2' | 1:A:453:C:H6 | 1.56 | 0.69 |
| 1:A:932:G:H21 | 1:A:1209:A:H62 | 1.40 | 0.69 |
| 3:C:8:ILE:HG23 | 3:C:16:ARG:HG2 | 1.73 | 0.69 |
| 5:E:15:ARG:O | 5:E:16:THR:HG22 | 1.93 | 0.69 |
| 18:R:36:ASN:O | 18:R:36:ASN:ND2 | 2.26 | 0.69 |
| 19:S:36:ARG:HH21 | 19:S:75:ALA:HB3 | 1.56 | 0.69 |
| 1:A:1355:U:H2' | 1:A:1356:G:O4' | 1.93 | 0.69 |
| 1:A:522:G:OP2 | 12:L:115:LYS:HG3 | 1.93 | 0.69 |
| 3:C:139:GLN:NE2 | 3:C:143:GLU:HB2 | 2.07 | 0.69 |
| 6:F:11:ASN:OD1 | 6:F:13:ASN:N | 2.22 | 0.69 |
| 12:L:75:HIS:HA | 12:L:102:ARG:NH2 | 2.06 | 0.69 |
| 1:A:65:G:H4' | 1:A:66:U:C5' | 2.21 | 0.69 |
| 2:B:31:TYR:HE1 | 2:B:200:ILE:HD12 | 1.56 | 0.69 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 1.75 | 0.69 |
| 5:E:15:ARG:O | 5:E:27:ARG:O | 2.11 | 0.69 |
| 11:K:73:MET:O | 11:K:76:GLY:N | 2.26 | 0.69 |
| 1:A:1260:U:C5' | 1:A:1261:A:O4' | 2.41 | 0.68 |
| 3:C:173:VAL:O | 3:C:173:VAL:HG12 | 1.94 | 0.68 |
| 5:E:43:LEU:C | 5:E:43:LEU:HD23 | 2.13 | 0.68 |
| 4:D:111:ALA:HB2 | 4:D:120:LEU:HD12 | 1.75 | 0.68 |
| 5:E:26:PHE:CD1 | 5:E:26:PHE:N | 2.60 | 0.68 |
| 18:R:36:ASN:C | 18:R:36:ASN:HD22 | 1.94 | 0.68 |
| 1:A:371:U:OP1 | 16:P:69:THR:HG21 | 1.94 | 0.68 |
| 9:I:32:ASP:O | 9:I:35:GLU:N | 2.22 | 0.68 |
| 20:T:33:ILE:CD1 | 20:T:63:ILE:HA | 2.24 | 0.68 |
| 1:A:247:G:H4' | 1:A:248:U:O5' | 1.92 | 0.68 |
| 1:A:407:A:N9 | 1:A:409:G:H1' | 2.08 | 0.68 |
| 1:A:822:G:C2' | 1:A:823:U:H5'' | 2.22 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1099:C:H2' | 1:A:1100:G:C5' | 2.23 | 0.68 |
| 3:C:177:THR:O | 3:C:177:THR:HG23 | 1.92 | 0.68 |
| 5:E:105:VAL:HB | 5:E:106:PRO:HD3 | 1.75 | 0.68 |
| 1:A:1355:U:H5'' | 9:I:71:SER:HB3 | 1.76 | 0.68 |
| 1:A:1385:C:H2' | 1:A:1386:C:O4' | 1.94 | 0.68 |
| 1:A:955:A:H2' | 1:A:956:A:H5'' | 1.74 | 0.68 |
| 4:D:70:ILE:CG2 | 4:D:71:SER:N | 2.57 | 0.68 |
| 6:F:10:LEU:HB3 | 6:F:85:VAL:HA | 1.74 | 0.68 |
| 7:G:141:VAL:O | 7:G:144:MET:HB2 | 1.94 | 0.68 |
| 13:M:5:ALA:HB2 | 13:M:22:ILE:HD13 | 1.76 | 0.68 |
| 21:U:12:LYS:O | 21:U:16:GLY:N | 2.26 | 0.68 |
| 1:A:1201:U:H2' | 1:A:1202:G:C8 | 2.29 | 0.68 |
| 1:A:608:C:O2' | 1:A:609:G:H5' | 1.93 | 0.68 |
| 1:A:1506:U:O2' | 1:A:1507:G:H3' | 1.94 | 0.68 |
| 1:A:168:U:H5' | 1:A:204:A:O4' | 1.93 | 0.68 |
| 1:A:769:G:C2 | 1:A:770:G:C8 | 2.82 | 0.68 |
| 1:A:964:A:H2' | 1:A:965:G:C8 | 2.29 | 0.68 |
| 7:G:24:THR:HA | 7:G:27:ILE:HD12 | 1.76 | 0.68 |
| 9:I:17:VAL:HG21 | 9:I:81:ILE:N | 2.07 | 0.68 |
| 10:J:81:THR:C | 10:J:83:GLU:H | 1.98 | 0.68 |
| 1:A:53:G:O2' | 1:A:54:A:H5' | 1.93 | 0.68 |
| 1:A:585:C:H2' | 1:A:586:A:H8 | 1.59 | 0.68 |
| 2:B:181:PHE:N | 2:B:181:PHE:HD1 | 1.92 | 0.68 |
| 4:D:70:ILE:HD11 | 4:D:100:ARG:CZ | 2.24 | 0.68 |
| 4:D:179:GLU:O | 4:D:181:MET:HG3 | 1.94 | 0.68 |
| 10:J:45:ARG:CB | 10:J:45:ARG:HH11 | 2.00 | 0.68 |
| 1:A:1207:A:C5' | 13:M:103:THR:OG1 | 2.41 | 0.68 |
| 4:D:35:ARG:O | 4:D:36:ARG:HB2 | 1.94 | 0.68 |
| 8:H:65:TYR:HA | 8:H:79:VAL:HG23 | 1.76 | 0.68 |
| 10:J:71:LEU:O | 10:J:72:VAL:HB | 1.93 | 0.68 |
| 13:M:24:GLY:HA3 | 13:M:66:LEU:HD22 | 1.75 | 0.68 |
| 1:A:97:C:OP1 | 20:T:17:ARG:HD2 | 1.94 | 0.68 |
| 20:T:42:GLN:O | 20:T:45:GLN:HB3 | 1.95 | 0.68 |
| 1:A:745:G:C5 | 1:A:746:C:C4 | 2.82 | 0.67 |
| 1:A:897:A:O2' | 1:A:898:U:H5' | 1.94 | 0.67 |
| 2:B:104:ASN:OD1 | 2:B:107:THR:HB | 1.94 | 0.67 |
| 2:B:181:PHE:N | 2:B:181:PHE:CD1 | 2.60 | 0.67 |
| 4:D:36:ARG:H | 4:D:37:PRO:HD3 | 1.59 | 0.67 |
| 9:I:48:GLU:OE1 | 9:I:51:ARG:HD2 | 1.93 | 0.67 |
| 1:A:1325:G:H1' | 9:I:121:ARG:NH1 | 2.08 | 0.67 |
| 2:B:155:LEU:HD22 | 2:B:157:ARG:O | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:15:ARG:NE | 5:E:26:PHE:CD2 | 2.62 | 0.67 |
| 5:E:36:ASP:O | 5:E:38:GLN:N | 2.27 | 0.67 |
| 1:A:943:A:C2 | 13:M:124:PRO:HB2 | 2.29 | 0.67 |
| 1:A:1287:G:O2' | 1:A:1288:A:H8 | 1.72 | 0.67 |
| 1:A:18:U:H2' | 1:A:19:C:C6 | 2.29 | 0.67 |
| 5:E:41:VAL:HG23 | 5:E:113:ALA:HA | 1.76 | 0.67 |
| 7:G:146:GLU:HA | 7:G:149:ARG:HB2 | 1.75 | 0.67 |
| 9:I:33:PHE:HZ | 9:I:46:ALA:HB3 | 1.59 | 0.67 |
| 17:Q:27:PHE:O | 17:Q:36:ILE:HG12 | 1.94 | 0.67 |
| 1:A:1269:A:H2' | 1:A:1270:A:C8 | 2.30 | 0.67 |
| 1:A:960:U:H4' | 1:A:961:A:O5' | 1.93 | 0.67 |
| 3:C:26:LYS:CD | 3:C:26:LYS:H | 2.00 | 0.67 |
| 5:E:91:LEU:HD12 | 5:E:138:ALA:HB1 | 1.76 | 0.67 |
| 5:E:80:ILE:CD1 | 5:E:91:LEU:HD12 | 2.24 | 0.67 |
| 1:A:1211:A:H2' | 1:A:1212:C:H6 | 1.59 | 0.67 |
| 1:A:647:A:H2' | 1:A:648:G:C8 | 2.29 | 0.67 |
| 2:B:28:PHE:CD2 | 2:B:190:THR:HA | 2.30 | 0.67 |
| 4:D:103:ASN:O | 4:D:106:TYR:N | 2.27 | 0.67 |
| 1:A:1486:G:H2' | 1:A:1487:C:C6 | 2.26 | 0.67 |
| 1:A:799:A:H5'' | 1:A:801:C:N4 | 2.10 | 0.67 |
| 1:A:1040:G:C5' | 3:C:154:SER:HB2 | 2.24 | 0.67 |
| 9:I:118:LYS:O | 9:I:119:ALA:HB3 | 1.94 | 0.67 |
| 12:L:28:LYS:CD | 12:L:33:ARG:HH22 | 1.92 | 0.67 |
| 1:A:386:C:O3' | 16:P:28:ARG:NH2 | 2.28 | 0.67 |
| 2:B:52:GLU:HG2 | 2:B:56:ARG:NH2 | 2.09 | 0.67 |
| 10:J:29:ARG:HB2 | 10:J:84:GLN:HE22 | 1.60 | 0.67 |
| 11:K:82:VAL:HB | 11:K:108:ILE:HA | 1.77 | 0.67 |
| 11:K:36:ASP:N | 11:K:36:ASP:OD2 | 2.28 | 0.67 |
| 20:T:56:MET:O | 20:T:59:ALA:HB3 | 1.94 | 0.67 |
| 1:A:1338:G:H2' | 1:A:1339:A:C8 | 2.30 | 0.67 |
| 1:A:1482:G:O2' | 1:A:1483:G:OP2 | 2.12 | 0.67 |
| 1:A:243:G:OP2 | 17:Q:99:SER:HB2 | 1.94 | 0.67 |
| 1:A:930:U:O2' | 1:A:931:G:H5' | 1.94 | 0.67 |
| 16:P:8:ARG:HG2 | 16:P:17:TYR:CE2 | 2.30 | 0.67 |
| 17:Q:20:THR:HG23 | 17:Q:43:LEU:HD21 | 1.77 | 0.67 |
| 1:A:1274:U:H5' | 9:I:38:GLN:HE22 | 1.59 | 0.67 |
| 1:A:1496:A:H2' | 1:A:1497:A:C8 | 2.30 | 0.67 |
| 2:B:152:PHE:CE1 | 2:B:155:LEU:HD12 | 2.30 | 0.67 |
| 4:D:61:LYS:HD2 | 4:D:207:TYR:OH | 1.95 | 0.67 |
| 15:O:27:VAL:HG12 | 15:O:31:LEU:HD11 | 1.77 | 0.67 |
| 15:O:7:GLU:O | 15:O:11:VAL:HG23 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:Q:56:VAL:HG12 | 17:Q:77:VAL:HB | 1.77 | 0.67 |
| 19:S:42:PRO:O | 19:S:45:VAL:HG23 | 1.95 | 0.67 |
| 1:A:1329:G:HO2' | 1:A:1330:U:P | 2.17 | 0.67 |
| 1:A:1377:A:N6 | 1:A:1479:C:H5' | 2.10 | 0.67 |
| 1:A:283:U:H2' | 1:A:284:A:H8 | 1.60 | 0.67 |
| 2:B:134:GLU:C | 2:B:136:VAL:H | 1.97 | 0.67 |
| 2:B:88:ALA:HB1 | 2:B:90:MET:HG2 | 1.77 | 0.67 |
| 3:C:13:GLY:O | 3:C:14:ILE:HD13 | 1.95 | 0.67 |
| 4:D:190:ASP:O | 4:D:192:GLU:N | 2.28 | 0.67 |
| 9:I:79:LEU:O | 9:I:82:ALA:HB3 | 1.95 | 0.67 |
| 13:M:36:LYS:HD2 | 13:M:59:TYR:CZ | 2.30 | 0.67 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N | 2.10 | 0.67 |
| 1:A:1047:G:H4' | 1:A:1048:U:H5'' | 1.76 | 0.66 |
| 1:A:529:C:O2' | 1:A:530:G:H5' | 1.95 | 0.66 |
| 1:A:720:C:H2' | 1:A:721:A:C8 | 2.30 | 0.66 |
| 2:B:100:GLY:O | 2:B:102:LEU:N | 2.28 | 0.66 |
| 5:E:75:THR:HG23 | 5:E:76:ILE:N | 2.08 | 0.66 |
| 10:J:94:VAL:HG12 | 10:J:95:GLU:N | 2.08 | 0.66 |
| 1:A:1020:C:H2' | 1:A:1021:C:C6 | 2.30 | 0.66 |
| 1:A:1263:U:H5' | 1:A:1264:C:H5 | 1.59 | 0.66 |
| 2:B:121:LEU:O | 2:B:127:ILE:HG12 | 1.94 | 0.66 |
| 6:F:46:ARG:HB2 | 6:F:60:PHE:CE1 | 2.30 | 0.66 |
| 10:J:45:ARG:HB3 | 10:J:45:ARG:NH1 | 1.99 | 0.66 |
| 1:A:1477:A:P | 22:A:1523:KSG:H12 | 2.35 | 0.66 |
| 1:A:250:G:OP1 | 17:Q:67:LYS:O | 2.13 | 0.66 |
| 1:A:721:A:H2' | 1:A:722:C:H6 | 1.60 | 0.66 |
| 2:B:142:LEU:CA | 2:B:146:GLN:HE22 | 2.08 | 0.66 |
| 5:E:121:LYS:HE3 | 5:E:122:GLU:O | 1.95 | 0.66 |
| 1:A:1135:A:H5'' | 10:J:13:HIS:HD2 | 1.59 | 0.66 |
| 1:A:1225:C:H2' | 1:A:1226:C:H6 | 1.61 | 0.66 |
| 1:A:1260:U:H5'' | 1:A:1261:A:O4' | 1.95 | 0.66 |
| 1:A:1403:C:H2' | 1:A:1404:G:H8 | 1.61 | 0.66 |
| 1:A:75:C:H2' | 1:A:76:G:H8 | 1.61 | 0.66 |
| 2:B:156:LYS:O | 2:B:156:LYS:HD3 | 1.95 | 0.66 |
| 1:A:474:C:H2' | 1:A:475:G:C8 | 2.31 | 0.66 |
| 1:A:501:G:HO2' | 1:A:514:G:H4' | 1.60 | 0.66 |
| 3:C:100:ALA:O | 3:C:101:LEU:HB2 | 1.94 | 0.66 |
| 7:G:75:VAL:HG11 | 7:G:86:GLN:HB3 | 1.77 | 0.66 |
| 1:A:1351:G:OP1 | 10:J:62:HIS:HE1 | 1.78 | 0.66 |
| 1:A:1225:C:H2' | 1:A:1226:C:C6 | 2.30 | 0.66 |
| 4:D:107:ARG:HH12 | 4:D:114:ARG:HH22 | 1.43 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:13:ARG:NH1 | 4:D:38:TYR:O | 2.29 | 0.66 |
| 19:S:28:LYS:CG | 19:S:29:ARG:H | 1.92 | 0.66 |
| 20:T:66:ALA:HB1 | 20:T:72:LEU:HB2 | 1.78 | 0.66 |
| 1:A:385:A:C2' | 1:A:386:C:H5' | 2.26 | 0.66 |
| 1:A:522:G:H4' | 12:L:114:LYS:HD3 | 1.78 | 0.66 |
| 1:A:579:G:H2' | 1:A:625:U:O4 | 1.96 | 0.66 |
| 2:B:93:VAL:HG11 | 2:B:97:TRP:CD1 | 2.31 | 0.66 |
| 9:I:43:ALA:HA | 9:I:74:ILE:HD13 | 1.77 | 0.66 |
| 17:Q:74:LEU:HD23 | 17:Q:74:LEU:O | 1.96 | 0.66 |
| 20:T:46:GLU:HB3 | 20:T:48:LYS:HZ2 | 1.61 | 0.66 |
| 21:U:12:LYS:HG3 | 21:U:17:THR:OG1 | 1.95 | 0.66 |
| 1:A:380:G:H2' | 1:A:381:C:C6 | 2.31 | 0.66 |
| 1:A:540:C:H2' | 1:A:541:G:H5' | 1.78 | 0.66 |
| 1:A:758:G:H1 | 1:A:789:C:H42 | 1.42 | 0.66 |
| 3:C:82:GLU:O | 3:C:85:ARG:HB3 | 1.94 | 0.66 |
| 16:P:22:THR:HA | 16:P:33:ILE:CD1 | 2.26 | 0.66 |
| 16:P:55:ARG:O | 16:P:58:TYR:HB3 | 1.95 | 0.66 |
| 1:A:1373:U:H2' | 1:A:1374:U:H6 | 1.61 | 0.66 |
| 1:A:802:G:O2' | 1:A:804:U:C5 | 2.48 | 0.66 |
| 3:C:23:TYR:CD2 | 3:C:24:ALA:N | 2.64 | 0.66 |
| 4:D:36:ARG:N | 4:D:37:PRO:HD3 | 2.10 | 0.66 |
| 7:G:12:LEU:HD12 | 7:G:12:LEU:N | 2.11 | 0.66 |
| 7:G:64:GLN:O | 7:G:67:GLU:HB3 | 1.96 | 0.66 |
| 8:H:86:ILE:HD12 | 8:H:133:LEU:HD22 | 1.78 | 0.66 |
| 11:K:57:THR:HG23 | 11:K:60:ALA:CB | 2.26 | 0.66 |
| 16:P:20:VAL:HG13 | 16:P:21:VAL:N | 2.09 | 0.66 |
| 1:A:271:G:H5' | 17:Q:14:LYS:HD3 | 1.76 | 0.66 |
| 17:Q:92:ARG:O | 17:Q:95:TYR:HB2 | 1.96 | 0.66 |
| 18:R:39:VAL:HG13 | 18:R:40:LEU:H | 1.60 | 0.66 |
| 1:A:1489:G:O2' | 1:A:1490:U:H5' | 1.96 | 0.66 |
| 1:A:749:G:N1 | 1:A:796:C:H2' | 2.10 | 0.66 |
| 1:A:767:C:O2' | 1:A:768:C:H5' | 1.94 | 0.66 |
| 4:D:31:CYS:SG | 4:D:31:CYS:O | 2.54 | 0.66 |
| 11:K:67:ASP:HA | 11:K:70:LYS:HD2 | 1.77 | 0.66 |
| 1:A:964:A:H1' | 19:S:54:GLY:O | 1.95 | 0.66 |
| 1:A:1488:U:H2' | 1:A:1489:G:C8 | 2.31 | 0.65 |
| 1:A:266:A:H2' | 1:A:267:C:C6 | 2.31 | 0.65 |
| 1:A:609:G:H2' | 1:A:610:U:H6 | 1.57 | 0.65 |
| 3:C:174:PRO:HB2 | 3:C:177:THR:HG22 | 1.77 | 0.65 |
| 5:E:144:THR:CG2 | 5:E:145:LYS:N | 2.57 | 0.65 |
| 7:G:148:ASN:O | 7:G:150:ALA:N | 2.28 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:73:GLU:HA | 15:O:73:GLU:OE1 | 1.95 | 0.65 |
| 19:S:16:LEU:O | 19:S:19:VAL:HG12 | 1.96 | 0.65 |
| 1:A:1151:A:H8 | 1:A:1151:A:O5' | 1.79 | 0.65 |
| 1:A:424:G:C2 | 1:A:426:A:N6 | 2.63 | 0.65 |
| 1:A:671:A:H4' | 1:A:672:G:O5' | 1.95 | 0.65 |
| 1:A:552:G:N2 | 1:A:861:C:C2 | 2.65 | 0.65 |
| 2:B:32:ILE:HD13 | 2:B:40:HIS:CD2 | 2.31 | 0.65 |
| 6:F:10:LEU:HA | 6:F:86:ARG:HG2 | 1.78 | 0.65 |
| 7:G:25:ALA:HA | 7:G:28:ASN:HD22 | 1.60 | 0.65 |
| 14:N:22:THR:HB | 14:N:33:VAL:CG2 | 2.25 | 0.65 |
| 4:D:140:VAL:CG1 | 4:D:146:ILE:HD11 | 2.21 | 0.65 |
| 5:E:115:VAL:HG21 | 5:E:118:ILE:HD11 | 1.78 | 0.65 |
| 17:Q:81:ARG:HG3 | 17:Q:81:ARG:O | 1.96 | 0.65 |
| 17:Q:82:MET:O | 17:Q:84:LEU:N | 2.29 | 0.65 |
| 18:R:87:ARG:HG2 | 18:R:87:ARG:NH1 | 2.11 | 0.65 |
| 20:T:67:ALA:HA | 20:T:73:HIS:H | 1.61 | 0.65 |
| 1:A:867:A:H4' | 1:A:868:G:OP1 | 1.96 | 0.65 |
| 4:D:104:VAL:HG21 | 4:D:140:VAL:HG21 | 1.77 | 0.65 |
| 4:D:96:LEU:O | 4:D:99:SER:N | 2.28 | 0.65 |
| 6:F:82:ARG:HE | 6:F:82:ARG:HA | 1.61 | 0.65 |
| 12:L:53:ARG:H | 12:L:53:ARG:HD2 | 1.61 | 0.65 |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:N | 2.11 | 0.65 |
| 1:A:483:A:H4' | 1:A:484:G:OP1 | 1.96 | 0.65 |
| 1:A:799:A:O2' | 1:A:800:A:P | 2.54 | 0.65 |
| 14:N:6:LEU:HB3 | 14:N:23:ARG:NH2 | 2.11 | 0.65 |
| 1:A:1295:U:OP2 | 19:S:6:LYS:HA | 1.96 | 0.65 |
| 1:A:622:G:O2' | 1:A:623:G:H5' | 1.96 | 0.65 |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:CG1 | 2.23 | 0.65 |
| 18:R:58:LEU:HD11 | 18:R:66:LEU:HD13 | 1.77 | 0.65 |
| 1:A:1251:A:C2 | 1:A:1295:U:O4' | 2.50 | 0.65 |
| 1:A:501:G:O2' | 1:A:514:G:H4' | 1.95 | 0.65 |
| 1:A:724:U:O2' | 1:A:725:G:H5' | 1.95 | 0.65 |
| 2:B:142:LEU:CD2 | 2:B:146:GLN:HE22 | 2.09 | 0.65 |
| 7:G:38:LEU:O | 7:G:42:ILE:HG13 | 1.96 | 0.65 |
| 10:J:38:ILE:HG13 | 10:J:71:LEU:HB3 | 1.79 | 0.65 |
| 10:J:78:ASN:O | 10:J:80:LYS:N | 2.30 | 0.65 |
| 12:L:53:ARG:HD2 | 12:L:53:ARG:N | 2.11 | 0.65 |
| 15:O:36:ILE:HA | 15:O:59:MET:CE | 2.27 | 0.65 |
| 18:R:29:PHE:HE1 | 18:R:31:LEU:CD2 | 2.10 | 0.65 |
| 1:A:1220:A:N7 | 1:A:1285:C:H1' | 2.11 | 0.65 |
| 1:A:860:C:O2' | 1:A:861:C:H5' | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:903:G:C6 | 1:A:905:G:N7 | 2.64 | 0.65 |
| 1:A:994:A:H2' | 1:A:995:A:C8 | 2.32 | 0.65 |
| 3:C:64:VAL:HB | 3:C:99:VAL:CB | 2.27 | 0.65 |
| 3:C:6:HIS:CD2 | 3:C:9:GLY:H | 2.07 | 0.65 |
| 1:A:1482:G:H4' | 1:A:1483:G:O5' | 1.97 | 0.65 |
| 1:A:199:U:H2' | 1:A:200:C:C6 | 2.31 | 0.65 |
| 3:C:54:ARG:HB3 | 3:C:69:HIS:CD2 | 2.32 | 0.65 |
| 7:G:46:ALA:O | 7:G:50:ILE:HG13 | 1.97 | 0.65 |
| 1:A:670:U:H1' | 11:K:42:TRP:HE1 | 1.62 | 0.65 |
| 19:S:22:LEU:HD11 | 19:S:31:ILE:HD11 | 1.79 | 0.65 |
| 1:A:106:G:H21 | 1:A:350:G:C5' | 2.03 | 0.65 |
| 1:A:1435:G:O2' | 1:A:1436:G:H5' | 1.98 | 0.65 |
| 3:C:112:SER:HB2 | 3:C:115:LEU:HB2 | 1.78 | 0.65 |
| 4:D:203:VAL:O | 4:D:206:PHE:N | 2.30 | 0.65 |
| 6:F:1:MET:SD | 6:F:67:MET:HA | 2.37 | 0.65 |
| 10:J:6:ILE:O | 10:J:71:LEU:O | 2.14 | 0.65 |
| 12:L:5:PRO:HA | 12:L:9:GLN:OE1 | 1.97 | 0.65 |
| 13:M:5:ALA:HB3 | 13:M:8:GLU:HG3 | 1.78 | 0.65 |
| 1:A:400:U:H2' | 1:A:401:U:H6 | 1.59 | 0.64 |
| 1:A:40:G:O2' | 1:A:41:C:H5' | 1.97 | 0.64 |
| 1:A:943:A:O2' | 1:A:944:G:H5' | 1.98 | 0.64 |
| 2:B:204:ASN:C | 2:B:204:ASN:HD22 | 2.00 | 0.64 |
| 1:A:1198:G:H5'' | 14:N:5:ALA:HB2 | 1.79 | 0.64 |
| 20:T:66:ALA:CB | 20:T:72:LEU:HB2 | 2.27 | 0.64 |
| 1:A:1108:U:H3 | 10:J:5:ARG:HH21 | 1.44 | 0.64 |
| 1:A:142:G:O2' | 1:A:143:G:H5' | 1.97 | 0.64 |
| 1:A:698:G:H2' | 1:A:699:A:C8 | 2.31 | 0.64 |
| 11:K:44:SER:OG | 11:K:47:VAL:HG23 | 1.97 | 0.64 |
| 13:M:108:ARG:O | 13:M:112:GLY:N | 2.24 | 0.64 |
| 14:N:26:ARG:NH1 | 14:N:47:LEU:HG | 2.11 | 0.64 |
| 16:P:21:VAL:HG12 | 16:P:33:ILE:HD12 | 1.79 | 0.64 |
| 19:S:30:LEU:HD23 | 19:S:48:THR:O | 1.97 | 0.64 |
| 1:A:1480:A:H2 | 1:A:1483:G:N1 | 1.85 | 0.64 |
| 5:E:88:LYS:HB3 | 5:E:123:LEU:HB2 | 1.79 | 0.64 |
| 13:M:65:LYS:CE | 13:M:69:GLU:HG2 | 2.25 | 0.64 |
| 17:Q:76:LEU:C | 17:Q:76:LEU:HD23 | 2.17 | 0.64 |
| 1:A:1465:G:H2' | 1:A:1466:G:H8 | 1.62 | 0.64 |
| 1:A:1491:A:H2' | 1:A:1492:C:C6 | 2.32 | 0.64 |
| 1:A:953:A:H4' | 1:A:954:G:OP2 | 1.96 | 0.64 |
| 2:B:97:TRP:HH2 | 2:B:176:GLU:CD | 2.00 | 0.64 |
| 3:C:113:ALA:HB3 | 3:C:114:PRO:HD3 | 1.77 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:203:VAL:HG12 | 4:D:204:ILE:N | 2.11 | 0.64 |
| 9:I:28:VAL:HA | 9:I:63:ILE:O | 1.97 | 0.64 |
| 1:A:1211:A:H2' | 1:A:1212:C:C6 | 2.32 | 0.64 |
| 1:A:1335:G:H2' | 1:A:1336:C:H6 | 1.61 | 0.64 |
| 1:A:647:A:H2' | 1:A:648:G:H8 | 1.63 | 0.64 |
| 3:C:52:LEU:HD21 | 3:C:118:GLN:HE22 | 1.62 | 0.64 |
| 4:D:104:VAL:HG11 | 4:D:146:ILE:CD1 | 2.27 | 0.64 |
| 5:E:39:GLY:HA2 | 5:E:113:ALA:O | 1.97 | 0.64 |
| 1:A:1354:G:O3' | 9:I:69:GLY:HA3 | 1.97 | 0.64 |
| 10:J:12:ASP:HB3 | 10:J:15:THR:CB | 2.27 | 0.64 |
| 12:L:55:VAL:HG13 | 12:L:68:ALA:O | 1.97 | 0.64 |
| 17:Q:10:VAL:O | 17:Q:53:LEU:HD12 | 1.97 | 0.64 |
| 19:S:47:HIS:O | 19:S:62:ILE:HG22 | 1.98 | 0.64 |
| 19:S:5:LEU:O | 19:S:6:LYS:HB2 | 1.97 | 0.64 |
| 1:A:646:G:H2' | 1:A:647:A:C8 | 2.32 | 0.64 |
| 1:A:900:G:H2' | 1:A:901:A:H8 | 1.62 | 0.64 |
| 1:A:926:C:O2' | 1:A:927:A:H5' | 1.96 | 0.64 |
| 3:C:83:ARG:C | 3:C:85:ARG:H | 2.00 | 0.64 |
| 1:A:1246:C:H2' | 1:A:1247:G:C8 | 2.32 | 0.64 |
| 1:A:1288:A:H62 | 1:A:1313:G:H1' | 1.59 | 0.64 |
| 1:A:1403:C:H2' | 1:A:1404:G:C8 | 2.32 | 0.64 |
| 1:A:271:G:H5' | 17:Q:14:LYS:HB3 | 1.80 | 0.64 |
| 1:A:776:A:H4' | 1:A:777:U:H5'' | 1.79 | 0.64 |
| 3:C:26:LYS:HD3 | 3:C:26:LYS:N | 2.11 | 0.64 |
| 7:G:24:THR:O | 7:G:28:ASN:ND2 | 2.31 | 0.64 |
| 9:I:48:GLU:N | 9:I:49:PRO:HD2 | 2.11 | 0.64 |
| 11:K:19:ALA:HB2 | 11:K:80:VAL:HG11 | 1.78 | 0.64 |
| 1:A:678:A:H5' | 11:K:53:SER:HB2 | 1.77 | 0.64 |
| 1:A:1109:U:H2' | 1:A:1110:G:O4' | 1.98 | 0.64 |
| 1:A:634:G:C2' | 1:A:635:C:H5' | 2.27 | 0.64 |
| 7:G:92:SER:HB2 | 7:G:93:PRO:HD2 | 1.80 | 0.64 |
| 9:I:17:VAL:HG22 | 9:I:63:ILE:HD13 | 1.79 | 0.64 |
| 12:L:117:ARG:O | 12:L:119:LYS:O | 2.16 | 0.64 |
| 18:R:66:LEU:HD21 | 18:R:70:ILE:HD11 | 1.79 | 0.64 |
| 1:A:1172:G:HO2' | 1:A:1173:A:P | 2.21 | 0.64 |
| 1:A:831:G:O2' | 1:A:832:G:H5' | 1.98 | 0.64 |
| 2:B:130:ARG:HH21 | 3:C:207:VAL:HG22 | 1.63 | 0.64 |
| 4:D:70:ILE:HG22 | 4:D:71:SER:N | 2.11 | 0.64 |
| 19:S:11:VAL:HG13 | 19:S:38:SER:HB2 | 1.80 | 0.64 |
| 1:A:1489:G:H2' | 1:A:1490:U:O4' | 1.97 | 0.64 |
| 1:A:540:C:C2' | 1:A:541:G:H5' | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:739:G:OP2 | 15:O:65:ARG:HG2 | 1.97 | 0.64 |
| 1:A:858:C:O2' | 1:A:859:G:H5' | 1.97 | 0.64 |
| 1:A:95:A:H2' | 1:A:96:G:H8 | 1.63 | 0.64 |
| 4:D:9:CYS:O | 4:D:13:ARG:HG3 | 1.98 | 0.64 |
| 12:L:93:LEU:HB3 | 12:L:96:VAL:HG21 | 1.80 | 0.64 |
| 1:A:340:A:H5'' | 1:A:341:C:H5 | 1.63 | 0.63 |
| 1:A:719:C:O2' | 1:A:720:C:H5' | 1.97 | 0.63 |
| 1:A:947:A:N6 | 13:M:126:LYS:HB2 | 2.13 | 0.63 |
| 2:B:178:ARG:NH2 | 8:H:74:PRO:HG3 | 2.12 | 0.63 |
| 4:D:119:GLN:HG2 | 4:D:123:HIS:CD2 | 2.32 | 0.63 |
| 10:J:19:SER:CB | 10:J:91:PRO:HG3 | 2.28 | 0.63 |
| 13:M:84:ILE:C | 13:M:86:CYS:H | 2.01 | 0.63 |
| 15:O:31:LEU:O | 15:O:34:LEU:HB3 | 1.98 | 0.63 |
| 1:A:25:U:H2' | 1:A:26:C:C6 | 2.32 | 0.63 |
| 1:A:835:C:H2' | 1:A:836:G:O4' | 1.98 | 0.63 |
| 1:A:952:A:P | 14:N:29:ARG:HH22 | 2.20 | 0.63 |
| 1:A:999:U:H2' | 1:A:1000:G:H8 | 1.62 | 0.63 |
| 4:D:82:ALA:HB1 | 4:D:92:VAL:HB | 1.79 | 0.63 |
| 5:E:76:ILE:O | 5:E:93:PRO:HB3 | 1.98 | 0.63 |
| 6:F:48:LEU:HD22 | 18:R:77:GLY:HA3 | 1.80 | 0.63 |
| 1:A:506:C:H41 | 12:L:53:ARG:HH22 | 1.45 | 0.63 |
| 12:L:86:ARG:HG3 | 12:L:86:ARG:HH11 | 1.62 | 0.63 |
| 1:A:1383:C:C4' | 1:A:1384:G:OP2 | 2.47 | 0.63 |
| 1:A:1465:G:O2' | 1:A:1466:G:H5' | 1.97 | 0.63 |
| 1:A:50:U:H1' | 12:L:28:LYS:NZ | 2.13 | 0.63 |
| 20:T:43:LEU:HD12 | 20:T:52:ALA:HA | 1.79 | 0.63 |
| 1:A:1385:C:O2 | 1:A:1478:A:N1 | 2.31 | 0.63 |
| 1:A:750:A:C8 | 1:A:798:A:N6 | 2.67 | 0.63 |
| 2:B:29:ALA:O | 2:B:31:TYR:N | 2.31 | 0.63 |
| 3:C:177:THR:O | 3:C:179:ARG:N | 2.31 | 0.63 |
| 1:A:781:C:OP1 | 11:K:124:LYS:HG3 | 1.99 | 0.63 |
| 11:K:17:GLY:O | 11:K:80:VAL:HA | 1.99 | 0.63 |
| 11:K:87:THR:HA | 11:K:91:ARG:HH21 | 1.63 | 0.63 |
| 12:L:119:LYS:O | 12:L:120:TYR:HB2 | 1.99 | 0.63 |
| 15:O:36:ILE:HA | 15:O:59:MET:HE3 | 1.80 | 0.63 |
| 1:A:181:C:H2' | 1:A:182:C:H6 | 1.63 | 0.63 |
| 1:A:545:U:O2' | 1:A:546:C:OP2 | 2.16 | 0.63 |
| 1:A:654:G:H2' | 1:A:655:G:O4' | 1.99 | 0.63 |
| 12:L:75:HIS:HD2 | 12:L:77:LEU:HB2 | 1.63 | 0.63 |
| 1:A:745:G:H4' | 17:Q:102:GLY:C | 2.19 | 0.63 |
| 20:T:26:ASN:O | 20:T:29:LYS:HB2 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:A:H2' | 1:A:34:A:C8 | 2.34 | 0.63 |
| 2:B:89:GLY:H | 2:B:226:ARG:HH22 | 1.45 | 0.63 |
| 3:C:105:GLU:O | 3:C:107:GLN:NE2 | 2.31 | 0.63 |
| 4:D:65:ARG:HD2 | 4:D:75:PHE:HB2 | 1.81 | 0.63 |
| 11:K:57:THR:HG23 | 11:K:60:ALA:HB2 | 1.80 | 0.63 |
| 17:Q:44:ALA:HB1 | 17:Q:73:VAL:HG22 | 1.79 | 0.63 |
| 18:R:37:VAL:CG2 | 18:R:78:LEU:HB3 | 2.27 | 0.63 |
| 1:A:1482:G:HO2' | 1:A:1483:G:P | 2.21 | 0.63 |
| 1:A:452:C:H2' | 1:A:453:C:C6 | 2.34 | 0.63 |
| 1:A:677:G:H1' | 22:A:1524:KSG:H6 | 1.79 | 0.63 |
| 1:A:675:G:O2' | 1:A:781:C:H4' | 1.99 | 0.63 |
| 2:B:89:GLY:H | 2:B:226:ARG:NH2 | 1.97 | 0.63 |
| 6:F:3:ARG:NH2 | 6:F:64:GLN:HE22 | 1.95 | 0.63 |
| 12:L:25:PRO:C | 12:L:27:LEU:H | 1.99 | 0.63 |
| 12:L:47:LYS:CB | 12:L:48:PRO:CD | 2.75 | 0.63 |
| 1:A:1120:C:H4' | 1:A:1121:G:N2 | 2.14 | 0.63 |
| 7:G:23:VAL:HG13 | 7:G:43:PHE:CE2 | 2.34 | 0.63 |
| 10:J:82:ILE:O | 10:J:86:MET:HB2 | 1.99 | 0.63 |
| 1:A:176:G:O2' | 1:A:177:U:OP2 | 2.10 | 0.63 |
| 1:A:199:U:H2' | 1:A:200:C:H6 | 1.64 | 0.63 |
| 3:C:83:ARG:C | 3:C:85:ARG:N | 2.51 | 0.63 |
| 6:F:40:VAL:HG23 | 6:F:62:TRP:O | 1.99 | 0.63 |
| 10:J:12:ASP:CB | 10:J:15:THR:HB | 2.28 | 0.63 |
| 10:J:54:PHE:HD2 | 10:J:55:LYS:HG2 | 1.64 | 0.63 |
| 12:L:60:LEU:HD21 | 12:L:66:VAL:HG22 | 1.80 | 0.63 |
| 13:M:23:TYR:HB3 | 13:M:67:GLU:HA | 1.80 | 0.63 |
| 1:A:372:G:H5' | 16:P:5:ARG:HD2 | 1.81 | 0.63 |
| 19:S:20:LEU:HD12 | 19:S:21:GLU:N | 2.14 | 0.63 |
| 1:A:1364:U:O2' | 1:A:1365:C:H5' | 1.98 | 0.62 |
| 1:A:146:A:H2' | 1:A:147:A:O4' | 1.99 | 0.62 |
| 1:A:889:U:O2' | 1:A:890:C:H5' | 1.99 | 0.62 |
| 3:C:47:LEU:CD1 | 3:C:47:LEU:H | 2.11 | 0.62 |
| 3:C:83:ARG:O | 3:C:85:ARG:N | 2.31 | 0.62 |
| 11:K:120:ARG:NH1 | 11:K:126:ARG:HD2 | 2.14 | 0.62 |
| 17:Q:17:LYS:HA | 17:Q:46:ASP:O | 1.99 | 0.62 |
| 1:A:1453:G:H2' | 1:A:1454:G:C8 | 2.34 | 0.62 |
| 1:A:170:C:H2' | 1:A:171:C:H6 | 1.63 | 0.62 |
| 1:A:287:C:O2' | 1:A:288:G:H5' | 1.98 | 0.62 |
| 1:A:42:G:H2' | 1:A:43:G:H8 | 1.63 | 0.62 |
| 3:C:174:PRO:O | 3:C:177:THR:HG22 | 1.98 | 0.62 |
| 4:D:150:GLU:HA | 4:D:153:ARG:HG3 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:71:LEU:CD1 | 5:E:114:GLY:HA3 | 2.28 | 0.62 |
| 1:A:20:C:H2' | 1:A:21:U:H6 | 1.63 | 0.62 |
| 1:A:552:G:O6 | 12:L:5:PRO:HG3 | 1.99 | 0.62 |
| 1:A:673:C:H42 | 1:A:682:G:H1 | 1.45 | 0.62 |
| 1:A:733:C:H2' | 1:A:734:G:H8 | 1.64 | 0.62 |
| 1:A:773:U:H2' | 1:A:775:G:OP2 | 1.99 | 0.62 |
| 3:C:92:ALA:C | 3:C:94:LEU:H | 2.03 | 0.62 |
| 12:L:47:LYS:HB3 | 12:L:48:PRO:HD3 | 1.81 | 0.62 |
| 15:O:32:LEU:HD13 | 15:O:63:ARG:HB2 | 1.82 | 0.62 |
| 17:Q:43:LEU:CD1 | 17:Q:68:ARG:NH1 | 2.62 | 0.62 |
| 18:R:39:VAL:CG1 | 18:R:40:LEU:N | 2.62 | 0.62 |
| 1:A:1012:G:O2' | 1:A:1013:A:H5' | 1.99 | 0.62 |
| 1:A:1020:C:H2' | 1:A:1021:C:H6 | 1.63 | 0.62 |
| 1:A:1373:U:H2' | 1:A:1374:U:C6 | 2.35 | 0.62 |
| 2:B:23:ARG:HH11 | 2:B:24:TRP:N | 1.97 | 0.62 |
| 11:K:34:ASP:OD2 | 11:K:38:ASN:HB2 | 2.00 | 0.62 |
| 17:Q:12:SER:HB3 | 17:Q:20:THR:CB | 2.29 | 0.62 |
| 18:R:39:VAL:CG1 | 18:R:40:LEU:H | 2.12 | 0.62 |
| 20:T:69:GLY:O | 20:T:73:HIS:ND1 | 2.33 | 0.62 |
| 1:A:1320:G:H2' | 1:A:1321:A:C8 | 2.33 | 0.62 |
| 1:A:1329:G:N2 | 1:A:1356:G:H2' | 2.13 | 0.62 |
| 1:A:1396:A:H2 | 1:A:1465:G:N2 | 1.91 | 0.62 |
| 1:A:1466:G:H2' | 1:A:1467:G:C8 | 2.35 | 0.62 |
| 1:A:925:G:H2' | 1:A:926:C:C6 | 2.35 | 0.62 |
| 2:B:25:ASN:HD22 | 2:B:26:PRO:HD2 | 1.65 | 0.62 |
| 5:E:11:ILE:O | 5:E:12:LEU:HB3 | 1.99 | 0.62 |
| 5:E:144:THR:CG2 | 5:E:145:LYS:H | 2.11 | 0.62 |
| 12:L:126:LYS:H | 12:L:126:LYS:HD2 | 1.64 | 0.62 |
| 15:O:87:ILE:O | 15:O:88:ARG:HB2 | 1.99 | 0.62 |
| 16:P:20:VAL:CG2 | 16:P:35:LYS:HA | 2.30 | 0.62 |
| 1:A:762:G:H8 | 1:A:762:G:O5' | 1.82 | 0.62 |
| 7:G:108:ALA:O | 7:G:111:ARG:HG3 | 2.00 | 0.62 |
| 11:K:48:ILE:HD11 | 11:K:64:ALA:N | 2.15 | 0.62 |
| 13:M:8:GLU:OE1 | 13:M:22:ILE:HA | 1.99 | 0.62 |
| 1:A:1192:C:H4' | 1:A:1196:C:C4 | 2.34 | 0.62 |
| 1:A:1437:C:H5'' | 20:T:27:LYS:NZ | 2.14 | 0.62 |
| 1:A:984:A:C2' | 1:A:985:C:H5' | 2.30 | 0.62 |
| 2:B:109:SER:HA | 2:B:112:VAL:HG23 | 1.82 | 0.62 |
| 3:C:3:ASN:C | 3:C:4:LYS:HG2 | 2.19 | 0.62 |
| 14:N:37:PHE:HB3 | 14:N:39:LEU:HD12 | 1.79 | 0.62 |
| 2:B:25:ASN:C | 2:B:25:ASN:HD22 | 2.03 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:93:VAL:HG11 | 2:B:97:TRP:HD1 | 1.63 | 0.62 |
| 3:C:119:ARG:O | 3:C:123:GLN:HG3 | 1.99 | 0.62 |
| 4:D:149:ALA:O | 4:D:150:GLU:C | 2.38 | 0.62 |
| 13:M:23:TYR:HE2 | 13:M:70:LEU:HB3 | 1.62 | 0.62 |
| 13:M:5:ALA:CB | 13:M:22:ILE:HD13 | 2.29 | 0.62 |
| 1:A:101:G:H2' | 1:A:102:G:H5' | 1.82 | 0.62 |
| 1:A:847:G:H4' | 1:A:850:A:C8 | 2.35 | 0.62 |
| 2:B:230:VAL:HG13 | 2:B:231:GLU:OE2 | 2.00 | 0.62 |
| 3:C:125:GLU:C | 3:C:127:ARG:H | 2.02 | 0.62 |
| 3:C:68:VAL:HG12 | 3:C:70:VAL:CG2 | 2.30 | 0.62 |
| 6:F:10:LEU:HD12 | 6:F:59:TYR:HB3 | 1.82 | 0.62 |
| 1:A:373:G:OP1 | 16:P:3:LYS:HD2 | 2.00 | 0.62 |
| 1:A:251:G:C1' | 17:Q:16:GLN:NE2 | 2.61 | 0.62 |
| 1:A:286:C:O2' | 1:A:287:C:H5' | 2.00 | 0.62 |
| 4:D:175:SER:O | 4:D:183:GLY:HA2 | 2.00 | 0.62 |
| 12:L:47:LYS:HB2 | 12:L:48:PRO:CD | 2.30 | 0.62 |
| 13:M:15:VAL:HG11 | 13:M:34:LEU:HD21 | 1.81 | 0.62 |
| 19:S:13:ASP:HA | 19:S:16:LEU:HB3 | 1.82 | 0.62 |
| 19:S:43:GLU:H | 19:S:43:GLU:CD | 2.04 | 0.62 |
| 20:T:31:SER:HA | 20:T:34:LYS:HD2 | 1.82 | 0.62 |
| 1:A:1421:G:H2' | 1:A:1422:C:C6 | 2.35 | 0.61 |
| 1:A:423:U:OP2 | 4:D:36:ARG:NH2 | 2.33 | 0.61 |
| 1:A:564:U:H2' | 1:A:565:G:O4' | 2.00 | 0.61 |
| 1:A:620:U:H2' | 1:A:621:G:H8 | 1.65 | 0.61 |
| 2:B:114:ARG:NH1 | 2:B:118:LEU:HD21 | 2.14 | 0.61 |
| 2:B:76:GLN:HG3 | 2:B:206:ASP:OD1 | 1.99 | 0.61 |
| 3:C:161:GLU:HG2 | 3:C:161:GLU:O | 2.00 | 0.61 |
| 3:C:201:TYR:N | 3:C:201:TYR:CD1 | 2.68 | 0.61 |
| 4:D:105:VAL:HA | 4:D:108:LEU:HD12 | 1.82 | 0.61 |
| 5:E:36:ASP:C | 5:E:38:GLN:H | 2.03 | 0.61 |
| 6:F:69:GLU:HA | 6:F:72:VAL:HG23 | 1.82 | 0.61 |
| 13:M:80:ARG:C | 13:M:82:MET:H | 2.03 | 0.61 |
| 1:A:1267:A:H4' | 1:A:1268:A:O5' | 1.98 | 0.61 |
| 1:A:212:G:H2' | 1:A:213:C:C6 | 2.34 | 0.61 |
| 1:A:407:A:C1' | 1:A:409:G:H1' | 2.30 | 0.61 |
| 5:E:80:ILE:HD11 | 5:E:91:LEU:CD1 | 2.28 | 0.61 |
| 1:A:1161:A:O3' | 9:I:103:THR:HG23 | 2.00 | 0.61 |
| 9:I:42:ARG:O | 9:I:43:ALA:C | 2.39 | 0.61 |
| 11:K:48:ILE:CD1 | 11:K:63:LEU:HB2 | 2.28 | 0.61 |
| 1:A:1050:A:O2' | 1:A:1051:G:P | 2.59 | 0.61 |
| 1:A:1127:G:N2 | 1:A:1129:A:H62 | 1.97 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:38:U:O2' | 1:A:484:G:H4' | 1.99 | 0.61 |
| 1:A:398:G:O2' | 1:A:399:C:H5' | 1.99 | 0.61 |
| 1:A:443:A:H2' | 1:A:444:C:C6 | 2.35 | 0.61 |
| 3:C:5:ILE:HD12 | 3:C:5:ILE:O | 2.00 | 0.61 |
| 5:E:11:ILE:HG22 | 5:E:31:LEU:HB2 | 1.81 | 0.61 |
| 14:N:11:LYS:O | 14:N:12:ARG:C | 2.38 | 0.61 |
| 16:P:8:ARG:HB2 | 16:P:28:ARG:NH1 | 2.15 | 0.61 |
| 1:A:290:U:H2' | 1:A:291:C:C6 | 2.34 | 0.61 |
| 1:A:454:G:H3' | 1:A:455:A:C5' | 2.31 | 0.61 |
| 5:E:42:GLY:HA3 | 5:E:62:ALA:O | 1.99 | 0.61 |
| 19:S:49:ILE:HD12 | 19:S:71:LEU:HD21 | 1.83 | 0.61 |
| 19:S:31:ILE:O | 19:S:50:ALA:N | 2.30 | 0.61 |
| 1:A:1169:G:C2 | 1:A:1170:A:C4 | 2.89 | 0.61 |
| 1:A:262:G:H5'' | 1:A:262:G:C8 | 2.36 | 0.61 |
| 1:A:706:A:H4' | 1:A:707:U:C5 | 2.35 | 0.61 |
| 2:B:121:LEU:HD23 | 2:B:121:LEU:N | 2.14 | 0.61 |
| 2:B:178:ARG:O | 8:H:71:GLY:HA2 | 2.01 | 0.61 |
| 9:I:111:ARG:HD2 | 9:I:113:LYS:HG3 | 1.83 | 0.61 |
| 18:R:47:THR:HG22 | 18:R:48:GLY:N | 2.15 | 0.61 |
| 1:A:945:C:C4' | 9:I:128:ARG:HG3 | 2.28 | 0.61 |
| 2:B:22:LYS:O | 2:B:23:ARG:HG3 | 2.00 | 0.61 |
| 2:B:30:ARG:HG3 | 2:B:31:TYR:CE2 | 2.35 | 0.61 |
| 8:H:88:LYS:HB3 | 8:H:89:PRO:HD2 | 1.83 | 0.61 |
| 12:L:6:THR:OG1 | 12:L:9:GLN:HG3 | 2.00 | 0.61 |
| 17:Q:97:SER:HB2 | 17:Q:102:GLY:C | 2.20 | 0.61 |
| 19:S:16:LEU:C | 19:S:18:LYS:H | 2.04 | 0.61 |
| 1:A:775:G:C2' | 1:A:776:A:H5' | 2.29 | 0.61 |
| 1:A:7:G:C4 | 5:E:119:LEU:HD11 | 2.36 | 0.61 |
| 2:B:149:LEU:O | 2:B:151:GLY:N | 2.34 | 0.61 |
| 4:D:65:ARG:HE | 4:D:72:GLU:N | 1.97 | 0.61 |
| 17:Q:43:LEU:HD11 | 17:Q:68:ARG:NH1 | 2.16 | 0.61 |
| 19:S:22:LEU:HD22 | 19:S:28:LYS:HB2 | 1.81 | 0.61 |
| 1:A:268:C:O2' | 1:A:269:A:H5' | 2.00 | 0.61 |
| 1:A:576:G:O2' | 1:A:577:G:H5' | 2.01 | 0.61 |
| 1:A:603:U:C2 | 4:D:135:LEU:HD11 | 2.36 | 0.61 |
| 4:D:26:CYS:HA | 4:D:31:CYS:HB2 | 1.82 | 0.61 |
| 5:E:41:VAL:HG21 | 5:E:113:ALA:HA | 1.79 | 0.61 |
| 7:G:83:ALA:HB3 | 7:G:85:TYR:HE2 | 1.65 | 0.61 |
| 1:A:1403:C:O5' | 1:A:1403:C:H6 | 1.83 | 0.61 |
| 1:A:402:G:H5'' | 4:D:5:ILE:HG21 | 1.83 | 0.61 |
| 1:A:407:A:C4 | 1:A:409:G:H1' | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:737:A:H5' | 1:A:738:C:C6 | 2.36 | 0.61 |
| 2:B:23:ARG:C | 2:B:23:ARG:NH1 | 2.55 | 0.61 |
| 4:D:194:LEU:HB3 | 4:D:196:LEU:HD12 | 1.82 | 0.61 |
| 4:D:61:LYS:HD3 | 4:D:206:PHE:CE2 | 2.36 | 0.61 |
| 5:E:139:LEU:HD22 | 5:E:142:LEU:CD1 | 2.22 | 0.61 |
| 1:A:359:A:OP1 | 12:L:33:ARG:HG3 | 2.00 | 0.61 |
| 1:A:372:G:O2' | 1:A:373:G:H5' | 2.00 | 0.61 |
| 1:A:964:A:H2' | 1:A:965:G:H8 | 1.66 | 0.61 |
| 2:B:17:PHE:HD1 | 2:B:18:GLY:N | 1.99 | 0.61 |
| 4:D:190:ASP:N | 4:D:193:ASP:OD2 | 2.34 | 0.61 |
| 4:D:30:LYS:C | 4:D:32:ALA:H | 2.04 | 0.61 |
| 8:H:44:PHE:HB3 | 8:H:80:ILE:HG12 | 1.83 | 0.61 |
| 9:I:5:TYR:CG | 9:I:6:GLY:N | 2.68 | 0.61 |
| 11:K:80:VAL:HG21 | 11:K:103:LEU:HD13 | 1.82 | 0.61 |
| 2:B:20:GLU:HG3 | 2:B:189:ASP:OD2 | 2.01 | 0.60 |
| 5:E:13:ILE:HG22 | 5:E:30:ALA:CB | 2.31 | 0.60 |
| 5:E:44:GLY:N | 5:E:62:ALA:HB2 | 2.16 | 0.60 |
| 10:J:92:THR:HG22 | 10:J:92:THR:O | 2.01 | 0.60 |
| 14:N:9:LYS:C | 14:N:9:LYS:HD3 | 2.22 | 0.60 |
| 16:P:39:TYR:HB2 | 16:P:49:LEU:HD12 | 1.83 | 0.60 |
| 1:A:745:G:H1' | 17:Q:103:GLY:O | 2.01 | 0.60 |
| 1:A:1203:G:OP1 | 1:A:1303:C:N3 | 2.33 | 0.60 |
| 1:A:51:A:O2' | 1:A:53:G:C8 | 2.54 | 0.60 |
| 4:D:5:ILE:HA | 4:D:115:ARG:NH2 | 2.16 | 0.60 |
| 4:D:151:LYS:N | 4:D:151:LYS:HD2 | 2.13 | 0.60 |
| 7:G:111:ARG:HB3 | 7:G:113:GLU:OE2 | 2.00 | 0.60 |
| 7:G:12:LEU:HD12 | 7:G:12:LEU:H | 1.63 | 0.60 |
| 13:M:87:TYR:CE1 | 13:M:91:ARG:HD3 | 2.35 | 0.60 |
| 20:T:44:ALA:HB1 | 20:T:92:LEU:HG | 1.83 | 0.60 |
| 1:A:1302:C:O2' | 1:A:1303:C:H5' | 2.01 | 0.60 |
| 1:A:332:C:H2' | 1:A:333:C:H6 | 1.65 | 0.60 |
| 1:A:980:G:H2' | 1:A:981:G:C8 | 2.36 | 0.60 |
| 1:A:993:A:H2' | 1:A:994:A:C8 | 2.36 | 0.60 |
| 3:C:132:ARG:HH22 | 4:D:47:ARG:NH1 | 1.97 | 0.60 |
| 3:C:179:ARG:C | 3:C:179:ARG:HD2 | 2.21 | 0.60 |
| 1:A:1350:C:H5' | 10:J:60:ARG:NH1 | 2.16 | 0.60 |
| 12:L:98:TYR:N | 12:L:98:TYR:CD1 | 2.69 | 0.60 |
| 14:N:9:LYS:HD3 | 14:N:9:LYS:O | 2.01 | 0.60 |
| 18:R:62:GLU:O | 18:R:65:ILE:N | 2.34 | 0.60 |
| 1:A:1342:A:H2' | 1:A:1343:G:O4' | 2.01 | 0.60 |
| 1:A:60:A:H3' | 1:A:327:G:H22 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:42:G:H2' | 1:A:43:G:C8 | 2.37 | 0.60 |
| 3:C:177:THR:HG23 | 3:C:180:ALA:HB2 | 1.83 | 0.60 |
| 4:D:187:ARG:HD2 | 4:D:188:LEU:H | 1.66 | 0.60 |
| 6:F:100:ASN:HD22 | 18:R:23:LYS:CG | 2.14 | 0.60 |
| 8:H:87:SER:HA | 8:H:93:VAL:CG2 | 2.22 | 0.60 |
| 12:L:45:PRO:HG2 | 12:L:51:ALA:N | 2.16 | 0.60 |
| 13:M:96:LEU:O | 13:M:110:ARG:NH1 | 2.34 | 0.60 |
| 1:A:205:G:H2' | 1:A:206:G:C8 | 2.35 | 0.60 |
| 3:C:188:LEU:O | 3:C:189:ALA:HB2 | 2.00 | 0.60 |
| 3:C:97:LYS:O | 3:C:98:ASN:HB3 | 2.01 | 0.60 |
| 14:N:44:LEU:O | 14:N:44:LEU:HD12 | 2.02 | 0.60 |
| 1:A:199:U:H1' | 20:T:103:GLY:HA2 | 1.83 | 0.60 |
| 1:A:1050:A:HO2' | 1:A:1051:G:H8 | 1.48 | 0.60 |
| 1:A:1205:C:P | 19:S:78:ARG:HH12 | 2.24 | 0.60 |
| 1:A:1333:U:H2' | 1:A:1334:C:H6 | 1.67 | 0.60 |
| 1:A:190:U:O4 | 17:Q:63:ARG:N | 2.31 | 0.60 |
| 1:A:702:G:H5' | 1:A:703:C:OP2 | 2.01 | 0.60 |
| 1:A:745:G:C2 | 17:Q:105:ALA:HB3 | 2.37 | 0.60 |
| 3:C:107:GLN:H | 3:C:107:GLN:CD | 2.05 | 0.60 |
| 7:G:68:ASN:ND2 | 7:G:128:ALA:HA | 2.17 | 0.60 |
| 14:N:3:ARG:NH1 | 14:N:6:LEU:HD11 | 2.17 | 0.60 |
| 16:P:74:LEU:O | 16:P:79:VAL:HG23 | 2.00 | 0.60 |
| 20:T:33:ILE:HD11 | 20:T:63:ILE:HA | 1.84 | 0.60 |
| 1:A:1140:A:H5'' | 1:A:1141:C:OP1 | 2.01 | 0.60 |
| 1:A:1175:G:O2' | 1:A:1176:U:H5' | 2.01 | 0.60 |
| 1:A:1245:C:H2' | 1:A:1246:C:H6 | 1.66 | 0.60 |
| 1:A:923:G:N2 | 1:A:1316:G:H4' | 2.16 | 0.60 |
| 1:A:1498:G:O2' | 1:A:1499:G:H5' | 2.01 | 0.60 |
| 1:A:1500:U:O2' | 1:A:1501:G:H5' | 2.01 | 0.60 |
| 1:A:521:G:H2' | 1:A:522:G:C8 | 2.36 | 0.60 |
| 4:D:12:CYS:HA | 4:D:19:LEU:HD12 | 1.83 | 0.60 |
| 5:E:70:PRO:O | 5:E:71:LEU:C | 2.39 | 0.60 |
| 7:G:25:ALA:CA | 7:G:28:ASN:HD22 | 2.14 | 0.60 |
| 10:J:30:SER:O | 10:J:78:ASN:HB2 | 2.02 | 0.60 |
| 13:M:13:LYS:O | 13:M:14:ARG:C | 2.39 | 0.60 |
| 16:P:74:LEU:CB | 16:P:79:VAL:HG21 | 2.25 | 0.60 |
| 20:T:39:LYS:HD2 | 20:T:55:ILE:HD13 | 1.82 | 0.60 |
| 1:A:1172:G:C2' | 1:A:1173:A:OP2 | 2.50 | 0.60 |
| 1:A:1245:C:H2' | 1:A:1246:C:C6 | 2.37 | 0.60 |
| 1:A:469:G:H4' | 1:A:470:G:O5' | 2.01 | 0.60 |
| 1:A:757:G:C6 | 1:A:791:A:N6 | 2.69 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:79:G:H3' | 1:A:80:U:H5'' | 1.83 | 0.60 |
| 2:B:137:ARG:HB3 | 2:B:137:ARG:NH1 | 2.15 | 0.60 |
| 4:D:90:GLY:N | 4:D:204:ILE:HD11 | 2.16 | 0.60 |
| 5:E:79:GLU:O | 5:E:80:ILE:HG23 | 2.02 | 0.60 |
| 7:G:148:ASN:C | 7:G:150:ALA:N | 2.55 | 0.60 |
| 7:G:96:GLN:O | 7:G:99:LEU:N | 2.35 | 0.60 |
| 8:H:91:ARG:NH1 | 17:Q:33:GLY:HA3 | 2.16 | 0.60 |
| 15:O:27:VAL:HG12 | 15:O:31:LEU:CD1 | 2.31 | 0.60 |
| 16:P:67:THR:HG22 | 16:P:68:ASP:H | 1.65 | 0.60 |
| 1:A:999:U:H2' | 1:A:1000:G:C8 | 2.36 | 0.60 |
| 1:A:1000:G:H2' | 1:A:1001:G:O4' | 2.02 | 0.60 |
| 1:A:1153:G:H2' | 1:A:1154:C:H6 | 1.67 | 0.60 |
| 1:A:47:G:O2' | 1:A:361:U:H1' | 2.02 | 0.60 |
| 1:A:486:G:C2 | 1:A:487:C:C2 | 2.89 | 0.60 |
| 1:A:763:C:H2' | 1:A:764:A:O4' | 2.01 | 0.60 |
| 3:C:134:ILE:O | 3:C:138:VAL:HG23 | 2.02 | 0.60 |
| 4:D:8:VAL:HG13 | 4:D:21:LEU:HD13 | 1.83 | 0.60 |
| 10:J:30:SER:HB2 | 10:J:81:THR:N | 2.16 | 0.60 |
| 14:N:14:PRO:C | 14:N:16:PHE:N | 2.55 | 0.60 |
| 18:R:45:SER:C | 18:R:47:THR:N | 2.52 | 0.60 |
| 18:R:65:ILE:C | 18:R:67:ALA:N | 2.55 | 0.60 |
| 1:A:1439:G:H2' | 1:A:1440:G:H8 | 1.67 | 0.60 |
| 1:A:214:C:H4' | 1:A:456:C:N4 | 2.16 | 0.60 |
| 6:F:75:LEU:HD13 | 6:F:75:LEU:O | 2.02 | 0.60 |
| 15:O:3:ILE:N | 15:O:3:ILE:HD12 | 2.17 | 0.60 |
| 18:R:47:THR:HG22 | 18:R:48:GLY:H | 1.65 | 0.60 |
| 19:S:51:VAL:HG12 | 19:S:52:TYR:N | 2.17 | 0.60 |
| 1:A:1336:C:O2' | 1:A:1337:G:H5' | 2.02 | 0.59 |
| 1:A:159:U:O2' | 1:A:160:C:H5' | 2.01 | 0.59 |
| 1:A:776:A:O2' | 1:A:777:U:P | 2.59 | 0.59 |
| 1:A:778:A:O2' | 1:A:779:C:H5' | 2.02 | 0.59 |
| 3:C:110:ASN:ND2 | 3:C:140:ARG:HB3 | 2.17 | 0.59 |
| 4:D:150:GLU:CD | 4:D:150:GLU:N | 2.53 | 0.59 |
| 7:G:20:ASP:O | 7:G:23:VAL:HB | 2.01 | 0.59 |
| 1:A:1324:C:O2' | 1:A:1325:G:H5' | 2.02 | 0.59 |
| 1:A:378:A:H2' | 1:A:379:A:H8 | 1.67 | 0.59 |
| 1:A:802:G:C3' | 1:A:803:A:C5' | 2.79 | 0.59 |
| 4:D:64:LEU:HD23 | 4:D:198:VAL:CG1 | 2.31 | 0.59 |
| 5:E:144:THR:HB | 5:E:147:ASP:OD2 | 2.02 | 0.59 |
| 11:K:99:GLN:HG2 | 11:K:105:VAL:HG21 | 1.84 | 0.59 |
| 1:A:1128:C:O2' | 1:A:1129:A:H8 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1232:A:H2' | 1:A:1233:A:C8 | 2.37 | 0.59 |
| 1:A:110:A:H61 | 1:A:309:A:H1' | 1.66 | 0.59 |
| 1:A:634:G:H2' | 1:A:635:C:H5' | 1.84 | 0.59 |
| 2:B:22:LYS:C | 2:B:23:ARG:HG3 | 2.23 | 0.59 |
| 1:A:1280:C:N4 | 7:G:114:ARG:HB3 | 2.17 | 0.59 |
| 7:G:115:ARG:HB2 | 7:G:118:VAL:HG23 | 1.84 | 0.59 |
| 7:G:25:ALA:HA | 7:G:28:ASN:ND2 | 2.16 | 0.59 |
| 15:O:9:GLN:HA | 15:O:12:ILE:HD12 | 1.84 | 0.59 |
| 16:P:45:THR:HB | 16:P:46:PRO:HD2 | 1.83 | 0.59 |
| 1:A:1103:G:H8 | 1:A:1103:G:O5' | 1.85 | 0.59 |
| 1:A:1220:A:H5' | 1:A:1318:C:H41 | 1.67 | 0.59 |
| 1:A:1302:C:H2' | 1:A:1303:C:O4' | 2.03 | 0.59 |
| 1:A:540:C:H2' | 1:A:541:G:C5' | 2.31 | 0.59 |
| 1:A:545:U:HO2' | 1:A:546:C:P | 2.24 | 0.59 |
| 5:E:145:LYS:O | 5:E:145:LYS:HG2 | 2.02 | 0.59 |
| 1:A:1208:C:H5" | 13:M:103:THR:HB | 1.83 | 0.59 |
| 20:T:93:GLU:OE2 | 20:T:93:GLU:HA | 2.01 | 0.59 |
| 1:A:1022:C:O2' | 1:A:1023:U:H5' | 2.03 | 0.59 |
| 1:A:1219:C:H4' | 1:A:1316:G:N2 | 2.15 | 0.59 |
| 1:A:1263:U:H5' | 1:A:1264:C:C5 | 2.36 | 0.59 |
| 1:A:548:C:C6 | 17:Q:31:LEU:HD11 | 2.37 | 0.59 |
| 1:A:902:C:O2' | 1:A:903:G:H5' | 2.02 | 0.59 |
| 1:A:908:C:O2' | 1:A:909:C:H5' | 2.01 | 0.59 |
| 13:M:65:LYS:O | 13:M:66:LEU:HD23 | 2.02 | 0.59 |
| 20:T:53:LEU:HD21 | 20:T:104:LEU:HD12 | 1.85 | 0.59 |
| 1:A:1164:G:O2' | 1:A:1165:A:OP2 | 2.20 | 0.59 |
| 1:A:1183:A:H4' | 1:A:1184:G:O5' | 2.02 | 0.59 |
| 1:A:1233:A:H2' | 1:A:1234:A:H8 | 1.66 | 0.59 |
| 1:A:443:A:OP2 | 1:A:470:G:N2 | 2.32 | 0.59 |
| 1:A:9:A:C6 | 4:D:209:ARG:HB2 | 2.36 | 0.59 |
| 3:C:10:PHE:CZ | 3:C:178:LEU:HD13 | 2.38 | 0.59 |
| 3:C:33:LEU:HD11 | 14:N:53:LEU:HD22 | 1.84 | 0.59 |
| 3:C:32:LEU:O | 3:C:35:GLU:HB3 | 2.02 | 0.59 |
| 5:E:36:ASP:C | 5:E:38:GLN:N | 2.55 | 0.59 |
| 7:G:151:TYR:HA | 7:G:153:HIS:CE1 | 2.36 | 0.59 |
| 10:J:85:LEU:O | 10:J:87:THR:N | 2.36 | 0.59 |
| 12:L:117:ARG:O | 12:L:119:LYS:N | 2.35 | 0.59 |
| 12:L:27:LEU:O | 12:L:29:GLY:N | 2.34 | 0.59 |
| 18:R:29:PHE:HE1 | 18:R:31:LEU:HD23 | 1.68 | 0.59 |
| 20:T:66:ALA:HB3 | 20:T:72:LEU:HD12 | 1.84 | 0.59 |
| 1:A:41:C:H2' | 1:A:42:G:C8 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:727:U:H2' | 1:A:728:C:C6 | 2.38 | 0.59 |
| 1:A:85:C:H2' | 1:A:86:U:O4' | 2.02 | 0.59 |
| 1:A:924:A:H2' | 1:A:925:G:C8 | 2.38 | 0.59 |
| 3:C:150:LYS:O | 3:C:200:ALA:HA | 2.02 | 0.59 |
| 4:D:109:GLY:C | 4:D:111:ALA:H | 2.05 | 0.59 |
| 4:D:176:LEU:HD23 | 4:D:176:LEU:O | 2.03 | 0.59 |
| 5:E:122:GLU:OE1 | 5:E:131:ILE:HG21 | 2.03 | 0.59 |
| 5:E:41:VAL:HG21 | 5:E:113:ALA:CA | 2.33 | 0.59 |
| 1:A:1135:A:C5' | 10:J:13:HIS:CD2 | 2.82 | 0.59 |
| 12:L:83:VAL:CG2 | 12:L:100:ILE:HG23 | 2.33 | 0.59 |
| 1:A:1423:C:H2' | 1:A:1424:G:O4' | 2.03 | 0.59 |
| 2:B:88:ALA:CB | 2:B:90:MET:HG2 | 2.32 | 0.59 |
| 6:F:82:ARG:HB2 | 6:F:85:VAL:HB | 1.84 | 0.59 |
| 8:H:83:ILE:CG2 | 8:H:83:ILE:O | 2.50 | 0.59 |
| 18:R:88:LYS:HG2 | 18:R:88:LYS:OXT | 2.02 | 0.59 |
| 1:A:1203:G:O3' | 19:S:77:THR:HG21 | 2.03 | 0.59 |
| 1:A:1436:G:O2' | 1:A:1437:C:H5' | 2.03 | 0.59 |
| 3:C:154:SER:CB | 3:C:197:GLY:H | 2.16 | 0.59 |
| 10:J:67:THR:HG22 | 10:J:67:THR:O | 2.03 | 0.59 |
| 12:L:47:LYS:HB2 | 12:L:48:PRO:HD3 | 1.84 | 0.59 |
| 13:M:87:TYR:CZ | 13:M:91:ARG:HD3 | 2.37 | 0.59 |
| 15:O:10:LYS:HG3 | 15:O:11:VAL:N | 2.17 | 0.59 |
| 1:A:1390:C:H2' | 1:A:1391:A:H8 | 1.67 | 0.59 |
| 1:A:270:A:HO2' | 1:A:271:G:H8 | 1.50 | 0.59 |
| 1:A:732:C:H1' | 1:A:733:C:H5 | 1.67 | 0.59 |
| 1:A:796:C:O2' | 1:A:797:U:P | 2.60 | 0.59 |
| 5:E:78:HIS:CD2 | 8:H:107:LEU:HD12 | 2.38 | 0.59 |
| 20:T:43:LEU:CD1 | 20:T:55:ILE:HD12 | 2.27 | 0.59 |
| 20:T:91:LEU:C | 20:T:93:GLU:H | 2.06 | 0.59 |
| 1:A:1440:G:H2' | 1:A:1441:C:H6 | 1.68 | 0.58 |
| 1:A:155:A:H2' | 1:A:156:A:O4' | 2.02 | 0.58 |
| 1:A:277:G:O2' | 1:A:278:A:P | 2.61 | 0.58 |
| 1:A:283:U:H2' | 1:A:284:A:C8 | 2.38 | 0.58 |
| 1:A:563:G:C5' | 1:A:712:A:H1' | 2.27 | 0.58 |
| 1:A:787:G:H2' | 1:A:788:U:C6 | 2.38 | 0.58 |
| 2:B:87:ARG:HD3 | 2:B:234:PRO:CD | 2.33 | 0.58 |
| 2:B:77:ALA:O | 2:B:78:GLN:C | 2.41 | 0.58 |
| 3:C:167:TRP:O | 3:C:168:ALA:CB | 2.51 | 0.58 |
| 3:C:113:ALA:HB1 | 3:C:185:GLY:N | 2.17 | 0.58 |
| 4:D:53:ASP:O | 4:D:57:ARG:HD3 | 2.03 | 0.58 |
| 5:E:13:ILE:HA | 5:E:29:GLY:O | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1111:C:H4' | 9:I:16:ARG:NH1 | 2.19 | 0.58 |
| 12:L:110:VAL:O | 12:L:122:THR:HG22 | 2.03 | 0.58 |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:HB3 | 1.84 | 0.58 |
| 16:P:20:VAL:HG22 | 16:P:35:LYS:HA | 1.85 | 0.58 |
| 16:P:58:TYR:O | 16:P:61:SER:HB3 | 2.02 | 0.58 |
| 17:Q:8:GLY:HA3 | 17:Q:22:LEU:O | 2.03 | 0.58 |
| 1:A:1305:G:H2' | 1:A:1306:A:H8 | 1.68 | 0.58 |
| 1:A:454:G:C3' | 1:A:455:A:H5'' | 2.33 | 0.58 |
| 1:A:635:C:N3 | 1:A:636:U:C4 | 2.71 | 0.58 |
| 2:B:46:LYS:O | 2:B:47:THR:C | 2.42 | 0.58 |
| 4:D:191:ARG:HD2 | 4:D:191:ARG:O | 2.02 | 0.58 |
| 9:I:26:VAL:CB | 9:I:33:PHE:HB2 | 2.30 | 0.58 |
| 1:A:1311:A:P | 13:M:28:ALA:HB3 | 2.43 | 0.58 |
| 18:R:55:ARG:O | 18:R:56:THR:C | 2.42 | 0.58 |
| 20:T:55:ILE:O | 20:T:56:MET:C | 2.41 | 0.58 |
| 1:A:1070:G:H2' | 1:A:1071:G:H8 | 1.67 | 0.58 |
| 1:A:1308:C:OP1 | 21:U:12:LYS:NZ | 2.36 | 0.58 |
| 1:A:362:C:O2' | 1:A:390:G:N2 | 2.36 | 0.58 |
| 4:D:152:SER:HB3 | 4:D:155:LEU:HD12 | 1.85 | 0.58 |
| 4:D:59:ARG:NH2 | 4:D:62:GLN:HG3 | 2.17 | 0.58 |
| 8:H:27:PRO:O | 8:H:32:LYS:HE3 | 2.03 | 0.58 |
| 10:J:5:ARG:HB3 | 10:J:99:LYS:O | 2.03 | 0.58 |
| 13:M:10:PRO:O | 13:M:45:VAL:HG11 | 2.04 | 0.58 |
| 15:O:56:LEU:HG | 15:O:57:LEU:N | 2.18 | 0.58 |
| 16:P:22:THR:HA | 16:P:33:ILE:CG1 | 2.33 | 0.58 |
| 1:A:1329:G:HO2' | 1:A:1356:G:H1 | 1.51 | 0.58 |
| 1:A:1329:G:O2' | 1:A:1330:U:P | 2.61 | 0.58 |
| 1:A:1395:C:H2' | 1:A:1396:A:C8 | 2.39 | 0.58 |
| 1:A:708:G:C2 | 1:A:709:G:C8 | 2.91 | 0.58 |
| 1:A:88:C:H2' | 1:A:89:G:C8 | 2.38 | 0.58 |
| 2:B:193:ASP:OD1 | 2:B:195:ASP:HB2 | 2.03 | 0.58 |
| 3:C:33:LEU:C | 3:C:33:LEU:HD23 | 2.23 | 0.58 |
| 4:D:177:ASP:O | 4:D:178:VAL:C | 2.40 | 0.58 |
| 7:G:145:ALA:C | 7:G:147:ALA:N | 2.51 | 0.58 |
| 8:H:120:THR:O | 8:H:121:ASP:C | 2.42 | 0.58 |
| 12:L:50:SER:O | 12:L:51:ALA:HB2 | 2.04 | 0.58 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H | 1.68 | 0.58 |
| 1:A:185:C:H2' | 1:A:186:C:C6 | 2.38 | 0.58 |
| 1:A:536:U:O2' | 1:A:537:A:H5' | 2.02 | 0.58 |
| 1:A:787:G:H2' | 1:A:788:U:H6 | 1.67 | 0.58 |
| 4:D:151:LYS:H | 4:D:151:LYS:CD | 2.15 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:39:PRO:HG2 | 4:D:44:GLY:HA2 | 1.85 | 0.58 |
| 6:F:3:ARG:NH2 | 6:F:64:GLN:NE2 | 2.52 | 0.58 |
| 16:P:57:ARG:NH1 | 16:P:79:VAL:O | 2.37 | 0.58 |
| 1:A:1287:G:C5' | 21:U:4:GLY:HA3 | 2.32 | 0.58 |
| 1:A:1021:C:H2' | 1:A:1022:C:H6 | 1.67 | 0.58 |
| 1:A:1065:G:H2' | 1:A:1066:U:O4' | 2.04 | 0.58 |
| 1:A:566:U:C2 | 1:A:744:G:C6 | 2.91 | 0.58 |
| 2:B:25:ASN:ND2 | 2:B:25:ASN:C | 2.56 | 0.58 |
| 3:C:20:SER:HB3 | 3:C:22:TRP:HE1 | 1.68 | 0.58 |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:CD1 | 2.33 | 0.58 |
| 8:H:111:ILE:HB | 8:H:135:CYS:SG | 2.44 | 0.58 |
| 8:H:44:PHE:CE1 | 8:H:137:VAL:HG12 | 2.38 | 0.58 |
| 11:K:33:THR:HA | 11:K:39:PRO:HA | 1.86 | 0.58 |
| 1:A:485:C:OP1 | 12:L:117:ARG:NH2 | 2.36 | 0.58 |
| 12:L:54:LYS:HD2 | 12:L:54:LYS:N | 2.19 | 0.58 |
| 12:L:60:LEU:HD11 | 12:L:85:ILE:HD12 | 1.84 | 0.58 |
| 16:P:67:THR:CG2 | 16:P:68:ASP:N | 2.67 | 0.58 |
| 13:M:94:ARG:HH12 | 19:S:81:ARG:HD3 | 1.68 | 0.58 |
| 1:A:398:G:H1' | 1:A:604:C:H42 | 1.69 | 0.58 |
| 1:A:707:U:H2' | 1:A:707:U:O2 | 2.03 | 0.58 |
| 3:C:74:GLY:O | 3:C:76:VAL:N | 2.36 | 0.58 |
| 4:D:122:ARG:NH2 | 4:D:134:ASP:OD2 | 2.36 | 0.58 |
| 4:D:8:VAL:HG11 | 4:D:21:LEU:CB | 2.33 | 0.58 |
| 16:P:39:TYR:HB2 | 16:P:49:LEU:CD1 | 2.34 | 0.58 |
| 1:A:1001:G:H2' | 1:A:1002:G:H8 | 1.67 | 0.58 |
| 1:A:1064:G:H5'' | 5:E:27:ARG:NH1 | 2.18 | 0.58 |
| 1:A:1099:C:C2' | 1:A:1100:G:C5' | 2.82 | 0.58 |
| 1:A:1287:G:OP1 | 21:U:2:GLY:N | 2.37 | 0.58 |
| 1:A:1340:U:H3' | 1:A:1341:C:C6 | 2.38 | 0.58 |
| 1:A:20:C:H2' | 1:A:21:U:C6 | 2.39 | 0.58 |
| 1:A:702:G:H4' | 11:K:117:ASN:HD21 | 1.67 | 0.58 |
| 1:A:757:G:O2' | 1:A:758:G:H5' | 2.03 | 0.58 |
| 1:A:925:G:C5 | 1:A:926:C:C4 | 2.92 | 0.58 |
| 2:B:209:ARG:NE | 2:B:239:VAL:HG11 | 2.18 | 0.58 |
| 4:D:149:ALA:O | 4:D:152:SER:N | 2.37 | 0.58 |
| 4:D:209:ARG:HG2 | 4:D:209:ARG:HH11 | 1.68 | 0.58 |
| 4:D:8:VAL:HG11 | 4:D:21:LEU:HB3 | 1.84 | 0.58 |
| 5:E:135:THR:O | 5:E:136:MET:C | 2.41 | 0.58 |
| 6:F:40:VAL:HG22 | 6:F:41:GLU:N | 2.19 | 0.58 |
| 7:G:122:HIS:HD2 | 7:G:125:MET:HE3 | 1.69 | 0.58 |
| 13:M:33:ALA:HA | 13:M:59:TYR:HE2 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:79:LYS:HD3 | 13:M:83:ASP:OD2 | 2.04 | 0.58 |
| 1:A:1131:U:H4' | 9:I:14:VAL:HG11 | 1.85 | 0.58 |
| 1:A:228:G:O2' | 1:A:229:C:H5' | 2.03 | 0.58 |
| 1:A:379:A:H2' | 1:A:380:G:H5' | 1.85 | 0.58 |
| 1:A:575:U:H2' | 1:A:576:G:C8 | 2.38 | 0.58 |
| 1:A:584:C:H42 | 1:A:622:G:H1 | 1.52 | 0.58 |
| 1:A:745:G:H2' | 1:A:746:C:C6 | 2.39 | 0.58 |
| 2:B:134:GLU:C | 2:B:136:VAL:N | 2.57 | 0.58 |
| 4:D:33:MET:SD | 4:D:37:PRO:HA | 2.44 | 0.58 |
| 4:D:64:LEU:O | 4:D:64:LEU:HD13 | 2.03 | 0.58 |
| 7:G:114:ARG:HG2 | 7:G:114:ARG:HH11 | 1.69 | 0.58 |
| 1:A:950:C:H4' | 10:J:57:LYS:HB3 | 1.86 | 0.58 |
| 13:M:80:ARG:HG2 | 13:M:81:LEU:N | 2.18 | 0.58 |
| 14:N:11:LYS:O | 14:N:13:THR:N | 2.37 | 0.58 |
| 21:U:2:GLY:O | 21:U:4:GLY:N | 2.36 | 0.58 |
| 1:A:1111:C:O2' | 1:A:1113:A:C8 | 2.54 | 0.58 |
| 1:A:1137:G:O2' | 1:A:1138:G:H5' | 2.03 | 0.58 |
| 1:A:187:C:H2' | 1:A:188:C:O4' | 2.03 | 0.58 |
| 1:A:241:C:O2' | 1:A:242:A:H5' | 2.03 | 0.58 |
| 1:A:340:A:H5'' | 1:A:341:C:C5 | 2.38 | 0.58 |
| 1:A:422:G:O2' | 1:A:423:U:H5' | 2.04 | 0.58 |
| 1:A:485:C:H2' | 1:A:486:G:C8 | 2.29 | 0.58 |
| 7:G:85:TYR:CD1 | 7:G:154:TYR:HE1 | 2.19 | 0.58 |
| 1:A:1274:U:C5' | 9:I:38:GLN:HE22 | 2.16 | 0.58 |
| 16:P:57:ARG:O | 16:P:61:SER:HB3 | 2.03 | 0.58 |
| 17:Q:87:LYS:O | 17:Q:88:TYR:C | 2.41 | 0.58 |
| 20:T:57:ARG:HH21 | 20:T:100:ILE:CG2 | 2.17 | 0.58 |
| 1:A:715:G:O2' | 1:A:716:C:H5' | 2.03 | 0.57 |
| 1:A:931:G:H2' | 1:A:932:G:O4' | 2.04 | 0.57 |
| 2:B:124:SER:O | 2:B:127:ILE:HG13 | 2.04 | 0.57 |
| 3:C:35:GLU:OE2 | 3:C:97:LYS:HG3 | 2.04 | 0.57 |
| 4:D:106:TYR:C | 4:D:106:TYR:CD2 | 2.76 | 0.57 |
| 4:D:36:ARG:HG3 | 4:D:38:TYR:CZ | 2.39 | 0.57 |
| 5:E:8:GLU:HG2 | 5:E:8:GLU:O | 2.04 | 0.57 |
| 13:M:65:LYS:HG3 | 13:M:69:GLU:OE2 | 2.02 | 0.57 |
| 1:A:262:G:O3' | 17:Q:67:LYS:HB2 | 2.04 | 0.57 |
| 20:T:50:GLU:HG3 | 20:T:99:LEU:HD12 | 1.84 | 0.57 |
| 1:A:421:G:O2' | 1:A:422:G:H5' | 2.02 | 0.57 |
| 1:A:50:U:O2 | 1:A:358:G:H1' | 2.04 | 0.57 |
| 2:B:100:GLY:C | 2:B:102:LEU:N | 2.57 | 0.57 |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:HG22 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:10:ARG:HG3 | 4:D:10:ARG:HH11 | 1.69 | 0.57 |
| 4:D:8:VAL:C | 4:D:10:ARG:H | 2.08 | 0.57 |
| 8:H:17:THR:HG22 | 8:H:63:LEU:HG | 1.86 | 0.57 |
| 10:J:3:LYS:C | 10:J:100:THR:HG23 | 2.24 | 0.57 |
| 10:J:51:ARG:H | 10:J:59:SER:HB2 | 1.68 | 0.57 |
| 16:P:39:TYR:CE1 | 16:P:41:PRO:HA | 2.39 | 0.57 |
| 17:Q:60:ILE:HD13 | 17:Q:61:GLU:O | 2.05 | 0.57 |
| 20:T:75:ASN:O | 20:T:78:ALA:HB3 | 2.04 | 0.57 |
| 1:A:41:C:H2' | 1:A:42:G:H8 | 1.69 | 0.57 |
| 2:B:68:ILE:HD12 | 2:B:222:ILE:HD11 | 1.86 | 0.57 |
| 3:C:195:VAL:C | 3:C:196:LEU:HD23 | 2.23 | 0.57 |
| 9:I:86:VAL:O | 9:I:87:GLN:C | 2.41 | 0.57 |
| 1:A:1102:C:O2' | 1:A:1103:G:H5' | 2.03 | 0.57 |
| 1:A:1483:G:H3' | 1:A:1483:G:H8 | 1.69 | 0.57 |
| 1:A:276:C:O2 | 17:Q:38:ARG:HG3 | 2.04 | 0.57 |
| 2:B:140:HIS:O | 2:B:141:GLU:C | 2.41 | 0.57 |
| 2:B:80:ILE:HD11 | 2:B:208:ILE:HG23 | 1.86 | 0.57 |
| 4:D:107:ARG:NH1 | 4:D:114:ARG:NH2 | 2.53 | 0.57 |
| 1:A:855:C:O2' | 8:H:4:ASP:HB2 | 2.03 | 0.57 |
| 10:J:20:ALA:O | 10:J:24:VAL:HG23 | 2.03 | 0.57 |
| 13:M:37:THR:CG2 | 13:M:39:ILE:HD11 | 2.35 | 0.57 |
| 17:Q:67:LYS:CA | 17:Q:70:ARG:HH12 | 2.15 | 0.57 |
| 18:R:40:LEU:HB2 | 18:R:79:LEU:HD11 | 1.87 | 0.57 |
| 1:A:1408:U:H2' | 1:A:1409:C:H6 | 1.69 | 0.57 |
| 1:A:390:G:H2' | 1:A:391:C:C6 | 2.40 | 0.57 |
| 3:C:5:ILE:HD13 | 3:C:10:PHE:HB2 | 1.85 | 0.57 |
| 3:C:150:LYS:HE2 | 3:C:152:ILE:HD11 | 1.85 | 0.57 |
| 3:C:180:ALA:O | 3:C:181:ASN:HB3 | 2.04 | 0.57 |
| 3:C:94:LEU:HD23 | 3:C:95:THR:CG2 | 2.28 | 0.57 |
| 4:D:160:GLN:O | 4:D:163:GLU:HB3 | 2.04 | 0.57 |
| 4:D:145:GLU:HG2 | 4:D:184:LYS:HE2 | 1.86 | 0.57 |
| 5:E:78:HIS:O | 5:E:78:HIS:ND1 | 2.38 | 0.57 |
| 5:E:80:ILE:CD1 | 5:E:91:LEU:HB2 | 2.34 | 0.57 |
| 8:H:113:SER:N | 8:H:134:ILE:HD11 | 2.19 | 0.57 |
| 9:I:27:THR:HG23 | 9:I:30:GLY:O | 2.03 | 0.57 |
| 12:L:39:VAL:HB | 12:L:57:LYS:CG | 2.34 | 0.57 |
| 13:M:77:ASN:O | 13:M:80:ARG:HB3 | 2.04 | 0.57 |
| 1:A:1085:A:O2' | 1:A:1086:C:H5' | 2.04 | 0.57 |
| 1:A:1132:C:OP1 | 9:I:9:ARG:HD3 | 2.03 | 0.57 |
| 1:A:1270:A:O4' | 1:A:1335:G:H4' | 2.05 | 0.57 |
| 1:A:291:C:C4 | 1:A:292:U:C4 | 2.92 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:342:G:H2' | 1:A:343:G:O4' | 2.05 | 0.57 |
| 1:A:850:A:C2 | 1:A:852:G:C6 | 2.92 | 0.57 |
| 1:A:888:C:H2' | 1:A:889:U:C6 | 2.39 | 0.57 |
| 1:A:906:G:O2' | 1:A:907:G:H5' | 2.05 | 0.57 |
| 3:C:72:LYS:O | 3:C:74:GLY:N | 2.38 | 0.57 |
| 5:E:5:ASP:CG | 5:E:6:PHE:H | 2.07 | 0.57 |
| 6:F:95:GLU:H | 6:F:95:GLU:CD | 2.06 | 0.57 |
| 12:L:53:ARG:CB | 12:L:93:LEU:HD11 | 2.35 | 0.57 |
| 12:L:92:ASP:O | 12:L:93:LEU:HD23 | 2.03 | 0.57 |
| 13:M:84:ILE:HG13 | 13:M:86:CYS:HB2 | 1.86 | 0.57 |
| 1:A:1291:G:P | 13:M:88:ARG:HH21 | 2.27 | 0.57 |
| 18:R:59:SER:H | 18:R:62:GLU:HB2 | 1.69 | 0.57 |
| 1:A:1202:G:H2' | 1:A:1203:G:C8 | 2.36 | 0.57 |
| 1:A:1335:G:O2' | 1:A:1336:C:H5' | 2.03 | 0.57 |
| 2:B:74:LYS:NZ | 2:B:206:ASP:HB2 | 2.17 | 0.57 |
| 3:C:14:ILE:CG2 | 3:C:15:THR:H | 2.15 | 0.57 |
| 3:C:33:LEU:HD23 | 3:C:34:LEU:N | 2.19 | 0.57 |
| 12:L:85:ILE:HA | 12:L:99:HIS:O | 2.05 | 0.57 |
| 1:A:1291:G:O2' | 1:A:1292:G:H5' | 2.05 | 0.57 |
| 1:A:190:U:H2' | 17:Q:63:ARG:NH2 | 2.20 | 0.57 |
| 1:A:453:C:C2 | 1:A:454:G:C8 | 2.93 | 0.57 |
| 1:A:515:U:H4' | 1:A:516:A:C5' | 2.33 | 0.57 |
| 1:A:623:G:O2' | 1:A:624:A:H5' | 2.05 | 0.57 |
| 1:A:902:C:H5' | 1:A:1382:C:OP2 | 2.04 | 0.57 |
| 3:C:201:TYR:N | 3:C:201:TYR:HD1 | 2.03 | 0.57 |
| 4:D:150:GLU:O | 4:D:153:ARG:HB2 | 2.04 | 0.57 |
| 7:G:21:VAL:HG23 | 7:G:22:LEU:N | 2.19 | 0.57 |
| 8:H:36:LEU:CD1 | 8:H:61:VAL:HG22 | 2.34 | 0.57 |
| 12:L:83:VAL:HG22 | 12:L:84:LEU:N | 2.20 | 0.57 |
| 16:P:81:ARG:CG | 16:P:83:GLU:HG2 | 2.35 | 0.57 |
| 18:R:17:SER:HA | 18:R:19:LYS:HZ1 | 1.69 | 0.57 |
| 1:A:1437:C:H5'' | 20:T:27:LYS:HZ3 | 1.70 | 0.57 |
| 1:A:410:A:C2 | 1:A:411:A:C4 | 2.93 | 0.57 |
| 2:B:28:PHE:O | 2:B:29:ALA:C | 2.43 | 0.57 |
| 5:E:7:GLU:OE2 | 5:E:37:ARG:NE | 2.23 | 0.57 |
| 13:M:17:VAL:O | 13:M:20:THR:HB | 2.05 | 0.57 |
| 20:T:50:GLU:O | 20:T:100:ILE:HD12 | 2.05 | 0.57 |
| 1:A:744:G:H2' | 1:A:745:G:H5' | 1.87 | 0.57 |
| 2:B:85:ALA:O | 2:B:88:ALA:O | 2.22 | 0.57 |
| 3:C:77:ILE:O | 3:C:83:ARG:HB3 | 2.05 | 0.57 |
| 1:A:1330:U:H4' | 9:I:120:ARG:HD2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:15:VAL:HB | 13:M:34:LEU:HD11 | 1.86 | 0.57 |
| 18:R:59:SER:OG | 18:R:62:GLU:HG3 | 2.05 | 0.57 |
| 1:A:1050:A:H1' | 1:A:1051:G:O4' | 2.04 | 0.56 |
| 1:A:1280:C:H4' | 1:A:1281:A:C8 | 2.40 | 0.56 |
| 1:A:444:C:H3' | 1:A:445:G:H8 | 1.69 | 0.56 |
| 1:A:446:A:H1' | 1:A:447:A:N7 | 2.20 | 0.56 |
| 1:A:812:A:H2' | 1:A:813:G:O4' | 2.05 | 0.56 |
| 2:B:31:TYR:CE1 | 2:B:200:ILE:HD12 | 2.37 | 0.56 |
| 5:E:144:THR:CG2 | 5:E:146:ALA:H | 2.17 | 0.56 |
| 6:F:67:MET:HB2 | 6:F:68:PRO:CD | 2.34 | 0.56 |
| 6:F:82:ARG:HA | 6:F:82:ARG:NE | 2.20 | 0.56 |
| 8:H:86:ILE:O | 8:H:88:LYS:HG3 | 2.05 | 0.56 |
| 1:A:702:G:C4' | 11:K:117:ASN:HD21 | 2.18 | 0.56 |
| 13:M:9:ILE:N | 13:M:9:ILE:HD12 | 2.19 | 0.56 |
| 1:A:1331:A:C2' | 1:A:1332:A:H8 | 2.10 | 0.56 |
| 1:A:1332:A:C2 | 1:A:1333:U:C2 | 2.92 | 0.56 |
| 1:A:778:A:H2' | 1:A:779:C:C6 | 2.40 | 0.56 |
| 2:B:18:GLY:HA3 | 2:B:41:ILE:HA | 1.86 | 0.56 |
| 3:C:3:ASN:O | 3:C:4:LYS:HG2 | 2.04 | 0.56 |
| 13:M:29:ARG:O | 13:M:32:GLU:HB3 | 2.05 | 0.56 |
| 1:A:1301:A:H2' | 1:A:1305:G:N7 | 2.20 | 0.56 |
| 1:A:1328:A:H1' | 1:A:1330:U:C5 | 2.39 | 0.56 |
| 1:A:1473:U:H2' | 1:A:1474:C:C6 | 2.40 | 0.56 |
| 1:A:239:A:H4' | 1:A:240:U:O5' | 2.04 | 0.56 |
| 1:A:353:G:O2' | 1:A:354:U:H5' | 2.03 | 0.56 |
| 3:C:188:LEU:HD13 | 3:C:189:ALA:N | 2.20 | 0.56 |
| 4:D:156:GLU:HG2 | 4:D:160:GLN:HE21 | 1.70 | 0.56 |
| 5:E:48:ALA:HB1 | 5:E:49:PRO:HD2 | 1.86 | 0.56 |
| 5:E:80:ILE:CD1 | 5:E:138:ALA:HB1 | 2.35 | 0.56 |
| 5:E:82:VAL:HG11 | 5:E:137:GLU:HB3 | 1.87 | 0.56 |
| 17:Q:44:ALA:HA | 17:Q:71:PHE:O | 2.04 | 0.56 |
| 1:A:1096:C:O5' | 1:A:1096:C:H6 | 1.87 | 0.56 |
| 1:A:1333:U:O2' | 1:A:1334:C:H5' | 2.05 | 0.56 |
| 1:A:1382:C:O2 | 1:A:1384:G:C5 | 2.59 | 0.56 |
| 1:A:442:G:H2' | 1:A:470:G:H22 | 1.69 | 0.56 |
| 1:A:995:A:H2' | 1:A:996:G:O4' | 2.04 | 0.56 |
| 2:B:106:LYS:O | 2:B:110:GLN:HG3 | 2.04 | 0.56 |
| 2:B:161:ALA:HA | 2:B:182:ILE:HG22 | 1.87 | 0.56 |
| 4:D:114:ARG:O | 4:D:117:ALA:HB3 | 2.05 | 0.56 |
| 14:N:37:PHE:HB3 | 14:N:39:LEU:CD1 | 2.36 | 0.56 |
| 1:A:1178:U:H5'' | 1:A:1179:G:C5' | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:938:U:C2 | 1:A:1207:A:N7 | 2.74 | 0.56 |
| 1:A:1302:C:N3 | 19:S:36:ARG:NH1 | 2.54 | 0.56 |
| 1:A:204:A:H4' | 1:A:205:G:O5' | 2.05 | 0.56 |
| 1:A:483:A:H1' | 1:A:531:A:N6 | 2.20 | 0.56 |
| 1:A:562:C:O2' | 1:A:712:A:N3 | 2.33 | 0.56 |
| 1:A:745:G:C6 | 1:A:746:C:C4 | 2.94 | 0.56 |
| 1:A:781:C:O2' | 1:A:782:G:H5' | 2.06 | 0.56 |
| 1:A:845:G:O2' | 1:A:851:A:N6 | 2.38 | 0.56 |
| 1:A:857:C:H2' | 1:A:858:C:H6 | 1.69 | 0.56 |
| 1:A:870:A:H2' | 1:A:871:C:C6 | 2.40 | 0.56 |
| 1:A:949:G:O2' | 1:A:1348:G:O2' | 2.22 | 0.56 |
| 3:C:35:GLU:O | 3:C:38:ARG:HB2 | 2.05 | 0.56 |
| 4:D:25:ARG:HA | 4:D:28:SER:OG | 2.05 | 0.56 |
| 12:L:34:ARG:O | 12:L:61:THR:HG23 | 2.06 | 0.56 |
| 19:S:80:TYR:CG | 19:S:81:ARG:N | 2.73 | 0.56 |
| 1:A:1207:A:H5' | 1:A:1208:C:OP2 | 2.05 | 0.56 |
| 1:A:1475:G:H1' | 1:A:1496:A:H2 | 1.71 | 0.56 |
| 1:A:211:U:H4' | 1:A:212:G:O5' | 2.04 | 0.56 |
| 1:A:367:G:C2' | 1:A:368:C:H5' | 2.35 | 0.56 |
| 2:B:47:THR:HA | 2:B:202:PRO:HG2 | 1.88 | 0.56 |
| 2:B:48:MET:O | 2:B:51:LEU:N | 2.38 | 0.56 |
| 13:M:52:GLU:HA | 13:M:55:ARG:HE | 1.70 | 0.56 |
| 17:Q:26:GLN:O | 17:Q:27:PHE:HB3 | 2.05 | 0.56 |
| 17:Q:66:SER:O | 17:Q:67:LYS:C | 2.44 | 0.56 |
| 18:R:34:TYR:HA | 18:R:69:THR:HG23 | 1.88 | 0.56 |
| 1:A:1309:C:H2' | 1:A:1310:C:C6 | 2.40 | 0.56 |
| 1:A:1351:G:H4' | 14:N:61:TRP:HZ2 | 1.70 | 0.56 |
| 1:A:208:C:H42 | 1:A:212:G:H1 | 1.53 | 0.56 |
| 1:A:251:G:C1' | 17:Q:16:GLN:HE21 | 2.19 | 0.56 |
| 1:A:674:G:N2 | 1:A:682:G:C6 | 2.74 | 0.56 |
| 1:A:561:G:H1' | 1:A:800:A:N3 | 2.20 | 0.56 |
| 6:F:36:ARG:HH12 | 6:F:38:GLU:HG2 | 1.68 | 0.56 |
| 12:L:126:LYS:H | 12:L:126:LYS:CD | 2.17 | 0.56 |
| 18:R:38:GLU:OE1 | 18:R:38:GLU:N | 2.38 | 0.56 |
| 18:R:76:LEU:O | 18:R:78:LEU:N | 2.39 | 0.56 |
| 20:T:54:LYS:HE2 | 20:T:100:ILE:HD11 | 1.87 | 0.56 |
| 1:A:101:G:C2' | 1:A:102:G:H5' | 2.35 | 0.56 |
| 1:A:1163:G:O2' | 1:A:1164:G:O4' | 2.24 | 0.56 |
| 1:A:1464:G:H2' | 1:A:1465:G:C8 | 2.40 | 0.56 |
| 1:A:334:A:H2' | 1:A:335:C:H6 | 1.70 | 0.56 |
| 1:A:438:C:H2' | 1:A:439:C:C6 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:23:G:H4' | 1:A:863:G:C8 | 2.41 | 0.56 |
| 1:A:994:A:H2' | 1:A:995:A:H8 | 1.70 | 0.56 |
| 2:B:100:GLY:C | 2:B:102:LEU:H | 2.06 | 0.56 |
| 4:D:90:GLY:CA | 4:D:204:ILE:HD11 | 2.36 | 0.56 |
| 6:F:38:GLU:O | 6:F:39:LYS:HB3 | 2.06 | 0.56 |
| 7:G:15:ASP:HB3 | 7:G:19:GLY:H | 1.70 | 0.56 |
| 19:S:10:PHE:C | 19:S:10:PHE:CD2 | 2.79 | 0.56 |
| 1:A:1103:G:O2' | 1:A:1104:U:H5' | 2.05 | 0.56 |
| 1:A:1195:A:N1 | 1:A:1197:G:H1' | 2.20 | 0.56 |
| 1:A:745:G:N2 | 17:Q:105:ALA:HB3 | 2.20 | 0.56 |
| 2:B:17:PHE:HD1 | 2:B:17:PHE:C | 2.09 | 0.56 |
| 5:E:41:VAL:CG2 | 5:E:113:ALA:CA | 2.80 | 0.56 |
| 7:G:113:GLU:H | 7:G:113:GLU:CD | 2.08 | 0.56 |
| 7:G:64:GLN:HG2 | 7:G:128:ALA:HB1 | 1.88 | 0.56 |
| 7:G:69:VAL:O | 7:G:71:PRO:HD3 | 2.06 | 0.56 |
| 8:H:97:VAL:HG13 | 8:H:98:LYS:N | 2.21 | 0.56 |
| 17:Q:19:VAL:HG23 | 17:Q:44:ALA:HB3 | 1.88 | 0.56 |
| 19:S:62:ILE:CD1 | 19:S:66:MET:HG3 | 2.34 | 0.56 |
| 1:A:1002:G:N3 | 1:A:1002:G:H2' | 2.20 | 0.56 |
| 1:A:1318:C:H1' | 1:A:1319:G:N1 | 2.21 | 0.56 |
| 1:A:258:A:C6 | 1:A:259:A:C6 | 2.94 | 0.56 |
| 1:A:273:C:O2' | 1:A:274:G:H5' | 2.06 | 0.56 |
| 1:A:485:C:H1' | 1:A:533:C:H1' | 1.88 | 0.56 |
| 1:A:639:A:C2 | 1:A:738:C:N3 | 2.74 | 0.56 |
| 1:A:79:G:C3' | 1:A:80:U:H5'' | 2.36 | 0.56 |
| 1:A:905:G:C2 | 1:A:906:G:C8 | 2.93 | 0.56 |
| 2:B:98:LEU:HB2 | 2:B:101:MET:CG | 2.36 | 0.56 |
| 3:C:132:ARG:HH22 | 4:D:47:ARG:HH12 | 1.52 | 0.56 |
| 3:C:116:VAL:HG21 | 3:C:202:ILE:HD11 | 1.88 | 0.56 |
| 5:E:139:LEU:HA | 5:E:142:LEU:HG | 1.88 | 0.56 |
| 6:F:3:ARG:HE | 6:F:64:GLN:HE21 | 1.53 | 0.56 |
| 16:P:21:VAL:HG11 | 16:P:59:TRP:CE2 | 2.40 | 0.56 |
| 20:T:76:ALA:HA | 20:T:79:ARG:NH1 | 2.21 | 0.56 |
| 1:A:1069:U:H3 | 1:A:1082:G:N2 | 2.03 | 0.56 |
| 1:A:1486:G:C5 | 1:A:1487:C:C5 | 2.93 | 0.56 |
| 1:A:879:A:N7 | 1:A:880:G:H1' | 2.22 | 0.56 |
| 1:A:896:A:H2' | 1:A:897:A:H8 | 1.70 | 0.56 |
| 1:A:9:A:H1' | 5:E:102:ALA:C | 2.27 | 0.56 |
| 2:B:17:PHE:CD1 | 2:B:17:PHE:C | 2.78 | 0.56 |
| 3:C:188:LEU:CD1 | 3:C:195:VAL:HG13 | 2.30 | 0.56 |
| 4:D:170:VAL:HG12 | 4:D:171:GLY:N | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:75:LEU:O | 6:F:79:LEU:HG | 2.06 | 0.56 |
| 6:F:25:ILE:HD12 | 6:F:82:ARG:HD2 | 1.88 | 0.56 |
| 18:R:19:LYS:O | 18:R:20:ALA:HB2 | 2.06 | 0.56 |
| 1:A:1109:U:P | 1:A:1109:U:H6 | 2.29 | 0.55 |
| 1:A:277:G:HO2' | 1:A:278:A:P | 2.28 | 0.55 |
| 1:A:405:G:OP1 | 4:D:24:GLU:O | 2.24 | 0.55 |
| 6:F:8:ILE:HB | 6:F:61:LEU:HB2 | 1.89 | 0.55 |
| 11:K:19:ALA:CB | 11:K:80:VAL:HG11 | 2.37 | 0.55 |
| 15:O:70:LEU:HD12 | 15:O:78:TYR:HB2 | 1.86 | 0.55 |
| 1:A:231:C:H5' | 17:Q:70:ARG:HG2 | 1.88 | 0.55 |
| 1:A:243:G:OP1 | 17:Q:100:LYS:HE2 | 2.06 | 0.55 |
| 1:A:70:G:H2' | 1:A:71:G:H8 | 1.70 | 0.55 |
| 2:B:174:VAL:O | 2:B:178:ARG:HB2 | 2.07 | 0.55 |
| 2:B:17:PHE:CD1 | 2:B:18:GLY:N | 2.74 | 0.55 |
| 2:B:26:PRO:O | 2:B:28:PHE:N | 2.39 | 0.55 |
| 4:D:38:TYR:HB2 | 4:D:39:PRO:HD2 | 1.88 | 0.55 |
| 5:E:38:GLN:O | 5:E:71:LEU:HD12 | 2.06 | 0.55 |
| 1:A:1328:A:C2' | 7:G:10:ARG:HH22 | 2.16 | 0.55 |
| 7:G:78:ARG:HB2 | 7:G:156:TRP:CZ3 | 2.41 | 0.55 |
| 8:H:96:GLY:O | 8:H:99:GLU:N | 2.26 | 0.55 |
| 9:I:59:PHE:O | 9:I:60:ASP:HB2 | 2.06 | 0.55 |
| 10:J:15:THR:HG23 | 10:J:94:VAL:HG22 | 1.87 | 0.55 |
| 1:A:891:A:P | 12:L:47:LYS:HZ2 | 2.29 | 0.55 |
| 17:Q:94:ASN:O | 17:Q:97:SER:OG | 2.20 | 0.55 |
| 1:A:1173:A:H2' | 1:A:1174:C:C6 | 2.42 | 0.55 |
| 1:A:1307:C:H2' | 1:A:1308:C:C6 | 2.41 | 0.55 |
| 1:A:67:G:H4' | 1:A:168:U:C5 | 2.42 | 0.55 |
| 1:A:75:C:O2' | 1:A:76:G:H5' | 2.06 | 0.55 |
| 2:B:25:ASN:HD22 | 2:B:26:PRO:CD | 2.18 | 0.55 |
| 4:D:118:ARG:O | 4:D:121:VAL:HB | 2.06 | 0.55 |
| 7:G:155:ARG:O | 7:G:156:TRP:CB | 2.54 | 0.55 |
| 13:M:11:ARG:HG2 | 13:M:12:ASN:N | 2.22 | 0.55 |
| 13:M:4:ILE:O | 13:M:5:ALA:O | 2.25 | 0.55 |
| 18:R:86:VAL:O | 18:R:87:ARG:CG | 2.52 | 0.55 |
| 1:A:1290:U:H2' | 1:A:1291:G:H8 | 1.71 | 0.55 |
| 1:A:1453:G:H2' | 1:A:1454:G:H8 | 1.70 | 0.55 |
| 1:A:412:G:C5 | 1:A:413:C:C4 | 2.95 | 0.55 |
| 2:B:35:GLU:O | 2:B:36:ARG:HG3 | 2.05 | 0.55 |
| 3:C:180:ALA:O | 3:C:181:ASN:CB | 2.54 | 0.55 |
| 3:C:35:GLU:CG | 3:C:59:ARG:HH22 | 2.19 | 0.55 |
| 4:D:177:ASP:OD1 | 4:D:177:ASP:O | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:24:ARG:HG2 | 5:E:24:ARG:HH11 | 1.70 | 0.55 |
| 5:E:83:GLU:HG2 | 5:E:88:LYS:HG3 | 1.88 | 0.55 |
| 11:K:123:LYS:O | 11:K:125:PHE:N | 2.39 | 0.55 |
| 11:K:66:LEU:HB3 | 11:K:70:LYS:CE | 2.34 | 0.55 |
| 14:N:14:PRO:HB2 | 14:N:16:PHE:O | 2.05 | 0.55 |
| 16:P:36:ILE:HG13 | 16:P:37:GLY:H | 1.72 | 0.55 |
| 1:A:263:C:OP2 | 17:Q:67:LYS:HD2 | 2.06 | 0.55 |
| 6:F:101:ALA:HA | 18:R:28:GLU:HG3 | 1.89 | 0.55 |
| 1:A:317:A:O2' | 1:A:318:C:H5' | 2.07 | 0.55 |
| 1:A:486:G:H2' | 1:A:487:C:H6 | 1.72 | 0.55 |
| 1:A:545:U:O2' | 1:A:546:C:P | 2.64 | 0.55 |
| 1:A:634:G:O2' | 1:A:635:C:H5' | 2.07 | 0.55 |
| 1:A:826:C:H2' | 1:A:827:C:H6 | 1.71 | 0.55 |
| 4:D:110:PHE:CD1 | 4:D:162:LEU:HD21 | 2.41 | 0.55 |
| 5:E:42:GLY:C | 5:E:62:ALA:HB1 | 2.26 | 0.55 |
| 7:G:36:LYS:O | 7:G:36:LYS:HD3 | 2.06 | 0.55 |
| 11:K:95:ILE:HG21 | 11:K:108:ILE:HD13 | 1.87 | 0.55 |
| 1:A:858:C:C5' | 12:L:12:ARG:HH21 | 2.15 | 0.55 |
| 12:L:33:ARG:HD2 | 12:L:62:SER:HB3 | 1.87 | 0.55 |
| 1:A:959:U:H4' | 14:N:21:TYR:CE2 | 2.42 | 0.55 |
| 16:P:53:VAL:HG23 | 16:P:54:GLU:N | 2.22 | 0.55 |
| 1:A:257:U:O2 | 1:A:259:A:C8 | 2.59 | 0.55 |
| 1:A:463:A:O2' | 1:A:464:C:H5' | 2.06 | 0.55 |
| 1:A:566:U:H2' | 1:A:567:A:O4' | 2.06 | 0.55 |
| 1:A:738:C:O2 | 1:A:738:C:C2' | 2.54 | 0.55 |
| 1:A:836:G:O6 | 1:A:847:G:C8 | 2.60 | 0.55 |
| 1:A:88:C:H2' | 1:A:89:G:H8 | 1.70 | 0.55 |
| 1:A:958:C:H2' | 1:A:959:U:H5' | 1.88 | 0.55 |
| 4:D:71:SER:O | 4:D:73:ARG:N | 2.40 | 0.55 |
| 9:I:92:TYR:O | 9:I:93:ARG:C | 2.45 | 0.55 |
| 9:I:93:ARG:CD | 9:I:97:LYS:HE3 | 2.27 | 0.55 |
| 13:M:14:ARG:CZ | 13:M:42:ALA:HA | 2.37 | 0.55 |
| 20:T:42:GLN:O | 20:T:46:GLU:HG3 | 2.05 | 0.55 |
| 1:A:1128:C:O2' | 1:A:1129:A:C8 | 2.60 | 0.55 |
| 1:A:270:A:O2' | 1:A:271:G:H8 | 1.90 | 0.55 |
| 1:A:846:C:O2' | 1:A:851:A:H2' | 2.07 | 0.55 |
| 1:A:959:U:H5'' | 14:N:21:TYR:CZ | 2.41 | 0.55 |
| 2:B:43:ASP:OD1 | 2:B:43:ASP:C | 2.45 | 0.55 |
| 3:C:5:ILE:CD1 | 3:C:10:PHE:HB2 | 2.36 | 0.55 |
| 4:D:23:GLY:HA3 | 4:D:112:VAL:CG1 | 2.37 | 0.55 |
| 4:D:201:GLN:O | 4:D:205:GLU:HG3 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:70:ILE:HD11 | 4:D:100:ARG:HD2 | 1.89 | 0.55 |
| 5:E:89:ILE:C | 5:E:89:ILE:CD1 | 2.68 | 0.55 |
| 9:I:108:VAL:CG1 | 9:I:109:VAL:H | 2.15 | 0.55 |
| 13:M:81:LEU:HA | 13:M:84:ILE:CD1 | 2.36 | 0.55 |
| 3:C:29:TYR:OH | 14:N:54:PRO:HG2 | 2.06 | 0.55 |
| 1:A:792:C:OP1 | 15:O:48:LYS:HE2 | 2.06 | 0.55 |
| 17:Q:43:LEU:HD11 | 17:Q:68:ARG:HH12 | 1.72 | 0.55 |
| 1:A:410:A:C2 | 1:A:411:A:N9 | 2.75 | 0.55 |
| 1:A:491:C:H2' | 1:A:492:C:C5 | 2.42 | 0.55 |
| 2:B:120:ALA:O | 2:B:122:PHE:N | 2.40 | 0.55 |
| 3:C:112:SER:O | 3:C:113:ALA:C | 2.45 | 0.55 |
| 3:C:15:THR:HG21 | 3:C:179:ARG:O | 2.07 | 0.55 |
| 3:C:64:VAL:O | 3:C:99:VAL:HG23 | 2.06 | 0.55 |
| 4:D:10:ARG:HG3 | 4:D:10:ARG:NH1 | 2.21 | 0.55 |
| 8:H:137:VAL:HG12 | 8:H:138:TRP:N | 2.21 | 0.55 |
| 10:J:25:GLU:O | 10:J:28:ARG:HB2 | 2.07 | 0.55 |
| 10:J:81:THR:O | 10:J:83:GLU:N | 2.39 | 0.55 |
| 11:K:43:SER:HB3 | 11:K:68:ALA:HB2 | 1.89 | 0.55 |
| 13:M:39:ILE:O | 13:M:41:PRO:HD3 | 2.07 | 0.55 |
| 15:O:45:VAL:HG12 | 15:O:46:HIS:H | 1.71 | 0.55 |
| 17:Q:67:LYS:O | 17:Q:68:ARG:CB | 2.50 | 0.55 |
| 1:A:1475:G:H2' | 1:A:1476:U:C6 | 2.37 | 0.55 |
| 1:A:407:A:H1' | 1:A:409:G:H1' | 1.89 | 0.55 |
| 1:A:939:U:C2' | 1:A:940:C:H5' | 2.37 | 0.55 |
| 2:B:120:ALA:C | 2:B:122:PHE:H | 2.09 | 0.55 |
| 3:C:108:ASN:OD1 | 3:C:110:ASN:HB2 | 2.07 | 0.55 |
| 3:C:142:MET:HE1 | 3:C:148:GLY:N | 2.22 | 0.55 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:CG2 | 2.29 | 0.55 |
| 4:D:32:ALA:C | 4:D:34:GLU:N | 2.56 | 0.55 |
| 9:I:33:PHE:CZ | 9:I:46:ALA:HB3 | 2.40 | 0.55 |
| 6:F:94:GLN:NE2 | 18:R:32:ARG:HD3 | 2.22 | 0.55 |
| 1:A:1287:G:OP1 | 21:U:2:GLY:CA | 2.54 | 0.55 |
| 1:A:124:G:O2' | 1:A:125:A:OP2 | 2.23 | 0.55 |
| 1:A:1287:G:N2 | 1:A:1313:G:C2' | 2.69 | 0.55 |
| 1:A:142:G:C2 | 1:A:143:G:C8 | 2.95 | 0.55 |
| 1:A:1485:A:H2' | 1:A:1486:G:C8 | 2.41 | 0.55 |
| 1:A:417:U:H5' | 1:A:418:C:OP2 | 2.07 | 0.55 |
| 2:B:142:LEU:O | 2:B:143:GLU:C | 2.44 | 0.55 |
| 4:D:18:LYS:HB3 | 4:D:20:TYR:HE2 | 1.72 | 0.55 |
| 5:E:107:ARG:O | 5:E:108:ALA:C | 2.44 | 0.55 |
| 7:G:96:GLN:O | 7:G:97:GLN:C | 2.45 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:3:ARG:HA | 13:M:8:GLU:O | 2.07 | 0.55 |
| 10:J:47:PHE:CE2 | 14:N:37:PHE:CE1 | 2.95 | 0.55 |
| 15:O:53:HIS:O | 15:O:56:LEU:HB3 | 2.07 | 0.55 |
| 16:P:9:PHE:HE2 | 16:P:18:ARG:HD2 | 1.70 | 0.55 |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:CB | 2.38 | 0.55 |
| 20:T:49:ALA:O | 20:T:50:GLU:C | 2.44 | 0.55 |
| 1:A:1050:A:O2' | 1:A:1051:G:C8 | 2.56 | 0.54 |
| 1:A:195:U:H2' | 1:A:196:G:C8 | 2.42 | 0.54 |
| 2:B:98:LEU:HB2 | 2:B:101:MET:HG3 | 1.90 | 0.54 |
| 5:E:141:GLN:O | 5:E:143:ARG:HG2 | 2.07 | 0.54 |
| 7:G:67:GLU:HA | 7:G:67:GLU:OE2 | 2.07 | 0.54 |
| 11:K:124:LYS:HB3 | 11:K:125:PHE:CD1 | 2.43 | 0.54 |
| 1:A:691:C:O2 | 11:K:39:PRO:HD3 | 2.07 | 0.54 |
| 12:L:35:GLY:HA3 | 12:L:58:VAL:HG12 | 1.87 | 0.54 |
| 1:A:1172:G:O2' | 1:A:1173:A:P | 2.64 | 0.54 |
| 1:A:1035:U:H2' | 1:A:1182:C:H41 | 1.72 | 0.54 |
| 1:A:11:A:O2' | 1:A:12:G:H5' | 2.07 | 0.54 |
| 1:A:1355:U:OP1 | 9:I:71:SER:HB3 | 2.06 | 0.54 |
| 1:A:1439:G:O2' | 1:A:1440:G:H5' | 2.07 | 0.54 |
| 1:A:475:G:H2' | 1:A:476:G:H8 | 1.72 | 0.54 |
| 1:A:591:A:C2' | 1:A:592:A:H5' | 2.37 | 0.54 |
| 1:A:736:G:O2' | 1:A:737:A:P | 2.65 | 0.54 |
| 3:C:35:GLU:HG2 | 3:C:59:ARG:HH22 | 1.71 | 0.54 |
| 4:D:90:GLY:H | 4:D:204:ILE:HD11 | 1.72 | 0.54 |
| 1:A:856:G:OP1 | 8:H:89:PRO:O | 2.25 | 0.54 |
| 9:I:38:GLN:OE1 | 9:I:39:GLY:N | 2.40 | 0.54 |
| 11:K:33:THR:OG1 | 11:K:37:GLY:C | 2.46 | 0.54 |
| 11:K:48:ILE:HD13 | 11:K:63:LEU:CB | 2.32 | 0.54 |
| 16:P:74:LEU:HB3 | 16:P:79:VAL:CG2 | 2.27 | 0.54 |
| 1:A:378:A:C2 | 1:A:379:A:C4 | 2.95 | 0.54 |
| 1:A:486:G:H2' | 1:A:487:C:O4' | 2.07 | 0.54 |
| 1:A:642:G:O2' | 1:A:643:U:H5' | 2.07 | 0.54 |
| 4:D:29:PRO:C | 4:D:30:LYS:HG3 | 2.28 | 0.54 |
| 8:H:16:ALA:HB3 | 8:H:63:LEU:HD21 | 1.89 | 0.54 |
| 10:J:47:PHE:CE2 | 14:N:37:PHE:HE1 | 2.25 | 0.54 |
| 13:M:40:ASN:HB3 | 13:M:43:THR:HG23 | 1.89 | 0.54 |
| 15:O:32:LEU:O | 15:O:33:THR:C | 2.44 | 0.54 |
| 1:A:1188:G:C6 | 1:A:1189:G:C5 | 2.96 | 0.54 |
| 1:A:1401:A:H3' | 1:A:1402:G:C8 | 2.42 | 0.54 |
| 1:A:1438:A:C2 | 1:A:1439:G:H1' | 2.43 | 0.54 |
| 1:A:904:G:H1 | 22:A:1523:KSG:H6 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:937:A:C3' | 1:A:938:U:H5'' | 2.29 | 0.54 |
| 2:B:137:ARG:HB3 | 2:B:137:ARG:HH11 | 1.71 | 0.54 |
| 2:B:200:ILE:HG22 | 2:B:201:ILE:N | 2.22 | 0.54 |
| 2:B:59:GLU:O | 2:B:60:ASP:C | 2.45 | 0.54 |
| 3:C:8:ILE:O | 3:C:11:ARG:N | 2.40 | 0.54 |
| 4:D:107:ARG:HH12 | 4:D:114:ARG:NH2 | 2.05 | 0.54 |
| 4:D:8:VAL:O | 4:D:11:LEU:HG | 2.07 | 0.54 |
| 6:F:24:GLU:HG3 | 6:F:25:ILE:N | 2.20 | 0.54 |
| 10:J:94:VAL:CG1 | 10:J:95:GLU:N | 2.71 | 0.54 |
| 14:N:12:ARG:O | 14:N:14:PRO:N | 2.40 | 0.54 |
| 15:O:24:SER:O | 15:O:25:THR:C | 2.46 | 0.54 |
| 15:O:66:LEU:O | 15:O:69:TYR:HB3 | 2.08 | 0.54 |
| 17:Q:97:SER:O | 17:Q:98:LEU:HD12 | 2.07 | 0.54 |
| 19:S:15:LEU:HD12 | 19:S:16:LEU:N | 2.22 | 0.54 |
| 1:A:182:C:C2 | 20:T:105:SER:HB3 | 2.42 | 0.54 |
| 20:T:57:ARG:HB2 | 20:T:57:ARG:HH11 | 1.72 | 0.54 |
| 1:A:1329:G:C4 | 9:I:107:ARG:NH1 | 2.75 | 0.54 |
| 1:A:544:U:H4' | 1:A:545:U:C5' | 2.38 | 0.54 |
| 1:A:585:C:H2' | 1:A:586:A:C8 | 2.41 | 0.54 |
| 1:A:855:C:O2' | 8:H:3:THR:HG23 | 2.07 | 0.54 |
| 1:A:923:G:H21 | 1:A:1316:G:H4' | 1.71 | 0.54 |
| 1:A:969:U:O2' | 1:A:970:U:H5' | 2.08 | 0.54 |
| 1:A:980:G:H2' | 1:A:981:G:O4' | 2.07 | 0.54 |
| 2:B:16:HIS:O | 2:B:17:PHE:O | 2.26 | 0.54 |
| 2:B:52:GLU:HG2 | 2:B:56:ARG:HH21 | 1.72 | 0.54 |
| 5:E:37:ARG:HG2 | 5:E:37:ARG:HH11 | 1.72 | 0.54 |
| 6:F:80:ARG:CZ | 6:F:88:VAL:HB | 2.38 | 0.54 |
| 1:A:626:A:N7 | 8:H:115:SER:HA | 2.23 | 0.54 |
| 9:I:69:GLY:O | 9:I:73:GLN:HG3 | 2.08 | 0.54 |
| 1:A:1430:C:O2' | 1:A:1431:U:H5' | 2.08 | 0.54 |
| 1:A:1428:G:N2 | 1:A:1438:A:H1' | 2.22 | 0.54 |
| 1:A:1464:G:H2' | 1:A:1465:G:O4' | 2.08 | 0.54 |
| 1:A:275:A:H5' | 1:A:277:G:O4' | 2.08 | 0.54 |
| 1:A:319:U:OP1 | 20:T:23:ARG:HA | 2.07 | 0.54 |
| 1:A:870:A:O2' | 1:A:1398:G:H4' | 2.07 | 0.54 |
| 2:B:148:TYR:CD2 | 2:B:148:TYR:N | 2.75 | 0.54 |
| 2:B:87:ARG:NH2 | 2:B:233:SER:HB2 | 2.22 | 0.54 |
| 3:C:14:ILE:CG2 | 3:C:15:THR:N | 2.71 | 0.54 |
| 3:C:38:ARG:HH11 | 3:C:38:ARG:HG3 | 1.72 | 0.54 |
| 4:D:10:ARG:NH1 | 4:D:40:PRO:HB2 | 2.21 | 0.54 |
| 7:G:122:HIS:HD2 | 7:G:125:MET:CE | 2.20 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:137:VAL:O | 8:H:138:TRP:HB3 | 2.07 | 0.54 |
| 9:I:93:ARG:HD3 | 9:I:97:LYS:CE | 2.28 | 0.54 |
| 10:J:90:LEU:N | 10:J:91:PRO:HD2 | 2.13 | 0.54 |
| 12:L:60:LEU:N | 12:L:60:LEU:HD22 | 2.23 | 0.54 |
| 14:N:16:PHE:O | 14:N:18:VAL:N | 2.41 | 0.54 |
| 16:P:22:THR:OG1 | 16:P:23:ASP:N | 2.40 | 0.54 |
| 18:R:25:THR:O | 18:R:25:THR:HG22 | 2.08 | 0.54 |
| 1:A:1415:G:H1' | 1:A:1447:G:N2 | 2.22 | 0.54 |
| 1:A:214:C:C4' | 1:A:456:C:N4 | 2.70 | 0.54 |
| 1:A:522:G:O2' | 1:A:523:A:H5' | 2.07 | 0.54 |
| 1:A:740:C:H2' | 1:A:741:U:O4' | 2.06 | 0.54 |
| 2:B:187:LEU:HD13 | 2:B:205:ASP:HA | 1.90 | 0.54 |
| 3:C:167:TRP:O | 3:C:168:ALA:HB2 | 2.06 | 0.54 |
| 4:D:8:VAL:HG13 | 4:D:21:LEU:CD1 | 2.38 | 0.54 |
| 5:E:86:ALA:HB3 | 5:E:125:SER:HB2 | 1.90 | 0.54 |
| 9:I:120:ARG:O | 9:I:122:ALA:N | 2.40 | 0.54 |
| 1:A:1325:G:C1' | 9:I:121:ARG:HH12 | 2.11 | 0.54 |
| 10:J:10:GLY:N | 10:J:16:LEU:HD11 | 2.23 | 0.54 |
| 12:L:119:LYS:O | 12:L:120:TYR:CB | 2.56 | 0.54 |
| 19:S:7:LYS:O | 19:S:7:LYS:HG3 | 2.08 | 0.54 |
| 1:A:1125:G:H2' | 1:A:1126:G:O4' | 2.07 | 0.54 |
| 1:A:124:G:H4' | 1:A:125:A:O5' | 2.08 | 0.54 |
| 1:A:698:G:N3 | 1:A:761:A:H1' | 2.23 | 0.54 |
| 1:A:893:A:H2' | 1:A:894:G:H5' | 1.90 | 0.54 |
| 2:B:134:GLU:O | 2:B:136:VAL:N | 2.41 | 0.54 |
| 3:C:52:LEU:CD2 | 3:C:52:LEU:H | 2.14 | 0.54 |
| 4:D:150:GLU:O | 4:D:153:ARG:N | 2.40 | 0.54 |
| 9:I:44:VAL:O | 9:I:46:ALA:N | 2.41 | 0.54 |
| 10:J:12:ASP:HB3 | 10:J:15:THR:CG2 | 2.37 | 0.54 |
| 13:M:79:LYS:C | 13:M:82:MET:HB3 | 2.27 | 0.54 |
| 17:Q:24:GLU:CD | 17:Q:37:LYS:HD3 | 2.28 | 0.54 |
| 20:T:57:ARG:O | 20:T:58:LYS:C | 2.45 | 0.54 |
| 20:T:72:LEU:CD2 | 20:T:76:ALA:HB3 | 2.38 | 0.54 |
| 1:A:1195:A:C2 | 1:A:1197:G:H1' | 2.43 | 0.54 |
| 1:A:1219:C:C4' | 1:A:1316:G:H21 | 2.21 | 0.54 |
| 1:A:1359:U:H2' | 1:A:1360:A:H8 | 1.70 | 0.54 |
| 1:A:1422:C:P | 20:T:38:LYS:HZ3 | 2.31 | 0.54 |
| 1:A:474:C:O2' | 1:A:475:G:H5' | 2.08 | 0.54 |
| 1:A:542:G:C8 | 1:A:543:A:C2 | 2.96 | 0.54 |
| 1:A:58:G:H2' | 1:A:59:C:C6 | 2.42 | 0.54 |
| 2:B:80:ILE:HG21 | 2:B:212:GLN:HA | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:D:5:ILE:HA | 4:D:115:ARG:HH22 | 1.71 | 0.54 |
| 4:D:179:GLU:O | 4:D:181:MET:N | 2.41 | 0.54 |
| 5:E:10:MET:HE1 | 5:E:13:ILE:HD13 | 1.89 | 0.54 |
| 1:A:637:A:P | 8:H:56:LYS:HZ1 | 2.31 | 0.54 |
| 10:J:19:SER:HB2 | 10:J:91:PRO:HG3 | 1.88 | 0.54 |
| 11:K:34:ASP:C | 11:K:36:ASP:H | 2.11 | 0.54 |
| 13:M:4:ILE:CG2 | 13:M:5:ALA:H | 2.11 | 0.54 |
| 14:N:24:CYS:SG | 14:N:26:ARG:HB3 | 2.48 | 0.54 |
| 14:N:36:PHE:O | 14:N:36:PHE:CD1 | 2.61 | 0.54 |
| 17:Q:97:SER:HB2 | 17:Q:103:GLY:N | 2.23 | 0.54 |
| 19:S:15:LEU:O | 19:S:19:VAL:N | 2.33 | 0.54 |
| 1:A:1096:C:H2' | 1:A:1097:C:H6 | 1.73 | 0.54 |
| 1:A:434:G:C4' | 1:A:435:A:OP1 | 2.50 | 0.54 |
| 1:A:803:A:H4' | 1:A:804:U:OP2 | 2.08 | 0.54 |
| 7:G:20:ASP:OD1 | 7:G:23:VAL:N | 2.38 | 0.54 |
| 7:G:76:ARG:HB2 | 7:G:89:MET:SD | 2.48 | 0.54 |
| 1:A:219:U:H5'' | 20:T:68:LYS:NZ | 2.23 | 0.54 |
| 1:A:1465:G:H2' | 1:A:1466:G:C8 | 2.43 | 0.53 |
| 1:A:1488:U:H2' | 1:A:1489:G:N7 | 2.22 | 0.53 |
| 1:A:55:C:H2' | 1:A:348:C:H41 | 1.73 | 0.53 |
| 1:A:699:A:H2' | 1:A:700:A:O4' | 2.08 | 0.53 |
| 1:A:802:G:O2' | 1:A:804:U:H5 | 1.90 | 0.53 |
| 1:A:826:C:H2' | 1:A:827:C:C6 | 2.43 | 0.53 |
| 1:A:918:C:H2' | 1:A:919:G:H8 | 1.71 | 0.53 |
| 8:H:120:THR:O | 8:H:122:ARG:N | 2.41 | 0.53 |
| 9:I:97:LYS:CE | 9:I:102:LEU:HD12 | 2.34 | 0.53 |
| 9:I:47:LEU:HB3 | 9:I:50:LEU:HD12 | 1.90 | 0.53 |
| 1:A:1135:A:C5' | 10:J:13:HIS:HD2 | 2.19 | 0.53 |
| 10:J:56:HIS:O | 10:J:59:SER:OG | 2.23 | 0.53 |
| 13:M:14:ARG:HB3 | 13:M:16:ASP:OD1 | 2.08 | 0.53 |
| 19:S:81:ARG:O | 19:S:81:ARG:HG2 | 2.07 | 0.53 |
| 1:A:1048:U:H4' | 1:A:1049:C:O5' | 2.09 | 0.53 |
| 1:A:1100:G:O3' | 9:I:104:ARG:NH1 | 2.28 | 0.53 |
| 1:A:1294:G:O2' | 1:A:1295:U:H5' | 2.09 | 0.53 |
| 1:A:1358:A:H2' | 1:A:1359:U:O4' | 2.07 | 0.53 |
| 1:A:444:C:H3' | 1:A:445:G:C8 | 2.43 | 0.53 |
| 1:A:447:A:O2' | 1:A:448:A:O4' | 2.27 | 0.53 |
| 3:C:40:ARG:O | 3:C:44:GLU:HG3 | 2.08 | 0.53 |
| 7:G:76:ARG:O | 7:G:156:TRP:HZ3 | 1.90 | 0.53 |
| 7:G:80:VAL:HB | 7:G:85:TYR:CD1 | 2.43 | 0.53 |
| 9:I:79:LEU:HD13 | 9:I:83:ARG:HG3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:95:LYS:C | 9:I:98:PRO:HD2 | 2.28 | 0.53 |
| 10:J:8:LEU:HD21 | 10:J:96:ILE:HG12 | 1.90 | 0.53 |
| 18:R:17:SER:HA | 18:R:19:LYS:HZ2 | 1.71 | 0.53 |
| 1:A:1010:G:H21 | 1:A:1012:G:H3' | 1.71 | 0.53 |
| 1:A:232:G:C5 | 1:A:233:C:C5 | 2.96 | 0.53 |
| 1:A:508:G:H2' | 1:A:509:C:C6 | 2.43 | 0.53 |
| 2:B:18:GLY:CA | 2:B:41:ILE:HA | 2.38 | 0.53 |
| 3:C:62:ASP:O | 3:C:97:LYS:O | 2.26 | 0.53 |
| 13:M:56:LEU:O | 13:M:60:VAL:HG23 | 2.07 | 0.53 |
| 16:P:73:LEU:O | 16:P:76:GLN:N | 2.38 | 0.53 |
| 1:A:334:A:H2' | 1:A:335:C:C6 | 2.43 | 0.53 |
| 1:A:472:A:C2 | 1:A:473:C:H1' | 2.44 | 0.53 |
| 1:A:730:A:O2' | 1:A:731:C:H5' | 2.09 | 0.53 |
| 1:A:803:A:H5'' | 1:A:804:U:OP2 | 2.08 | 0.53 |
| 1:A:887:A:H2' | 1:A:888:C:O4' | 2.09 | 0.53 |
| 2:B:125:PRO:C | 2:B:127:ILE:H | 2.12 | 0.53 |
| 2:B:88:ALA:C | 2:B:90:MET:N | 2.55 | 0.53 |
| 4:D:162:LEU:HD12 | 4:D:181:MET:HE2 | 1.89 | 0.53 |
| 5:E:53:LEU:O | 5:E:54:ALA:C | 2.46 | 0.53 |
| 7:G:155:ARG:O | 7:G:156:TRP:HB2 | 2.07 | 0.53 |
| 12:L:27:LEU:C | 12:L:29:GLY:N | 2.60 | 0.53 |
| 16:P:32:TYR:CE2 | 16:P:35:LYS:HB2 | 2.43 | 0.53 |
| 1:A:1070:G:H2' | 1:A:1071:G:C8 | 2.43 | 0.53 |
| 1:A:1377:A:C5 | 1:A:1479:C:H4' | 2.44 | 0.53 |
| 1:A:1475:G:O2' | 1:A:1476:U:H5' | 2.09 | 0.53 |
| 1:A:278:A:H3' | 1:A:279:C:C5 | 2.43 | 0.53 |
| 1:A:369:A:C2 | 1:A:467:A:C6 | 2.96 | 0.53 |
| 1:A:418:C:H4' | 1:A:419:G:C4 | 2.44 | 0.53 |
| 1:A:45:G:H2' | 1:A:46:U:C6 | 2.43 | 0.53 |
| 3:C:99:VAL:CG2 | 3:C:100:ALA:N | 2.72 | 0.53 |
| 4:D:70:ILE:CD1 | 4:D:100:ARG:CZ | 2.86 | 0.53 |
| 4:D:88:VAL:O | 4:D:92:VAL:HG23 | 2.08 | 0.53 |
| 5:E:152:ARG:HB3 | 8:H:43:GLY:HA3 | 1.91 | 0.53 |
| 7:G:80:VAL:HG11 | 7:G:154:TYR:CZ | 2.44 | 0.53 |
| 7:G:41:ARG:O | 7:G:44:TYR:N | 2.42 | 0.53 |
| 7:G:8:GLU:OE1 | 7:G:8:GLU:O | 2.26 | 0.53 |
| 9:I:126:SER:C | 9:I:128:ARG:H | 2.12 | 0.53 |
| 12:L:111:LYS:O | 12:L:112:ASP:HB2 | 2.08 | 0.53 |
| 12:L:28:LYS:O | 12:L:29:GLY:C | 2.46 | 0.53 |
| 12:L:59:ARG:NH1 | 12:L:65:GLU:HG2 | 2.22 | 0.53 |
| 15:O:45:VAL:HB | 15:O:46:HIS:ND1 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:S:5:LEU:O | 19:S:6:LYS:CB | 2.57 | 0.53 |
| 1:A:206:G:O2' | 1:A:207:G:H5' | 2.09 | 0.53 |
| 1:A:466:G:O2' | 1:A:467:A:C8 | 2.60 | 0.53 |
| 2:B:170:GLU:O | 2:B:172:ILE:N | 2.42 | 0.53 |
| 4:D:156:GLU:O | 4:D:160:GLN:HG3 | 2.09 | 0.53 |
| 4:D:200:GLU:HG2 | 4:D:201:GLN:H | 1.73 | 0.53 |
| 7:G:113:GLU:CD | 7:G:113:GLU:N | 2.62 | 0.53 |
| 8:H:104:ARG:O | 8:H:107:LEU:N | 2.42 | 0.53 |
| 9:I:43:ALA:HA | 9:I:74:ILE:CD1 | 2.38 | 0.53 |
| 10:J:51:ARG:HB2 | 10:J:59:SER:HB3 | 1.89 | 0.53 |
| 19:S:33:THR:HG22 | 19:S:35:SER:N | 2.22 | 0.53 |
| 20:T:26:ASN:O | 20:T:29:LYS:N | 2.39 | 0.53 |
| 20:T:60:GLU:HA | 20:T:63:ILE:HD12 | 1.89 | 0.53 |
| 1:A:1099:C:O2' | 1:A:1100:G:H5'' | 2.09 | 0.53 |
| 1:A:1481:A:O2' | 1:A:1482:G:OP1 | 2.20 | 0.53 |
| 1:A:181:C:H2' | 1:A:182:C:C6 | 2.43 | 0.53 |
| 1:A:198:G:H2' | 1:A:199:U:H6 | 1.74 | 0.53 |
| 1:A:531:A:C4' | 1:A:532:G:O5' | 2.50 | 0.53 |
| 5:E:128:PRO:O | 5:E:129:ILE:C | 2.44 | 0.53 |
| 5:E:72:GLN:O | 5:E:73:ASN:HB3 | 2.09 | 0.53 |
| 8:H:90:GLY:O | 8:H:91:ARG:HB2 | 2.09 | 0.53 |
| 10:J:7:LYS:HG3 | 10:J:71:LEU:HD22 | 1.91 | 0.53 |
| 11:K:67:ASP:O | 11:K:70:LYS:HB2 | 2.09 | 0.53 |
| 14:N:24:CYS:SG | 14:N:39:LEU:HA | 2.47 | 0.53 |
| 16:P:82:GLN:O | 16:P:82:GLN:HG3 | 2.07 | 0.53 |
| 17:Q:20:THR:HG23 | 17:Q:43:LEU:CD2 | 2.38 | 0.53 |
| 19:S:35:SER:C | 19:S:37:ARG:H | 2.10 | 0.53 |
| 19:S:42:PRO:HA | 19:S:45:VAL:CG2 | 2.37 | 0.53 |
| 1:A:1111:C:H2' | 1:A:1112:C:H5'' | 1.90 | 0.53 |
| 1:A:117:C:OP1 | 1:A:308:C:H5' | 2.09 | 0.53 |
| 1:A:328:G:O2' | 1:A:329:G:H5' | 2.08 | 0.53 |
| 1:A:59:C:H1' | 1:A:384:G:O6 | 2.09 | 0.53 |
| 1:A:51:A:N6 | 1:A:357:G:H4' | 2.23 | 0.53 |
| 1:A:687:G:H3' | 1:A:687:G:OP2 | 2.09 | 0.53 |
| 1:A:899:U:H2' | 1:A:900:G:O4' | 2.08 | 0.53 |
| 2:B:101:MET:HA | 2:B:108:ILE:CD1 | 2.39 | 0.53 |
| 2:B:24:TRP:CG | 2:B:25:ASN:N | 2.74 | 0.53 |
| 5:E:132:ALA:O | 5:E:135:THR:HB | 2.08 | 0.53 |
| 5:E:141:GLN:O | 5:E:142:LEU:C | 2.47 | 0.53 |
| 6:F:52:ILE:HD11 | 18:R:77:GLY:HA3 | 1.91 | 0.53 |
| 10:J:98:ILE:O | 10:J:99:LYS:HG3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:45:PRO:HG2 | 12:L:50:SER:C | 2.29 | 0.53 |
| 19:S:16:LEU:O | 19:S:18:LYS:N | 2.42 | 0.53 |
| 1:A:18:U:H4' | 1:A:1063:A:O4' | 2.09 | 0.53 |
| 1:A:709:G:H2' | 1:A:710:C:H6 | 1.74 | 0.53 |
| 1:A:872:G:H2' | 1:A:873:G:C8 | 2.44 | 0.53 |
| 3:C:140:ARG:HA | 3:C:143:GLU:HB3 | 1.91 | 0.53 |
| 3:C:33:LEU:O | 3:C:34:LEU:C | 2.44 | 0.53 |
| 5:E:57:LYS:O | 5:E:60:TYR:N | 2.42 | 0.53 |
| 9:I:31:GLN:NE2 | 9:I:35:GLU:HG3 | 2.23 | 0.53 |
| 16:P:20:VAL:CG1 | 16:P:21:VAL:N | 2.71 | 0.53 |
| 1:A:1041:G:C5 | 1:A:1042:C:C4 | 2.96 | 0.53 |
| 1:A:1036:G:H2' | 1:A:1181:U:H5 | 1.74 | 0.53 |
| 1:A:1338:G:H2' | 1:A:1339:A:H8 | 1.72 | 0.53 |
| 1:A:18:U:O4' | 1:A:1063:A:H1' | 2.09 | 0.53 |
| 1:A:21:U:H2' | 1:A:22:G:C8 | 2.44 | 0.53 |
| 1:A:546:C:N4 | 1:A:862:U:H2' | 2.23 | 0.53 |
| 1:A:673:C:N4 | 1:A:682:G:H1 | 2.07 | 0.53 |
| 4:D:179:GLU:C | 4:D:181:MET:H | 2.13 | 0.53 |
| 4:D:68:TYR:OH | 4:D:98:GLU:OE1 | 2.21 | 0.53 |
| 7:G:113:GLU:OE2 | 7:G:113:GLU:N | 2.42 | 0.53 |
| 7:G:31:MET:SD | 7:G:34:GLY:HA2 | 2.49 | 0.53 |
| 10:J:38:ILE:HG13 | 10:J:71:LEU:CB | 2.39 | 0.53 |
| 12:L:10:LEU:HD23 | 12:L:10:LEU:N | 2.24 | 0.53 |
| 12:L:32:PHE:HB3 | 12:L:85:ILE:O | 2.10 | 0.53 |
| 13:M:14:ARG:HG2 | 13:M:42:ALA:HA | 1.90 | 0.53 |
| 1:A:1219:C:O3' | 1:A:1282:G:N2 | 2.41 | 0.52 |
| 1:A:670:U:O4 | 1:A:687:G:O2' | 2.19 | 0.52 |
| 4:D:199:ASN:O | 4:D:200:GLU:C | 2.47 | 0.52 |
| 5:E:24:ARG:HG2 | 5:E:24:ARG:NH1 | 2.23 | 0.52 |
| 8:H:48:TYR:HA | 8:H:60:ARG:O | 2.09 | 0.52 |
| 11:K:49:GLY:O | 11:K:50:TYR:O | 2.27 | 0.52 |
| 12:L:59:ARG:CZ | 12:L:65:GLU:HG2 | 2.39 | 0.52 |
| 14:N:14:PRO:CG | 14:N:17:LYS:HA | 2.38 | 0.52 |
| 14:N:3:ARG:O | 14:N:7:ILE:HG13 | 2.09 | 0.52 |
| 15:O:11:VAL:HG21 | 15:O:34:LEU:HD12 | 1.90 | 0.52 |
| 16:P:67:THR:CG2 | 16:P:68:ASP:H | 2.23 | 0.52 |
| 17:Q:29:HIS:CE1 | 17:Q:32:TYR:H | 2.25 | 0.52 |
| 19:S:80:TYR:CD1 | 19:S:81:ARG:N | 2.77 | 0.52 |
| 1:A:1431:U:HO2' | 1:A:1432:A:H8 | 1.57 | 0.52 |
| 1:A:1458:G:O2' | 1:A:1459:U:H5' | 2.09 | 0.52 |
| 1:A:1473:U:H2' | 1:A:1474:C:H6 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:200:C:H2' | 1:A:201:C:C6 | 2.44 | 0.52 |
| 1:A:528:G:C5 | 1:A:529:C:C5 | 2.96 | 0.52 |
| 1:A:35:C:H42 | 1:A:534:G:H1 | 1.57 | 0.52 |
| 1:A:561:G:H1' | 1:A:800:A:C4 | 2.43 | 0.52 |
| 2:B:234:PRO:O | 2:B:237:ALA:HB3 | 2.09 | 0.52 |
| 2:B:53:ARG:HG3 | 2:B:56:ARG:HH12 | 1.73 | 0.52 |
| 10:J:39:PRO:O | 10:J:40:LEU:HB2 | 2.08 | 0.52 |
| 10:J:26:ALA:HB1 | 10:J:84:GLN:HB3 | 1.91 | 0.52 |
| 18:R:29:PHE:CE1 | 18:R:31:LEU:HD23 | 2.45 | 0.52 |
| 18:R:85:LEU:HD12 | 18:R:86:VAL:N | 2.24 | 0.52 |
| 1:A:480:A:H1' | 1:A:481:A:C8 | 2.44 | 0.52 |
| 2:B:75:LYS:HE3 | 2:B:78:GLN:OE1 | 2.09 | 0.52 |
| 3:C:91:LEU:HD23 | 3:C:92:ALA:N | 2.24 | 0.52 |
| 4:D:25:ARG:NH2 | 4:D:30:LYS:HB3 | 2.24 | 0.52 |
| 5:E:9:LYS:CG | 5:E:112:LEU:HD11 | 2.39 | 0.52 |
| 6:F:36:ARG:NH1 | 6:F:38:GLU:HG2 | 2.25 | 0.52 |
| 1:A:486:G:OP1 | 12:L:118:SER:CB | 2.57 | 0.52 |
| 13:M:58:GLU:O | 13:M:62:ASN:HB2 | 2.08 | 0.52 |
| 17:Q:29:HIS:C | 17:Q:29:HIS:ND1 | 2.62 | 0.52 |
| 1:A:1293:G:O6 | 19:S:2:PRO:HB2 | 2.09 | 0.52 |
| 1:A:1048:U:O2' | 1:A:1049:C:OP2 | 2.25 | 0.52 |
| 1:A:1228:C:H2' | 1:A:1229:U:H6 | 1.75 | 0.52 |
| 1:A:1325:G:H2' | 1:A:1326:C:C6 | 2.44 | 0.52 |
| 1:A:1436:G:H8 | 1:A:1436:G:O5' | 1.92 | 0.52 |
| 1:A:335:C:H2' | 1:A:336:U:C6 | 2.44 | 0.52 |
| 1:A:542:G:C4 | 1:A:543:A:C2 | 2.97 | 0.52 |
| 1:A:962:C:O2' | 1:A:963:C:H5' | 2.09 | 0.52 |
| 3:C:33:LEU:HD11 | 14:N:53:LEU:CD2 | 2.40 | 0.52 |
| 3:C:34:LEU:O | 3:C:34:LEU:HD23 | 2.09 | 0.52 |
| 3:C:68:VAL:HG12 | 3:C:70:VAL:HG22 | 1.90 | 0.52 |
| 3:C:6:HIS:NE2 | 3:C:8:ILE:HB | 2.22 | 0.52 |
| 9:I:71:SER:O | 9:I:74:ILE:N | 2.42 | 0.52 |
| 13:M:33:ALA:HA | 13:M:59:TYR:CE2 | 2.44 | 0.52 |
| 21:U:5:ASP:OD1 | 21:U:8:THR:HG23 | 2.09 | 0.52 |
| 1:A:1141:C:H42 | 1:A:1163:G:H1 | 1.56 | 0.52 |
| 1:A:1282:G:O2' | 1:A:1283:U:P | 2.67 | 0.52 |
| 1:A:1325:G:H2' | 1:A:1326:C:O4' | 2.09 | 0.52 |
| 1:A:1382:C:C2 | 1:A:1480:A:N6 | 2.78 | 0.52 |
| 1:A:1422:C:P | 20:T:38:LYS:NZ | 2.83 | 0.52 |
| 1:A:600:G:O2' | 1:A:601:G:H5' | 2.08 | 0.52 |
| 1:A:657:G:O3' | 6:F:87:ARG:NH2 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:737:A:H4' | 1:A:738:C:C5' | 2.39 | 0.52 |
| 1:A:9:A:H1' | 5:E:102:ALA:O | 2.10 | 0.52 |
| 1:A:9:A:H4' | 1:A:10:G:OP1 | 2.09 | 0.52 |
| 1:A:529:C:H5'' | 4:D:72:GLU:HG2 | 1.92 | 0.52 |
| 5:E:87:SER:HB3 | 5:E:131:ILE:CD1 | 2.39 | 0.52 |
| 8:H:28:ALA:O | 8:H:29:SER:HB3 | 2.09 | 0.52 |
| 12:L:84:LEU:O | 12:L:101:VAL:N | 2.33 | 0.52 |
| 13:M:18:ALA:O | 13:M:20:THR:N | 2.43 | 0.52 |
| 15:O:39:LEU:HD13 | 15:O:56:LEU:CB | 2.37 | 0.52 |
| 18:R:38:GLU:HA | 18:R:41:LYS:HE3 | 1.92 | 0.52 |
| 1:A:1151:A:H2' | 1:A:1152:A:C8 | 2.44 | 0.52 |
| 1:A:1263:U:H4' | 1:A:1264:C:OP2 | 2.10 | 0.52 |
| 1:A:271:G:H5' | 17:Q:14:LYS:CB | 2.40 | 0.52 |
| 1:A:715:G:H5' | 1:A:750:A:H4' | 1.90 | 0.52 |
| 1:A:732:C:H1' | 1:A:733:C:C5 | 2.43 | 0.52 |
| 1:A:745:G:C1' | 17:Q:103:GLY:O | 2.58 | 0.52 |
| 1:A:751:A:H2' | 1:A:752:A:C8 | 2.44 | 0.52 |
| 5:E:102:ALA:HB1 | 5:E:120:THR:HG21 | 1.91 | 0.52 |
| 8:H:53:VAL:HB | 8:H:58:TYR:CE1 | 2.45 | 0.52 |
| 11:K:109:VAL:HG22 | 18:R:86:VAL:HA | 1.91 | 0.52 |
| 12:L:59:ARG:HD3 | 12:L:65:GLU:OE2 | 2.10 | 0.52 |
| 16:P:20:VAL:HG21 | 16:P:32:TYR:CD2 | 2.45 | 0.52 |
| 17:Q:66:SER:O | 17:Q:70:ARG:NH1 | 2.42 | 0.52 |
| 20:T:36:LEU:HD12 | 20:T:62:LEU:HD11 | 1.90 | 0.52 |
| 1:A:197:U:O2' | 1:A:198:G:H5' | 2.10 | 0.52 |
| 1:A:224:A:H2' | 1:A:225:U:H6 | 1.73 | 0.52 |
| 1:A:444:C:C5 | 1:A:445:G:C5 | 2.98 | 0.52 |
| 1:A:681:U:O4' | 1:A:770:G:H4' | 2.10 | 0.52 |
| 1:A:838:A:H2' | 1:A:839:G:O4' | 2.09 | 0.52 |
| 1:A:984:A:H2' | 1:A:985:C:C5' | 2.39 | 0.52 |
| 3:C:112:SER:O | 3:C:116:VAL:HG23 | 2.09 | 0.52 |
| 3:C:91:LEU:C | 3:C:91:LEU:HD23 | 2.30 | 0.52 |
| 4:D:118:ARG:HG3 | 4:D:136:PRO:HB3 | 1.92 | 0.52 |
| 6:F:10:LEU:CD1 | 6:F:59:TYR:HB3 | 2.40 | 0.52 |
| 7:G:123:GLU:O | 7:G:127:ALA:HB2 | 2.10 | 0.52 |
| 12:L:59:ARG:CZ | 12:L:65:GLU:CG | 2.87 | 0.52 |
| 14:N:35:ARG:O | 14:N:37:PHE:N | 2.43 | 0.52 |
| 17:Q:62:SER:HB2 | 17:Q:72:ARG:HG3 | 1.92 | 0.52 |
| 18:R:56:THR:OG1 | 18:R:57:GLY:N | 2.43 | 0.52 |
| 21:U:24:ARG:HH11 | 21:U:24:ARG:HG3 | 1.75 | 0.52 |
| 1:A:1334:C:H1' | 1:A:1354:G:N2 | 2.23 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1425:G:H2' | 1:A:1425:G:N3 | 2.25 | 0.52 |
| 1:A:751:A:H2' | 1:A:752:A:H8 | 1.74 | 0.52 |
| 1:A:837:A:H2' | 1:A:838:A:H8 | 1.73 | 0.52 |
| 2:B:12:GLU:OE1 | 2:B:12:GLU:HA | 2.09 | 0.52 |
| 3:C:114:PRO:O | 3:C:117:ALA:HB3 | 2.10 | 0.52 |
| 3:C:22:TRP:O | 3:C:22:TRP:CE3 | 2.63 | 0.52 |
| 4:D:25:ARG:C | 4:D:27:TYR:H | 2.12 | 0.52 |
| 6:F:56:PRO:C | 6:F:57:GLN:HG3 | 2.30 | 0.52 |
| 1:A:582:U:H4' | 8:H:94:TYR:CG | 2.45 | 0.52 |
| 9:I:10:ARG:HD3 | 9:I:105:ASP:HB3 | 1.92 | 0.52 |
| 9:I:121:ARG:C | 9:I:121:ARG:HD3 | 2.30 | 0.52 |
| 9:I:122:ALA:HB1 | 9:I:123:PRO:HD2 | 1.92 | 0.52 |
| 10:J:39:PRO:O | 10:J:40:LEU:CB | 2.57 | 0.52 |
| 11:K:122:LYS:O | 11:K:123:LYS:C | 2.47 | 0.52 |
| 13:M:31:LYS:O | 13:M:35:GLU:HB2 | 2.09 | 0.52 |
| 16:P:11:SER:OG | 16:P:14:ASN:HB3 | 2.10 | 0.52 |
| 20:T:46:GLU:HB3 | 20:T:48:LYS:HZ3 | 1.75 | 0.52 |
| 1:A:1021:C:H2' | 1:A:1022:C:C6 | 2.45 | 0.52 |
| 1:A:1077:G:H5'' | 1:A:1078:U:H5 | 1.75 | 0.52 |
| 1:A:1299:C:O2' | 1:A:1300:A:H5' | 2.10 | 0.52 |
| 1:A:1308:C:OP2 | 21:U:6:ARG:CZ | 2.58 | 0.52 |
| 1:A:270:A:O2' | 1:A:271:G:P | 2.68 | 0.52 |
| 1:A:801:C:H4' | 1:A:802:G:O5' | 2.09 | 0.52 |
| 2:B:147:LYS:HB3 | 2:B:148:TYR:CD2 | 2.45 | 0.52 |
| 2:B:46:LYS:O | 2:B:48:MET:N | 2.43 | 0.52 |
| 1:A:1358:A:H4' | 7:G:29:LYS:HE2 | 1.91 | 0.52 |
| 9:I:121:ARG:NH1 | 9:I:121:ARG:HG2 | 2.22 | 0.52 |
| 10:J:8:LEU:CD2 | 10:J:96:ILE:HG12 | 2.40 | 0.52 |
| 13:M:11:ARG:CG | 13:M:12:ASN:N | 2.73 | 0.52 |
| 3:C:34:LEU:CD1 | 14:N:25:VAL:HG21 | 2.39 | 0.52 |
| 1:A:121:G:N2 | 17:Q:61:GLU:OE1 | 2.42 | 0.52 |
| 17:Q:78:GLU:OE1 | 17:Q:81:ARG:HD2 | 2.09 | 0.52 |
| 20:T:76:ALA:O | 20:T:80:ARG:HG2 | 2.10 | 0.52 |
| 1:A:1328:A:H5' | 9:I:120:ARG:HH12 | 1.75 | 0.52 |
| 1:A:1355:U:O2' | 1:A:1356:G:H5' | 2.10 | 0.52 |
| 1:A:366:C:C2' | 1:A:367:G:H5' | 2.39 | 0.52 |
| 1:A:823:U:O2 | 1:A:823:U:H2' | 2.09 | 0.52 |
| 2:B:132:LYS:HA | 2:B:135:GLN:HB3 | 1.92 | 0.52 |
| 2:B:182:ILE:O | 2:B:183:PRO:C | 2.47 | 0.52 |
| 2:B:78:GLN:O | 2:B:94:ASN:OD1 | 2.28 | 0.52 |
| 8:H:111:ILE:HD12 | 8:H:135:CYS:SG | 2.50 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:53:ARG:HB2 | 12:L:93:LEU:HD11 | 1.92 | 0.52 |
| 3:C:33:LEU:CD1 | 14:N:53:LEU:HD22 | 2.40 | 0.52 |
| 16:P:67:THR:HB | 16:P:70:ALA:HB2 | 1.92 | 0.52 |
| 1:A:1220:A:C8 | 1:A:1285:C:H1' | 2.44 | 0.51 |
| 1:A:1331:A:C4 | 1:A:1332:A:C8 | 2.98 | 0.51 |
| 1:A:1422:C:OP1 | 20:T:38:LYS:NZ | 2.43 | 0.51 |
| 1:A:239:A:C4' | 1:A:240:U:H5' | 2.27 | 0.51 |
| 1:A:366:C:C2 | 1:A:367:G:C8 | 2.99 | 0.51 |
| 1:A:574:C:C2 | 1:A:575:U:C5 | 2.99 | 0.51 |
| 1:A:959:U:H4' | 14:N:21:TYR:CD2 | 2.46 | 0.51 |
| 2:B:126:GLU:O | 2:B:129:GLU:HB2 | 2.11 | 0.51 |
| 4:D:110:PHE:HD1 | 4:D:162:LEU:HD21 | 1.75 | 0.51 |
| 4:D:170:VAL:HG21 | 4:D:176:LEU:HD22 | 1.92 | 0.51 |
| 4:D:158:ILE:CG2 | 4:D:181:MET:HE2 | 2.40 | 0.51 |
| 4:D:61:LYS:HD3 | 4:D:206:PHE:CD2 | 2.46 | 0.51 |
| 4:D:18:LYS:HB3 | 4:D:20:TYR:CE2 | 2.46 | 0.51 |
| 6:F:6:VAL:HG22 | 6:F:90:VAL:HG22 | 1.92 | 0.51 |
| 7:G:44:TYR:O | 7:G:47:CYS:HB2 | 2.10 | 0.51 |
| 14:N:23:ARG:HA | 14:N:30:ALA:HA | 1.92 | 0.51 |
| 14:N:57:ARG:HG2 | 14:N:58:LYS:H | 1.75 | 0.51 |
| 15:O:34:LEU:HD23 | 15:O:34:LEU:C | 2.31 | 0.51 |
| 17:Q:76:LEU:HD23 | 17:Q:77:VAL:N | 2.25 | 0.51 |
| 20:T:45:GLN:HA | 20:T:91:LEU:HD22 | 1.92 | 0.51 |
| 20:T:49:ALA:O | 20:T:52:ALA:N | 2.43 | 0.51 |
| 1:A:1417:A:H2' | 1:A:1418:G:O4' | 2.09 | 0.51 |
| 1:A:307:C:O2' | 1:A:308:C:H5' | 2.09 | 0.51 |
| 1:A:850:A:C2 | 1:A:852:G:C5 | 2.99 | 0.51 |
| 3:C:52:LEU:O | 3:C:53:ALA:HB2 | 2.10 | 0.51 |
| 7:G:110:GLN:OE1 | 7:G:110:GLN:HA | 2.10 | 0.51 |
| 9:I:26:VAL:HA | 9:I:61:ALA:O | 2.10 | 0.51 |
| 13:M:84:ILE:O | 13:M:86:CYS:N | 2.43 | 0.51 |
| 20:T:14:LYS:O | 20:T:18:GLN:HG3 | 2.09 | 0.51 |
| 1:A:1287:G:N2 | 1:A:1313:G:O2' | 2.42 | 0.51 |
| 1:A:23:G:H2' | 1:A:24:C:H6 | 1.72 | 0.51 |
| 1:A:462:G:H2' | 1:A:463:A:H8 | 1.75 | 0.51 |
| 1:A:45:G:H2' | 1:A:46:U:O4' | 2.10 | 0.51 |
| 1:A:541:G:H2' | 1:A:542:G:O4' | 2.11 | 0.51 |
| 1:A:857:C:H2' | 1:A:858:C:C6 | 2.45 | 0.51 |
| 2:B:98:LEU:CB | 2:B:101:MET:SD | 2.93 | 0.51 |
| 2:B:222:ILE:HG22 | 2:B:223:ILE:N | 2.24 | 0.51 |
| 2:B:87:ARG:HD3 | 2:B:234:PRO:HD2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:11:ARG:O | 3:C:12:LEU:C | 2.49 | 0.51 |
| 9:I:127:LYS:HD2 | 9:I:127:LYS:N | 2.26 | 0.51 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:CB | 2.38 | 0.51 |
| 13:M:17:VAL:O | 13:M:20:THR:CB | 2.58 | 0.51 |
| 13:M:60:VAL:O | 13:M:62:ASN:N | 2.43 | 0.51 |
| 14:N:41:ARG:CG | 14:N:41:ARG:NH1 | 2.66 | 0.51 |
| 15:O:75:PRO:O | 15:O:78:TYR:HB3 | 2.09 | 0.51 |
| 18:R:37:VAL:HG21 | 18:R:78:LEU:HB3 | 1.92 | 0.51 |
| 20:T:15:ARG:O | 20:T:18:GLN:N | 2.42 | 0.51 |
| 20:T:33:ILE:HD13 | 20:T:63:ILE:HA | 1.91 | 0.51 |
| 1:A:1149:G:N2 | 1:A:1151:A:H3' | 2.25 | 0.51 |
| 1:A:1328:A:H61 | 1:A:1357:A:H3' | 1.75 | 0.51 |
| 1:A:163:G:O2' | 1:A:164:C:H5' | 2.11 | 0.51 |
| 1:A:276:C:H4' | 1:A:277:G:OP2 | 2.10 | 0.51 |
| 1:A:43:G:C4 | 1:A:44:C:C5 | 2.98 | 0.51 |
| 1:A:982:G:C2 | 1:A:983:A:H1' | 2.44 | 0.51 |
| 1:A:983:A:N7 | 1:A:1020:C:N3 | 2.59 | 0.51 |
| 2:B:23:ARG:O | 2:B:24:TRP:O | 2.28 | 0.51 |
| 3:C:147:LYS:O | 3:C:203:PHE:CD2 | 2.63 | 0.51 |
| 4:D:78:LEU:HB3 | 4:D:93:PHE:HE2 | 1.75 | 0.51 |
| 5:E:136:MET:O | 5:E:139:LEU:N | 2.36 | 0.51 |
| 8:H:24:THR:HG23 | 8:H:24:THR:O | 2.10 | 0.51 |
| 9:I:26:VAL:HB | 9:I:33:PHE:CB | 2.33 | 0.51 |
| 9:I:84:ALA:O | 9:I:86:VAL:N | 2.44 | 0.51 |
| 12:L:92:ASP:C | 12:L:93:LEU:HD23 | 2.30 | 0.51 |
| 18:R:48:GLY:H | 18:R:82:THR:HA | 1.75 | 0.51 |
| 20:T:39:LYS:O | 20:T:43:LEU:HG | 2.11 | 0.51 |
| 21:U:5:ASP:O | 21:U:11:GLY:HA3 | 2.10 | 0.51 |
| 1:A:211:U:H5' | 1:A:212:G:OP1 | 2.10 | 0.51 |
| 1:A:74:G:O2' | 1:A:75:C:H5' | 2.10 | 0.51 |
| 1:A:937:A:H3' | 1:A:938:U:C5' | 2.32 | 0.51 |
| 3:C:155:GLY:HA3 | 3:C:163:ALA:CB | 2.36 | 0.51 |
| 4:D:25:ARG:CZ | 4:D:30:LYS:HB3 | 2.40 | 0.51 |
| 4:D:3:ARG:NH2 | 4:D:74:GLN:OE1 | 2.43 | 0.51 |
| 5:E:43:LEU:C | 5:E:43:LEU:CD2 | 2.78 | 0.51 |
| 8:H:47:GLY:O | 8:H:62:TYR:HB2 | 2.11 | 0.51 |
| 10:J:15:THR:CG2 | 10:J:16:LEU:N | 2.73 | 0.51 |
| 10:J:42:THR:HG23 | 10:J:67:THR:C | 2.30 | 0.51 |
| 10:J:96:ILE:HG22 | 10:J:97:GLU:N | 2.25 | 0.51 |
| 11:K:115:PRO:C | 11:K:117:ASN:H | 2.14 | 0.51 |
| 12:L:117:ARG:O | 12:L:118:SER:C | 2.47 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:26:GLY:O | 13:M:28:ALA:N | 2.43 | 0.51 |
| 13:M:6:GLY:O | 13:M:7:VAL:CG2 | 2.53 | 0.51 |
| 16:P:36:ILE:HG13 | 16:P:37:GLY:N | 2.26 | 0.51 |
| 1:A:263:C:P | 17:Q:67:LYS:HB2 | 2.50 | 0.51 |
| 1:A:1114:G:H1 | 1:A:1126:G:H21 | 1.59 | 0.51 |
| 1:A:1143:G:O2' | 1:A:1144:C:H5' | 2.11 | 0.51 |
| 1:A:198:G:C4 | 20:T:105:SER:HB2 | 2.45 | 0.51 |
| 1:A:470:G:HO2' | 1:A:471:U:H6 | 1.57 | 0.51 |
| 1:A:673:C:OP2 | 11:K:46:GLY:HA3 | 2.10 | 0.51 |
| 1:A:896:A:C6 | 1:A:897:A:C6 | 2.98 | 0.51 |
| 4:D:76:ARG:O | 4:D:79:PHE:HB3 | 2.10 | 0.51 |
| 5:E:133:TYR:O | 5:E:134:ALA:C | 2.49 | 0.51 |
| 5:E:34:VAL:N | 5:E:42:GLY:O | 2.44 | 0.51 |
| 5:E:65:ASN:CG | 5:E:65:ASN:O | 2.49 | 0.51 |
| 6:F:100:ASN:ND2 | 18:R:23:LYS:O | 2.44 | 0.51 |
| 8:H:31:PHE:HE1 | 8:H:118:VAL:CG2 | 2.24 | 0.51 |
| 9:I:118:LYS:O | 9:I:119:ALA:CB | 2.58 | 0.51 |
| 12:L:78:GLN:N | 12:L:81:SER:OG | 2.39 | 0.51 |
| 3:C:12:LEU:HD21 | 14:N:51:GLY:HA3 | 1.92 | 0.51 |
| 15:O:24:SER:O | 15:O:27:VAL:N | 2.43 | 0.51 |
| 17:Q:29:HIS:CE1 | 17:Q:31:LEU:H | 2.29 | 0.51 |
| 1:A:1208:C:H5'' | 13:M:103:THR:CB | 2.40 | 0.51 |
| 1:A:170:C:O2' | 1:A:171:C:H5' | 2.11 | 0.51 |
| 1:A:676:U:H1' | 1:A:679:A:N7 | 2.25 | 0.51 |
| 1:A:804:U:C4' | 1:A:805:G:OP2 | 2.54 | 0.51 |
| 1:A:917:G:C6 | 1:A:918:C:N4 | 2.79 | 0.51 |
| 3:C:120:VAL:O | 3:C:121:ALA:C | 2.49 | 0.51 |
| 5:E:129:ILE:O | 5:E:132:ALA:HB3 | 2.10 | 0.51 |
| 13:M:86:CYS:O | 13:M:89:GLY:N | 2.40 | 0.51 |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:CG | 2.22 | 0.51 |
| 15:O:67:LEU:O | 15:O:70:LEU:N | 2.44 | 0.51 |
| 17:Q:97:SER:O | 17:Q:99:SER:N | 2.43 | 0.51 |
| 1:A:703:C:O2 | 18:R:50:ILE:HG13 | 2.10 | 0.51 |
| 20:T:57:ARG:NH2 | 20:T:100:ILE:HG21 | 2.26 | 0.51 |
| 20:T:82:SER:O | 20:T:86:ARG:HB2 | 2.11 | 0.51 |
| 1:A:126:C:H2' | 1:A:127:C:C6 | 2.46 | 0.51 |
| 1:A:1380:C:OP2 | 5:E:24:ARG:NH2 | 2.44 | 0.51 |
| 1:A:154:G:H2' | 1:A:156:A:OP2 | 2.11 | 0.51 |
| 1:A:209:U:O2' | 1:A:210:U:OP1 | 2.24 | 0.51 |
| 1:A:36:G:H2' | 1:A:37:C:C6 | 2.46 | 0.51 |
| 1:A:480:A:H5' | 1:A:481:A:OP1 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:549:U:C4 | 1:A:550:G:C5 | 2.98 | 0.51 |
| 1:A:547:A:HO2' | 1:A:550:G:HO2' | 1.57 | 0.51 |
| 1:A:591:A:O2' | 1:A:592:A:H5' | 2.11 | 0.51 |
| 1:A:679:A:H2' | 1:A:680:A:C8 | 2.45 | 0.51 |
| 1:A:76:G:O2' | 1:A:77:G:H5' | 2.11 | 0.51 |
| 1:A:864:G:C6 | 1:A:865:G:C5 | 2.99 | 0.51 |
| 2:B:200:ILE:HG22 | 2:B:201:ILE:H | 1.75 | 0.51 |
| 4:D:194:LEU:HD22 | 4:D:194:LEU:N | 2.25 | 0.51 |
| 4:D:78:LEU:CD1 | 4:D:97:LEU:HD23 | 2.41 | 0.51 |
| 4:D:77:ASN:O | 4:D:78:LEU:C | 2.49 | 0.51 |
| 4:D:64:LEU:HD21 | 4:D:94:LEU:HD21 | 1.93 | 0.51 |
| 10:J:75:ILE:HG22 | 10:J:76:ASN:N | 2.25 | 0.51 |
| 13:M:23:TYR:O | 13:M:23:TYR:CG | 2.64 | 0.51 |
| 14:N:27:CYS:SG | 14:N:29:ARG:HB3 | 2.49 | 0.51 |
| 15:O:55:GLY:O | 15:O:58:MET:HB2 | 2.11 | 0.51 |
| 15:O:76:GLU:OE2 | 15:O:80:ALA:HB2 | 2.10 | 0.51 |
| 18:R:66:LEU:HD21 | 18:R:70:ILE:CD1 | 2.41 | 0.51 |
| 1:A:1072:G:N2 | 1:A:1073:U:H1' | 2.26 | 0.51 |
| 1:A:1172:G:H2' | 1:A:1173:A:OP2 | 2.11 | 0.51 |
| 1:A:1299:C:H2' | 1:A:1300:A:O4' | 2.11 | 0.51 |
| 1:A:1309:C:H2' | 1:A:1310:C:H6 | 1.76 | 0.51 |
| 1:A:1397:U:H2' | 1:A:1398:G:H8 | 1.76 | 0.51 |
| 1:A:1443:C:H2' | 1:A:1444:C:O4' | 2.11 | 0.51 |
| 1:A:517:A:O2' | 1:A:519:A:OP2 | 2.27 | 0.51 |
| 1:A:618:C:O2' | 1:A:619:G:H5' | 2.11 | 0.51 |
| 1:A:649:A:N3 | 1:A:716:C:H2' | 2.26 | 0.51 |
| 1:A:732:C:O2' | 1:A:733:C:OP2 | 2.28 | 0.51 |
| 1:A:736:G:H4' | 1:A:738:C:H5 | 1.75 | 0.51 |
| 1:A:959:U:H2' | 1:A:960:U:C5 | 2.46 | 0.51 |
| 2:B:74:LYS:NZ | 2:B:205:ASP:O | 2.42 | 0.51 |
| 2:B:93:VAL:HG22 | 2:B:101:MET:HE1 | 1.93 | 0.51 |
| 3:C:162:GLN:O | 3:C:163:ALA:C | 2.47 | 0.51 |
| 4:D:109:GLY:C | 4:D:111:ALA:N | 2.63 | 0.51 |
| 8:H:1:MET:CG | 8:H:2:LEU:N | 2.73 | 0.51 |
| 11:K:18:ARG:NH1 | 11:K:36:ASP:HA | 2.25 | 0.51 |
| 15:O:4:THR:O | 15:O:5:LYS:C | 2.49 | 0.51 |
| 19:S:35:SER:C | 19:S:37:ARG:N | 2.61 | 0.51 |
| 21:U:20:LYS:HG2 | 21:U:20:LYS:O | 2.10 | 0.51 |
| 1:A:104:C:C4 | 1:A:105:G:C5 | 2.99 | 0.51 |
| 1:A:1032:U:H1' | 1:A:1183:A:N7 | 2.25 | 0.51 |
| 1:A:1270:A:C2 | 1:A:1271:A:C4 | 2.99 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1301:A:H5' | 1:A:1302:C:OP1 | 2.11 | 0.51 |
| 1:A:1329:G:C2' | 1:A:1330:U:OP2 | 2.58 | 0.51 |
| 1:A:1408:U:H2' | 1:A:1409:C:C6 | 2.45 | 0.51 |
| 1:A:271:G:C5' | 17:Q:14:LYS:HD3 | 2.41 | 0.51 |
| 1:A:521:G:H2' | 1:A:522:G:H8 | 1.75 | 0.51 |
| 1:A:522:G:O3' | 12:L:114:LYS:HD3 | 2.11 | 0.51 |
| 1:A:805:G:N1 | 1:A:858:C:C4 | 2.79 | 0.51 |
| 1:A:981:G:N2 | 1:A:1022:C:C2 | 2.79 | 0.51 |
| 5:E:98:THR:N | 5:E:117:ASP:OD1 | 2.41 | 0.51 |
| 7:G:79:ARG:HA | 7:G:83:ALA:O | 2.09 | 0.51 |
| 1:A:1231:C:O2' | 9:I:73:GLN:NE2 | 2.43 | 0.51 |
| 17:Q:27:PHE:HB2 | 17:Q:28:PRO:HD2 | 1.92 | 0.51 |
| 18:R:53:ARG:CG | 18:R:63:GLN:HG2 | 2.37 | 0.51 |
| 18:R:47:THR:HA | 18:R:83:GLU:HB2 | 1.92 | 0.51 |
| 11:K:91:ARG:CD | 18:R:88:LYS:HE2 | 2.38 | 0.51 |
| 1:A:10:G:N2 | 1:A:11:A:C4 | 2.79 | 0.50 |
| 1:A:1307:C:H2' | 1:A:1308:C:H6 | 1.76 | 0.50 |
| 1:A:738:C:H2' | 1:A:738:C:O2 | 2.11 | 0.50 |
| 1:A:796:C:O2' | 1:A:797:U:OP2 | 2.28 | 0.50 |
| 2:B:19:HIS:NE2 | 2:B:206:ASP:HB3 | 2.26 | 0.50 |
| 2:B:53:ARG:O | 2:B:56:ARG:HB3 | 2.10 | 0.50 |
| 3:C:84:ILE:O | 3:C:84:ILE:HG12 | 2.10 | 0.50 |
| 4:D:150:GLU:O | 4:D:151:LYS:C | 2.49 | 0.50 |
| 5:E:128:PRO:HG2 | 5:E:129:ILE:H | 1.76 | 0.50 |
| 7:G:144:MET:O | 7:G:147:ALA:HB3 | 2.11 | 0.50 |
| 7:G:23:VAL:O | 7:G:24:THR:C | 2.49 | 0.50 |
| 8:H:26:VAL:HG22 | 8:H:59:LEU:HB2 | 1.93 | 0.50 |
| 14:N:41:ARG:CG | 14:N:41:ARG:HH11 | 2.08 | 0.50 |
| 16:P:13:HIS:O | 16:P:15:PRO:HD2 | 2.12 | 0.50 |
| 16:P:34:GLU:OE2 | 16:P:55:ARG:HD3 | 2.10 | 0.50 |
| 18:R:28:GLU:OE1 | 18:R:28:GLU:N | 2.44 | 0.50 |
| 19:S:16:LEU:C | 19:S:18:LYS:N | 2.64 | 0.50 |
| 19:S:34:TRP:O | 19:S:36:ARG:N | 2.41 | 0.50 |
| 20:T:51:GLU:HA | 20:T:54:LYS:HB2 | 1.93 | 0.50 |
| 1:A:170:C:H2' | 1:A:171:C:C6 | 2.44 | 0.50 |
| 1:A:324:C:O2' | 1:A:325:A:P | 2.68 | 0.50 |
| 1:A:368:C:N4 | 1:A:384:G:OP2 | 2.44 | 0.50 |
| 1:A:892:A:O2' | 1:A:893:A:H5' | 2.11 | 0.50 |
| 2:B:101:MET:HA | 2:B:108:ILE:HD12 | 1.92 | 0.50 |
| 4:D:203:VAL:O | 4:D:206:PHE:HB3 | 2.10 | 0.50 |
| 4:D:57:ARG:HH22 | 5:E:107:ARG:HD3 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:51:VAL:O | 8:H:58:TYR:N | 2.43 | 0.50 |
| 8:H:63:LEU:HB3 | 8:H:65:TYR:CE1 | 2.46 | 0.50 |
| 8:H:83:ILE:HG13 | 8:H:137:VAL:CG2 | 2.35 | 0.50 |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:H | 1.76 | 0.50 |
| 17:Q:104:LYS:O | 17:Q:105:ALA:HB2 | 2.11 | 0.50 |
| 1:A:1408:U:O2' | 1:A:1409:C:H5' | 2.10 | 0.50 |
| 1:A:281:G:O2' | 1:A:282:G:H5' | 2.11 | 0.50 |
| 1:A:390:G:H2' | 1:A:391:C:H6 | 1.75 | 0.50 |
| 1:A:493:A:O5' | 1:A:493:A:H8 | 1.94 | 0.50 |
| 1:A:63:U:H2' | 1:A:64:C:C6 | 2.47 | 0.50 |
| 1:A:720:C:H2' | 1:A:721:A:H8 | 1.73 | 0.50 |
| 2:B:142:LEU:HA | 2:B:146:GLN:HE22 | 1.74 | 0.50 |
| 2:B:204:ASN:ND2 | 2:B:206:ASP:N | 2.56 | 0.50 |
| 2:B:213:LEU:HD23 | 2:B:213:LEU:C | 2.31 | 0.50 |
| 11:K:85:ARG:HE | 11:K:111:ASP:HB3 | 1.77 | 0.50 |
| 13:M:4:ILE:O | 13:M:5:ALA:C | 2.49 | 0.50 |
| 17:Q:74:LEU:HD23 | 17:Q:74:LEU:C | 2.31 | 0.50 |
| 19:S:22:LEU:HD21 | 19:S:28:LYS:HD2 | 1.93 | 0.50 |
| 19:S:11:VAL:HA | 19:S:38:SER:HB2 | 1.92 | 0.50 |
| 1:A:172:C:P | 20:T:65:LYS:NZ | 2.85 | 0.50 |
| 1:A:1290:U:OP1 | 13:M:98:VAL:N | 2.43 | 0.50 |
| 1:A:536:U:H2' | 1:A:537:A:H8 | 1.77 | 0.50 |
| 1:A:763:C:N4 | 1:A:764:A:C6 | 2.79 | 0.50 |
| 1:A:868:G:O2' | 1:A:869:U:OP2 | 2.29 | 0.50 |
| 2:B:20:GLU:CG | 2:B:189:ASP:OD2 | 2.60 | 0.50 |
| 4:D:10:ARG:CG | 4:D:10:ARG:HH11 | 2.25 | 0.50 |
| 4:D:64:LEU:HD12 | 4:D:75:PHE:CE1 | 2.47 | 0.50 |
| 5:E:93:PRO:CG | 8:H:105:ARG:HE | 2.25 | 0.50 |
| 6:F:8:ILE:HD11 | 6:F:79:LEU:HD13 | 1.92 | 0.50 |
| 9:I:100:GLY:C | 9:I:102:LEU:N | 2.65 | 0.50 |
| 12:L:49:ASN:N | 12:L:49:ASN:HD22 | 2.08 | 0.50 |
| 13:M:15:VAL:O | 13:M:18:ALA:HB3 | 2.12 | 0.50 |
| 16:P:11:SER:O | 16:P:14:ASN:N | 2.39 | 0.50 |
| 19:S:39:THR:HA | 19:S:70:LYS:HG2 | 1.94 | 0.50 |
| 1:A:1249:C:O2 | 21:U:20:LYS:HD3 | 2.12 | 0.50 |
| 1:A:484:G:N2 | 1:A:530:G:H1' | 2.27 | 0.50 |
| 1:A:741:U:O2' | 1:A:857:C:H1' | 2.11 | 0.50 |
| 1:A:982:G:C6 | 1:A:983:A:N3 | 2.79 | 0.50 |
| 2:B:196:LEU:N | 2:B:196:LEU:HD23 | 2.27 | 0.50 |
| 2:B:33:TYR:O | 2:B:34:ALA:HB2 | 2.11 | 0.50 |
| 4:D:161:ASN:O | 4:D:162:LEU:C | 2.49 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:64:LEU:HD23 | 4:D:198:VAL:CB | 2.40 | 0.50 |
| 1:A:1280:C:C4 | 7:G:114:ARG:HD3 | 2.46 | 0.50 |
| 1:A:485:C:O3' | 12:L:118:SER:HB2 | 2.12 | 0.50 |
| 13:M:26:GLY:O | 13:M:27:LYS:C | 2.49 | 0.50 |
| 13:M:40:ASN:O | 13:M:43:THR:HG23 | 2.12 | 0.50 |
| 18:R:34:TYR:CD2 | 18:R:34:TYR:N | 2.78 | 0.50 |
| 21:U:17:THR:O | 21:U:22:ARG:HD3 | 2.12 | 0.50 |
| 1:A:232:G:C6 | 1:A:233:C:C4 | 2.99 | 0.50 |
| 2:B:126:GLU:HG2 | 2:B:129:GLU:OE1 | 2.11 | 0.50 |
| 4:D:200:GLU:HG2 | 4:D:201:GLN:N | 2.27 | 0.50 |
| 2:B:178:ARG:HH21 | 8:H:74:PRO:HG3 | 1.77 | 0.50 |
| 14:N:18:VAL:O | 14:N:20:ALA:N | 2.39 | 0.50 |
| 14:N:24:CYS:N | 14:N:33:VAL:HG11 | 2.27 | 0.50 |
| 15:O:32:LEU:CD1 | 15:O:63:ARG:HB2 | 2.42 | 0.50 |
| 15:O:46:HIS:O | 15:O:48:LYS:N | 2.45 | 0.50 |
| 1:A:1298:G:N2 | 1:A:1300:A:H3' | 2.27 | 0.50 |
| 1:A:736:G:O2' | 1:A:737:A:O5' | 2.30 | 0.50 |
| 1:A:866:G:N1 | 1:A:867:A:N6 | 2.60 | 0.50 |
| 1:A:976:G:O2' | 1:A:977:C:H5' | 2.11 | 0.50 |
| 2:B:97:TRP:CH2 | 2:B:176:GLU:CD | 2.83 | 0.50 |
| 5:E:15:ARG:O | 5:E:16:THR:CG2 | 2.58 | 0.50 |
| 1:A:723:C:P | 6:F:2:ARG:HH22 | 2.35 | 0.50 |
| 10:J:81:THR:C | 10:J:83:GLU:N | 2.65 | 0.50 |
| 15:O:32:LEU:O | 15:O:34:LEU:N | 2.45 | 0.50 |
| 1:A:1062:G:H2' | 1:A:1063:A:C8 | 2.47 | 0.50 |
| 1:A:231:C:H2' | 1:A:232:G:H8 | 1.77 | 0.50 |
| 1:A:528:G:H2' | 1:A:529:C:H6 | 1.77 | 0.50 |
| 1:A:536:U:H2' | 1:A:537:A:C8 | 2.46 | 0.50 |
| 1:A:609:G:C4 | 1:A:610:U:C5 | 2.99 | 0.50 |
| 1:A:745:G:O2' | 17:Q:104:LYS:HA | 2.11 | 0.50 |
| 3:C:130:VAL:O | 3:C:134:ILE:HG13 | 2.12 | 0.50 |
| 3:C:79:ARG:HG3 | 3:C:82:GLU:HB3 | 1.94 | 0.50 |
| 4:D:137:SER:O | 4:D:138:TYR:C | 2.48 | 0.50 |
| 6:F:22:GLU:OE2 | 6:F:84:ASN:HB2 | 2.11 | 0.50 |
| 7:G:42:ILE:CG2 | 7:G:120:ILE:HD12 | 2.40 | 0.50 |
| 11:K:34:ASP:CG | 11:K:38:ASN:HB2 | 2.32 | 0.50 |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA | 1.93 | 0.50 |
| 13:M:81:LEU:HA | 13:M:84:ILE:HD11 | 1.94 | 0.50 |
| 15:O:82:ILE:O | 15:O:85:LEU:N | 2.36 | 0.50 |
| 20:T:57:ARG:HD2 | 20:T:103:GLY:H | 1.77 | 0.50 |
| 1:A:1342:A:H2' | 1:A:1343:G:C8 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:212:G:H2' | 1:A:213:C:H6 | 1.77 | 0.50 |
| 1:A:289:G:C6 | 1:A:290:U:C4 | 3.00 | 0.50 |
| 1:A:298:G:N3 | 1:A:540:C:H4' | 2.27 | 0.50 |
| 2:B:142:LEU:CB | 2:B:146:GLN:HE22 | 2.25 | 0.50 |
| 3:C:10:PHE:CE2 | 3:C:178:LEU:HD13 | 2.46 | 0.50 |
| 3:C:178:LEU:O | 3:C:179:ARG:HB2 | 2.12 | 0.50 |
| 4:D:103:ASN:O | 4:D:106:TYR:HB3 | 2.12 | 0.50 |
| 7:G:65:ALA:HB1 | 7:G:127:ALA:CB | 2.42 | 0.50 |
| 9:I:86:VAL:HG13 | 9:I:90:PRO:HA | 1.94 | 0.50 |
| 9:I:93:ARG:O | 9:I:96:LEU:N | 2.45 | 0.50 |
| 12:L:27:LEU:C | 12:L:29:GLY:H | 2.15 | 0.50 |
| 16:P:8:ARG:HG2 | 16:P:17:TYR:HE2 | 1.75 | 0.50 |
| 18:R:65:ILE:O | 18:R:67:ALA:N | 2.45 | 0.50 |
| 19:S:47:HIS:H | 19:S:62:ILE:CG2 | 2.25 | 0.50 |
| 1:A:1099:C:C2' | 1:A:1100:G:H5'' | 2.42 | 0.49 |
| 1:A:1230:A:H1' | 9:I:70:LYS:HZ3 | 1.76 | 0.49 |
| 1:A:1292:G:C2 | 1:A:1310:C:N3 | 2.80 | 0.49 |
| 1:A:654:G:C2 | 1:A:721:A:C2 | 3.00 | 0.49 |
| 1:A:639:A:C2 | 1:A:738:C:N4 | 2.80 | 0.49 |
| 1:A:84:A:H2' | 1:A:85:C:O4' | 2.12 | 0.49 |
| 2:B:80:ILE:HD13 | 2:B:212:GLN:HB2 | 1.94 | 0.49 |
| 3:C:201:TYR:O | 3:C:202:ILE:HG13 | 2.13 | 0.49 |
| 1:A:856:G:C5' | 8:H:89:PRO:HG2 | 2.42 | 0.49 |
| 12:L:39:VAL:HB | 12:L:57:LYS:HG2 | 1.93 | 0.49 |
| 13:M:62:ASN:O | 13:M:63:THR:CB | 2.52 | 0.49 |
| 17:Q:86:GLU:O | 17:Q:87:LYS:C | 2.49 | 0.49 |
| 1:A:1205:C:OP1 | 1:A:1206:G:H3' | 2.12 | 0.49 |
| 1:A:1227:A:H2' | 1:A:1228:C:C6 | 2.47 | 0.49 |
| 22:A:1524:KSG:O6 | 22:A:1524:KSG:H1 | 2.13 | 0.49 |
| 1:A:222:G:C6 | 1:A:223:G:N7 | 2.80 | 0.49 |
| 1:A:238:C:H2' | 1:A:239:A:H5' | 1.94 | 0.49 |
| 1:A:311:A:H4' | 1:A:349:A:N1 | 2.27 | 0.49 |
| 1:A:338:C:H2' | 1:A:339:U:O4' | 2.12 | 0.49 |
| 1:A:341:C:H4' | 1:A:342:G:C5' | 2.42 | 0.49 |
| 1:A:385:A:C6 | 1:A:386:C:H1' | 2.47 | 0.49 |
| 1:A:540:C:O2' | 1:A:541:G:H5' | 2.11 | 0.49 |
| 1:A:820:G:C6 | 1:A:829:G:C6 | 3.00 | 0.49 |
| 1:A:90:U:H2' | 1:A:91:G:H8 | 1.77 | 0.49 |
| 1:A:1087:G:OP1 | 2:B:111:ARG:HD2 | 2.11 | 0.49 |
| 3:C:119:ARG:HG2 | 3:C:140:ARG:HH12 | 1.76 | 0.49 |
| 4:D:162:LEU:O | 4:D:165:MET:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:62:GLN:O | 4:D:63:LYS:C | 2.50 | 0.49 |
| 5:E:11:ILE:HG22 | 5:E:31:LEU:CB | 2.42 | 0.49 |
| 8:H:20:TYR:HA | 8:H:65:TYR:CZ | 2.48 | 0.49 |
| 17:Q:91:ARG:O | 17:Q:92:ARG:C | 2.49 | 0.49 |
| 18:R:53:ARG:HH12 | 18:R:59:SER:HA | 1.76 | 0.49 |
| 1:A:1047:G:O2' | 1:A:1172:G:N2 | 2.45 | 0.49 |
| 1:A:1258:G:O5' | 1:A:1258:G:H8 | 1.96 | 0.49 |
| 1:A:434:G:O3' | 1:A:478:G:N1 | 2.45 | 0.49 |
| 1:A:850:A:C4' | 1:A:851:A:OP1 | 2.58 | 0.49 |
| 1:A:918:C:H2' | 1:A:919:G:C8 | 2.47 | 0.49 |
| 3:C:42:LEU:O | 3:C:45:LYS:N | 2.44 | 0.49 |
| 4:D:78:LEU:HD13 | 4:D:97:LEU:HD23 | 1.94 | 0.49 |
| 5:E:144:THR:HG22 | 5:E:146:ALA:N | 2.26 | 0.49 |
| 13:M:15:VAL:CG1 | 13:M:34:LEU:HD11 | 2.42 | 0.49 |
| 16:P:48:TRP:CE3 | 16:P:49:LEU:HB2 | 2.47 | 0.49 |
| 17:Q:82:MET:C | 17:Q:84:LEU:N | 2.65 | 0.49 |
| 18:R:45:SER:OG | 18:R:49:LYS:HB2 | 2.12 | 0.49 |
| 20:T:10:LEU:C | 20:T:12:ALA:H | 2.15 | 0.49 |
| 1:A:202:A:H2' | 1:A:203:A:C8 | 2.47 | 0.49 |
| 1:A:246:A:C2 | 1:A:270:A:C6 | 3.00 | 0.49 |
| 1:A:296:A:H2' | 1:A:297:G:O4' | 2.12 | 0.49 |
| 1:A:341:C:H4' | 1:A:342:G:H5'' | 1.94 | 0.49 |
| 1:A:39:G:C2 | 1:A:393:A:C2 | 3.00 | 0.49 |
| 1:A:605:A:O5' | 1:A:605:A:H8 | 1.95 | 0.49 |
| 2:B:126:GLU:HA | 2:B:129:GLU:HG3 | 1.94 | 0.49 |
| 2:B:46:LYS:O | 2:B:49:GLU:N | 2.46 | 0.49 |
| 5:E:40:ARG:CG | 5:E:40:ARG:HH11 | 2.23 | 0.49 |
| 8:H:5:PRO:O | 8:H:8:ASP:HB3 | 2.11 | 0.49 |
| 8:H:91:ARG:CG | 12:L:7:ILE:HG13 | 2.39 | 0.49 |
| 12:L:111:LYS:O | 12:L:112:ASP:CB | 2.60 | 0.49 |
| 12:L:117:ARG:C | 12:L:119:LYS:N | 2.66 | 0.49 |
| 12:L:9:GLN:O | 12:L:10:LEU:C | 2.50 | 0.49 |
| 1:A:1078:U:H2' | 1:A:1079:C:O4' | 2.12 | 0.49 |
| 1:A:382:C:C2' | 1:A:383:U:H5' | 2.42 | 0.49 |
| 1:A:470:G:C2' | 1:A:471:U:OP2 | 2.60 | 0.49 |
| 1:A:795:C:H4' | 1:A:878:A:N6 | 2.27 | 0.49 |
| 1:A:510:C:OP1 | 1:A:891:A:H3' | 2.12 | 0.49 |
| 1:A:952:A:C4 | 14:N:31:ARG:NH2 | 2.81 | 0.49 |
| 2:B:44:LEU:O | 2:B:45:GLN:C | 2.50 | 0.49 |
| 3:C:118:GLN:O | 3:C:121:ALA:HB3 | 2.12 | 0.49 |
| 3:C:119:ARG:CG | 3:C:140:ARG:HH12 | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 6:F:56:PRO:O | 6:F:57:GLN:HG3 | 2.11 | 0.49 |
| 8:H:52:ASP:HA | 8:H:56:LYS:O | 2.12 | 0.49 |
| 13:M:80:ARG:C | 13:M:82:MET:N | 2.65 | 0.49 |
| 1:A:1110:G:N1 | 1:A:1128:C:N3 | 2.59 | 0.49 |
| 1:A:1192:C:H5' | 1:A:1196:C:N4 | 2.28 | 0.49 |
| 1:A:1429:C:C2 | 1:A:1430:C:C5 | 3.01 | 0.49 |
| 1:A:208:C:N4 | 1:A:210:U:H1' | 2.27 | 0.49 |
| 1:A:324:C:H4' | 1:A:325:A:C5' | 2.41 | 0.49 |
| 1:A:397:C:O2' | 1:A:398:G:H5' | 2.13 | 0.49 |
| 1:A:670:U:H2' | 1:A:671:A:C8 | 2.47 | 0.49 |
| 1:A:702:G:O4' | 11:K:117:ASN:ND2 | 2.45 | 0.49 |
| 1:A:739:G:OP2 | 15:O:65:ARG:CG | 2.61 | 0.49 |
| 1:A:823:U:O2 | 1:A:823:U:C2' | 2.61 | 0.49 |
| 1:A:970:U:O2' | 1:A:971:G:OP2 | 2.28 | 0.49 |
| 2:B:15:VAL:HG11 | 2:B:209:ARG:C | 2.33 | 0.49 |
| 3:C:38:ARG:HG3 | 3:C:38:ARG:NH1 | 2.27 | 0.49 |
| 4:D:194:LEU:H | 4:D:194:LEU:HD22 | 1.77 | 0.49 |
| 4:D:54:TYR:O | 4:D:55:ALA:C | 2.50 | 0.49 |
| 4:D:65:ARG:NE | 4:D:72:GLU:HA | 2.27 | 0.49 |
| 5:E:102:ALA:CB | 5:E:120:THR:HG21 | 2.42 | 0.49 |
| 7:G:107:ALA:O | 7:G:108:ALA:C | 2.50 | 0.49 |
| 9:I:18:PHE:HB2 | 9:I:62:TYR:O | 2.12 | 0.49 |
| 9:I:80:GLY:O | 9:I:81:ILE:C | 2.50 | 0.49 |
| 12:L:113:ARG:CB | 12:L:122:THR:HG21 | 2.43 | 0.49 |
| 13:M:54:VAL:O | 13:M:55:ARG:C | 2.51 | 0.49 |
| 20:T:63:ILE:O | 20:T:66:ALA:N | 2.35 | 0.49 |
| 1:A:1113:A:P | 1:A:1114:G:OP2 | 2.71 | 0.49 |
| 1:A:1204:G:O2' | 1:A:1205:C:H5' | 2.13 | 0.49 |
| 1:A:1313:G:C2' | 1:A:1314:A:OP2 | 2.60 | 0.49 |
| 1:A:199:U:H4' | 20:T:102:GLY:C | 2.33 | 0.49 |
| 1:A:21:U:H2' | 1:A:22:G:H8 | 1.77 | 0.49 |
| 1:A:373:G:P | 16:P:5:ARG:HH11 | 2.36 | 0.49 |
| 1:A:581:G:C8 | 1:A:582:U:C5 | 3.00 | 0.49 |
| 1:A:768:C:C2 | 1:A:769:G:C8 | 3.01 | 0.49 |
| 1:A:791:A:C4 | 1:A:792:C:C5 | 3.00 | 0.49 |
| 1:A:981:G:C2 | 1:A:982:G:C6 | 3.01 | 0.49 |
| 2:B:120:ALA:C | 2:B:122:PHE:N | 2.66 | 0.49 |
| 2:B:12:GLU:C | 2:B:14:GLY:N | 2.64 | 0.49 |
| 3:C:145:GLY:O | 3:C:146:ALA:HB3 | 2.12 | 0.49 |
| 3:C:147:LYS:HE2 | 3:C:205:GLY:HA2 | 1.94 | 0.49 |
| 3:C:155:GLY:HA2 | 3:C:164:ARG:H | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:186:PHE:CD1 | 3:C:187:ALA:N | 2.80 | 0.49 |
| 3:C:70:VAL:O | 3:C:106:VAL:HG23 | 2.12 | 0.49 |
| 4:D:191:ARG:NH2 | 4:D:198:VAL:O | 2.44 | 0.49 |
| 4:D:61:LYS:HD2 | 4:D:207:TYR:CZ | 2.48 | 0.49 |
| 4:D:88:VAL:O | 4:D:89:THR:C | 2.50 | 0.49 |
| 12:L:79:GLU:HB3 | 12:L:80:HIS:CE1 | 2.48 | 0.49 |
| 13:M:117:VAL:HG12 | 13:M:118:ALA:N | 2.23 | 0.49 |
| 19:S:16:LEU:HA | 19:S:19:VAL:HG12 | 1.94 | 0.49 |
| 1:A:1173:A:H2' | 1:A:1174:C:H6 | 1.78 | 0.49 |
| 1:A:1044:G:C2 | 1:A:1179:G:N3 | 2.81 | 0.49 |
| 1:A:1358:A:C6 | 1:A:1359:U:N3 | 2.81 | 0.49 |
| 1:A:166:A:O2' | 1:A:167:A:H5' | 2.13 | 0.49 |
| 1:A:497:C:O2' | 1:A:498:C:H5' | 2.12 | 0.49 |
| 1:A:620:U:H2' | 1:A:621:G:C8 | 2.46 | 0.49 |
| 1:A:667:G:H2' | 1:A:668:A:C8 | 2.48 | 0.49 |
| 1:A:762:G:C2' | 1:A:763:C:H5' | 2.43 | 0.49 |
| 3:C:191:THR:HG22 | 3:C:192:THR:N | 2.27 | 0.49 |
| 3:C:3:ASN:O | 3:C:4:LYS:CG | 2.61 | 0.49 |
| 5:E:141:GLN:O | 5:E:142:LEU:O | 2.30 | 0.49 |
| 5:E:89:ILE:HD12 | 5:E:91:LEU:HG | 1.95 | 0.49 |
| 6:F:38:GLU:OE1 | 6:F:66:GLU:HB2 | 2.13 | 0.49 |
| 8:H:14:ARG:O | 8:H:17:THR:OG1 | 2.30 | 0.49 |
| 9:I:73:GLN:O | 9:I:76:ALA:HB3 | 2.13 | 0.49 |
| 16:P:67:THR:HB | 16:P:70:ALA:CB | 2.42 | 0.49 |
| 1:A:1000:G:C2 | 1:A:1001:G:H1' | 2.48 | 0.49 |
| 1:A:1221:A:H2' | 1:A:1280:C:N4 | 2.28 | 0.49 |
| 1:A:961:A:OP1 | 14:N:6:LEU:HD21 | 2.12 | 0.49 |
| 3:C:139:GLN:C | 3:C:139:GLN:HE21 | 2.15 | 0.49 |
| 3:C:42:LEU:O | 3:C:43:LEU:C | 2.51 | 0.49 |
| 4:D:101:LEU:C | 4:D:103:ASN:H | 2.14 | 0.49 |
| 4:D:199:ASN:O | 4:D:202:LEU:N | 2.44 | 0.49 |
| 10:J:30:SER:HB3 | 10:J:84:GLN:HE21 | 1.78 | 0.49 |
| 11:K:97:ALA:O | 11:K:101:SER:HB3 | 2.13 | 0.49 |
| 11:K:34:ASP:OD1 | 11:K:38:ASN:N | 2.46 | 0.49 |
| 13:M:104:ARG:O | 13:M:105:THR:HG23 | 2.13 | 0.49 |
| 18:R:37:VAL:HG21 | 18:R:78:LEU:HD22 | 1.95 | 0.49 |
| 19:S:44:MET:O | 19:S:47:HIS:CD2 | 2.65 | 0.49 |
| 19:S:44:MET:HA | 19:S:47:HIS:HD2 | 1.78 | 0.49 |
| 20:T:32:ALA:O | 20:T:35:THR:HB | 2.13 | 0.49 |
| 1:A:182:C:P | 20:T:82:SER:HB3 | 2.52 | 0.49 |
| 1:A:1141:C:C2' | 1:A:1141:C:O2 | 2.61 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1199:C:C4 | 1:A:1200:C:C5 | 3.01 | 0.49 |
| 1:A:1396:A:O2' | 1:A:1397:U:H5' | 2.13 | 0.49 |
| 1:A:215:C:H2' | 1:A:216:G:O4' | 2.13 | 0.49 |
| 1:A:445:G:N7 | 1:A:466:G:O6 | 2.46 | 0.49 |
| 1:A:542:G:C5 | 1:A:543:A:C2 | 3.00 | 0.49 |
| 1:A:685:C:H5'' | 1:A:687:G:O4' | 2.12 | 0.49 |
| 1:A:744:G:C2' | 1:A:745:G:H5' | 2.43 | 0.49 |
| 1:A:751:A:H2' | 1:A:752:A:O4' | 2.12 | 0.49 |
| 1:A:76:G:H2' | 1:A:77:G:O4' | 2.12 | 0.49 |
| 1:A:853:C:O2' | 8:H:14:ARG:NH1 | 2.43 | 0.49 |
| 1:A:856:G:C6 | 1:A:857:C:C4 | 3.01 | 0.49 |
| 3:C:79:ARG:HG2 | 3:C:82:GLU:HG2 | 1.94 | 0.49 |
| 4:D:34:GLU:O | 4:D:35:ARG:HB2 | 2.12 | 0.49 |
| 4:D:76:ARG:HG2 | 4:D:76:ARG:HH11 | 1.77 | 0.49 |
| 5:E:57:LYS:O | 5:E:60:TYR:HB3 | 2.13 | 0.49 |
| 5:E:64:ARG:O | 5:E:65:ASN:HB3 | 2.12 | 0.49 |
| 6:F:67:MET:HB2 | 6:F:68:PRO:HD2 | 1.94 | 0.49 |
| 10:J:29:ARG:CB | 10:J:84:GLN:HE22 | 2.25 | 0.49 |
| 1:A:745:G:H4' | 17:Q:102:GLY:CA | 2.42 | 0.49 |
| 18:R:43:PHE:CG | 18:R:66:LEU:HD11 | 2.48 | 0.49 |
| 20:T:55:ILE:O | 20:T:58:LYS:N | 2.46 | 0.49 |
| 1:A:1030:G:OP1 | 14:N:4:LYS:NZ | 2.44 | 0.48 |
| 1:A:1435:G:H8 | 1:A:1435:G:O5' | 1.96 | 0.48 |
| 1:A:21:U:O2' | 1:A:22:G:H5' | 2.12 | 0.48 |
| 1:A:305:G:H2' | 1:A:306:G:H8 | 1.77 | 0.48 |
| 1:A:649:A:H2' | 1:A:709:G:N2 | 2.28 | 0.48 |
| 1:A:886:A:O2' | 1:A:887:A:H5' | 2.12 | 0.48 |
| 2:B:29:ALA:O | 2:B:32:ILE:N | 2.34 | 0.48 |
| 3:C:177:THR:CG2 | 3:C:180:ALA:HB2 | 2.42 | 0.48 |
| 4:D:195:ALA:O | 4:D:196:LEU:C | 2.50 | 0.48 |
| 5:E:50:GLU:O | 5:E:53:LEU:HB2 | 2.13 | 0.48 |
| 9:I:15:ALA:HA | 9:I:64:THR:O | 2.13 | 0.48 |
| 9:I:79:LEU:HD13 | 9:I:79:LEU:C | 2.33 | 0.48 |
| 12:L:25:PRO:C | 12:L:27:LEU:N | 2.64 | 0.48 |
| 12:L:75:HIS:CD2 | 12:L:77:LEU:HB2 | 2.46 | 0.48 |
| 16:P:14:ASN:OD1 | 16:P:16:HIS:HE1 | 1.96 | 0.48 |
| 17:Q:84:LEU:O | 17:Q:85:VAL:C | 2.51 | 0.48 |
| 18:R:76:LEU:O | 18:R:78:LEU:HG | 2.12 | 0.48 |
| 19:S:42:PRO:O | 19:S:45:VAL:N | 2.46 | 0.48 |
| 19:S:53:ASN:N | 19:S:56:GLN:O | 2.42 | 0.48 |
| 19:S:51:VAL:O | 19:S:57:HIS:HA | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:1230:A:H1' | 9:I:70:LYS:HZ1 | 1.73 | 0.48 |
| 1:A:1270:A:H1' | 1:A:1334:C:O2' | 2.12 | 0.48 |
| 1:A:469:G:O2' | 1:A:470:G:OP2 | 2.29 | 0.48 |
| 1:A:576:G:H2' | 1:A:577:G:H8 | 1.77 | 0.48 |
| 1:A:627:C:H2' | 1:A:628:G:C8 | 2.41 | 0.48 |
| 1:A:811:U:C4 | 1:A:848:U:C2 | 3.02 | 0.48 |
| 3:C:125:GLU:C | 3:C:127:ARG:N | 2.65 | 0.48 |
| 4:D:185:PHE:HE2 | 4:D:188:LEU:HD23 | 1.78 | 0.48 |
| 5:E:33:VAL:HB | 5:E:112:LEU:HD12 | 1.95 | 0.48 |
| 9:I:79:LEU:HD23 | 9:I:101:PHE:O | 2.12 | 0.48 |
| 1:A:1160:G:P | 9:I:97:LYS:HZ3 | 2.36 | 0.48 |
| 12:L:45:PRO:HB2 | 12:L:49:ASN:O | 2.12 | 0.48 |
| 12:L:5:PRO:HB2 | 12:L:10:LEU:HD21 | 1.94 | 0.48 |
| 12:L:34:ARG:HG3 | 12:L:61:THR:CG2 | 2.43 | 0.48 |
| 13:M:98:VAL:CG2 | 13:M:110:ARG:HH12 | 2.19 | 0.48 |
| 19:S:49:ILE:O | 19:S:60:VAL:N | 2.45 | 0.48 |
| 1:A:1169:G:OP1 | 9:I:113:LYS:HE2 | 2.12 | 0.48 |
| 1:A:1192:C:H5' | 1:A:1196:C:H42 | 1.78 | 0.48 |
| 1:A:1216:C:H4' | 1:A:1347:U:H1' | 1.95 | 0.48 |
| 1:A:1357:A:O2' | 1:A:1358:A:H5' | 2.13 | 0.48 |
| 1:A:1422:C:H2' | 1:A:1423:C:C6 | 2.49 | 0.48 |
| 1:A:1450:U:O2' | 1:A:1451:A:H5' | 2.12 | 0.48 |
| 1:A:1483:G:C3' | 1:A:1483:G:C8 | 2.89 | 0.48 |
| 1:A:125:A:H5'' | 1:A:191:G:H2' | 1.96 | 0.48 |
| 1:A:725:G:O2' | 1:A:726:G:H5' | 2.13 | 0.48 |
| 3:C:94:LEU:HD23 | 3:C:94:LEU:O | 2.13 | 0.48 |
| 6:F:3:ARG:HE | 6:F:64:GLN:NE2 | 2.10 | 0.48 |
| 7:G:22:LEU:HD11 | 7:G:101:LEU:HD21 | 1.95 | 0.48 |
| 11:K:58:PRO:HA | 11:K:90:GLY:HA3 | 1.95 | 0.48 |
| 12:L:84:LEU:HB3 | 12:L:101:VAL:HB | 1.96 | 0.48 |
| 15:O:18:PHE:HB2 | 15:O:19:PRO:CD | 2.43 | 0.48 |
| 15:O:27:VAL:O | 15:O:31:LEU:CD1 | 2.61 | 0.48 |
| 15:O:6:GLU:O | 15:O:7:GLU:C | 2.52 | 0.48 |
| 17:Q:97:SER:OG | 17:Q:103:GLY:CA | 2.61 | 0.48 |
| 1:A:1001:G:H2' | 1:A:1002:G:C8 | 2.47 | 0.48 |
| 1:A:1245:C:O2' | 1:A:1246:C:H5' | 2.13 | 0.48 |
| 1:A:1299:C:C6 | 14:N:16:PHE:CD2 | 3.01 | 0.48 |
| 1:A:198:G:H2' | 1:A:199:U:C6 | 2.49 | 0.48 |
| 1:A:406:G:H2' | 1:A:425:U:C4 | 2.49 | 0.48 |
| 1:A:486:G:H2' | 1:A:487:C:C6 | 2.48 | 0.48 |
| 1:A:865:G:H2' | 1:A:866:G:O4' | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:975:U:O2' | 1:A:976:G:H5' | 2.14 | 0.48 |
| 2:B:230:VAL:HG12 | 2:B:231:GLU:O | 2.13 | 0.48 |
| 2:B:31:TYR:HE1 | 2:B:200:ILE:CD1 | 2.26 | 0.48 |
| 3:C:202:ILE:CG2 | 3:C:204:LEU:HD21 | 2.44 | 0.48 |
| 4:D:5:ILE:O | 4:D:5:ILE:HG22 | 2.12 | 0.48 |
| 10:J:49:VAL:HG12 | 10:J:50:ILE:N | 2.27 | 0.48 |
| 16:P:38:TYR:CE2 | 16:P:50:LYS:HD3 | 2.49 | 0.48 |
| 20:T:53:LEU:HD13 | 20:T:101:GLY:H | 1.77 | 0.48 |
| 1:A:1340:U:H3' | 1:A:1341:C:C5 | 2.48 | 0.48 |
| 1:A:193:G:O2' | 1:A:194:G:H5' | 2.14 | 0.48 |
| 1:A:208:C:N3 | 1:A:212:G:N2 | 2.51 | 0.48 |
| 1:A:254:G:O2' | 1:A:255:G:H5' | 2.14 | 0.48 |
| 1:A:352:A:C5 | 1:A:353:G:C8 | 3.01 | 0.48 |
| 1:A:542:G:H2' | 1:A:543:A:H2 | 1.78 | 0.48 |
| 1:A:582:U:H2' | 1:A:583:C:C6 | 2.48 | 0.48 |
| 2:B:125:PRO:C | 2:B:127:ILE:N | 2.65 | 0.48 |
| 3:C:154:SER:OG | 3:C:196:LEU:HB3 | 2.14 | 0.48 |
| 3:C:46:GLU:HB2 | 3:C:47:LEU:HD12 | 1.95 | 0.48 |
| 3:C:58:GLU:HB2 | 3:C:65:ALA:HB2 | 1.96 | 0.48 |
| 7:G:93:PRO:CG | 7:G:94:ARG:H | 2.24 | 0.48 |
| 10:J:27:ALA:HB1 | 10:J:74:ILE:HD13 | 1.96 | 0.48 |
| 12:L:75:HIS:HD2 | 12:L:77:LEU:CB | 2.24 | 0.48 |
| 14:N:18:VAL:HG23 | 14:N:19:ARG:N | 2.29 | 0.48 |
| 14:N:41:ARG:C | 14:N:41:ARG:HD2 | 2.34 | 0.48 |
| 17:Q:103:GLY:O | 17:Q:104:LYS:O | 2.30 | 0.48 |
| 17:Q:61:GLU:HA | 17:Q:71:PHE:CD1 | 2.49 | 0.48 |
| 19:S:36:ARG:NH2 | 19:S:75:ALA:HB3 | 2.25 | 0.48 |
| 19:S:11:VAL:HG22 | 19:S:39:THR:O | 2.13 | 0.48 |
| 1:A:1089:G:O2' | 1:A:1090:C:H5' | 2.13 | 0.48 |
| 1:A:1322:A:O2' | 1:A:1323:U:H5' | 2.14 | 0.48 |
| 1:A:1361:C:C5 | 1:A:1362:G:C8 | 3.01 | 0.48 |
| 1:A:168:U:C2 | 1:A:204:A:C2 | 3.01 | 0.48 |
| 1:A:190:U:O4 | 17:Q:62:SER:CB | 2.58 | 0.48 |
| 2:B:213:LEU:O | 2:B:214:ILE:C | 2.51 | 0.48 |
| 2:B:25:ASN:HD22 | 2:B:26:PRO:N | 2.11 | 0.48 |
| 3:C:139:GLN:HE22 | 3:C:143:GLU:HB2 | 1.78 | 0.48 |
| 4:D:187:ARG:CD | 4:D:188:LEU:H | 2.26 | 0.48 |
| 5:E:12:LEU:O | 5:E:30:ALA:HA | 2.14 | 0.48 |
| 9:I:13:ALA:HA | 9:I:67:GLY:O | 2.13 | 0.48 |
| 9:I:48:GLU:HA | 9:I:48:GLU:OE1 | 2.14 | 0.48 |
| 9:I:99:LEU:N | 9:I:99:LEU:HD22 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:K:110:ASP:C | 11:K:110:ASP:OD1 | 2.51 | 0.48 |
| 14:N:44:LEU:C | 14:N:44:LEU:HD12 | 2.33 | 0.48 |
| 19:S:23:ASN:HA | 19:S:26:GLY:O | 2.12 | 0.48 |
| 20:T:94:ALA:O | 20:T:95:ALA:CB | 2.61 | 0.48 |
| 1:A:1096:C:H1' | 3:C:178:LEU:HD21 | 1.95 | 0.48 |
| 1:A:1236:C:OP1 | 10:J:45:ARG:HD2 | 2.14 | 0.48 |
| 1:A:1280:C:O2 | 1:A:1280:C:H2' | 2.13 | 0.48 |
| 1:A:1311:A:O2' | 1:A:1312:U:H5' | 2.14 | 0.48 |
| 1:A:1374:U:H2' | 1:A:1375:G:H8 | 1.76 | 0.48 |
| 1:A:275:A:OP2 | 17:Q:95:TYR:CE2 | 2.67 | 0.48 |
| 1:A:446:A:C1' | 1:A:447:A:C8 | 2.97 | 0.48 |
| 1:A:447:A:O2' | 1:A:448:A:P | 2.72 | 0.48 |
| 1:A:620:U:O2' | 1:A:621:G:H5' | 2.13 | 0.48 |
| 1:A:682:G:H2' | 1:A:683:C:C6 | 2.49 | 0.48 |
| 1:A:844:C:H2' | 1:A:845:G:O4' | 2.14 | 0.48 |
| 1:A:928:U:H2' | 1:A:929:G:H8 | 1.78 | 0.48 |
| 2:B:115:LEU:O | 2:B:118:LEU:N | 2.44 | 0.48 |
| 2:B:172:ILE:O | 2:B:175:ARG:HB3 | 2.14 | 0.48 |
| 2:B:48:MET:O | 2:B:50:GLU:N | 2.47 | 0.48 |
| 2:B:82:ARG:O | 2:B:83:MET:C | 2.52 | 0.48 |
| 3:C:34:LEU:C | 3:C:34:LEU:HD23 | 2.33 | 0.48 |
| 3:C:21:ARG:NH2 | 3:C:56:ASP:OD2 | 2.46 | 0.48 |
| 5:E:115:VAL:HG11 | 5:E:118:ILE:HD12 | 1.96 | 0.48 |
| 5:E:45:PHE:CE2 | 5:E:47:LYS:HE3 | 2.49 | 0.48 |
| 5:E:81:GLU:HB3 | 5:E:88:LYS:NZ | 2.29 | 0.48 |
| 7:G:72:ARG:HG2 | 7:G:142:GLU:OE1 | 2.14 | 0.48 |
| 9:I:111:ARG:HG3 | 9:I:111:ARG:HH11 | 1.78 | 0.48 |
| 13:M:18:ALA:O | 13:M:21:TYR:N | 2.38 | 0.48 |
| 15:O:10:LYS:HD2 | 15:O:10:LYS:C | 2.34 | 0.48 |
| 15:O:25:THR:O | 15:O:28:GLN:HB2 | 2.13 | 0.48 |
| 1:A:1036:G:H2' | 1:A:1181:U:C5 | 2.47 | 0.48 |
| 1:A:1219:C:C4' | 1:A:1316:G:N2 | 2.77 | 0.48 |
| 1:A:1218:A:H2' | 1:A:1219:C:C6 | 2.49 | 0.48 |
| 1:A:1274:U:P | 7:G:41:ARG:NH2 | 2.81 | 0.48 |
| 1:A:1291:G:C6 | 1:A:1311:A:C2 | 3.02 | 0.48 |
| 1:A:1310:C:O2' | 1:A:1311:A:H5' | 2.14 | 0.48 |
| 1:A:210:U:H5'' | 1:A:211:U:OP1 | 2.14 | 0.48 |
| 1:A:254:G:H2' | 1:A:255:G:H8 | 1.79 | 0.48 |
| 1:A:354:U:H2' | 1:A:355:U:C6 | 2.49 | 0.48 |
| 1:A:409:G:H2' | 1:A:424:G:N2 | 2.28 | 0.48 |
| 1:A:46:U:H2' | 1:A:47:G:C8 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:501:G:O2' | 1:A:514:G:C4' | 2.62 | 0.48 |
| 1:A:799:A:HO2' | 1:A:800:A:P | 2.35 | 0.48 |
| 1:A:818:C:O5' | 1:A:818:C:H6 | 1.97 | 0.48 |
| 2:B:19:HIS:CD2 | 2:B:204:ASN:ND2 | 2.82 | 0.48 |
| 3:C:129:ALA:CB | 3:C:132:ARG:HD2 | 2.43 | 0.48 |
| 4:D:8:VAL:CG2 | 4:D:115:ARG:NH1 | 2.76 | 0.48 |
| 7:G:41:ARG:O | 7:G:42:ILE:C | 2.52 | 0.48 |
| 1:A:855:C:O2 | 8:H:3:THR:HG21 | 2.14 | 0.48 |
| 10:J:12:ASP:OD1 | 10:J:14:LYS:N | 2.47 | 0.48 |
| 11:K:85:ARG:NE | 11:K:111:ASP:OD2 | 2.47 | 0.48 |
| 13:M:68:GLY:O | 13:M:72:ALA:N | 2.41 | 0.48 |
| 15:O:46:HIS:C | 15:O:48:LYS:N | 2.66 | 0.48 |
| 1:A:97:C:P | 20:T:17:ARG:HH11 | 2.36 | 0.48 |
| 1:A:1088:A:O2' | 1:A:1089:G:H5' | 2.14 | 0.48 |
| 1:A:1429:C:H2' | 1:A:1430:C:C6 | 2.40 | 0.48 |
| 1:A:1459:U:H2' | 1:A:1460:G:O4' | 2.13 | 0.48 |
| 1:A:298:G:O5' | 1:A:298:G:H8 | 1.97 | 0.48 |
| 1:A:490:G:C6 | 1:A:491:C:C4 | 3.02 | 0.48 |
| 1:A:698:G:C2 | 1:A:761:A:H1' | 2.48 | 0.48 |
| 1:A:95:A:H2' | 1:A:96:G:C8 | 2.46 | 0.48 |
| 2:B:75:LYS:HD3 | 2:B:75:LYS:O | 2.12 | 0.48 |
| 3:C:130:VAL:HG11 | 3:C:157:ILE:HD13 | 1.95 | 0.48 |
| 4:D:131:ARG:HD2 | 4:D:131:ARG:N | 2.11 | 0.48 |
| 4:D:96:LEU:O | 4:D:99:SER:HB2 | 2.13 | 0.48 |
| 8:H:104:ARG:O | 8:H:105:ARG:C | 2.52 | 0.48 |
| 1:A:1181:U:H4' | 10:J:54:PHE:CD1 | 2.49 | 0.48 |
| 10:J:71:LEU:O | 10:J:72:VAL:CB | 2.58 | 0.48 |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:N | 2.21 | 0.48 |
| 13:M:49:THR:O | 13:M:53:VAL:HG23 | 2.14 | 0.48 |
| 15:O:5:LYS:O | 15:O:9:GLN:HG3 | 2.12 | 0.48 |
| 16:P:52:ASP:O | 16:P:52:ASP:OD1 | 2.31 | 0.48 |
| 18:R:70:ILE:HG22 | 18:R:70:ILE:O | 2.13 | 0.48 |
| 1:A:1301:A:H5' | 19:S:70:LYS:HZ2 | 1.78 | 0.48 |
| 1:A:1112:C:O2' | 1:A:1113:A:OP2 | 2.24 | 0.48 |
| 1:A:113:A:C5 | 1:A:236:C:C4 | 3.02 | 0.48 |
| 1:A:1349:C:H2' | 1:A:1350:C:H6 | 1.75 | 0.48 |
| 1:A:1506:U:HO2' | 1:A:1507:G:P | 2.37 | 0.48 |
| 1:A:191:G:H1 | 1:A:260:U:P | 2.37 | 0.48 |
| 1:A:317:A:H2 | 1:A:328:G:H22 | 1.59 | 0.48 |
| 1:A:567:A:H1' | 1:A:743:A:N6 | 2.28 | 0.48 |
| 1:A:713:A:H2' | 1:A:714:G:H8 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:981:G:H2' | 1:A:982:G:C8 | 2.49 | 0.48 |
| 3:C:19:GLU:O | 3:C:56:ASP:HA | 2.14 | 0.48 |
| 6:F:30:LEU:HB3 | 6:F:35:ALA:HB3 | 1.96 | 0.48 |
| 8:H:38:ILE:HG22 | 8:H:39:LEU:N | 2.28 | 0.48 |
| 9:I:97:LYS:C | 9:I:100:GLY:H | 2.16 | 0.48 |
| 10:J:91:PRO:HB2 | 10:J:94:VAL:CG2 | 2.44 | 0.48 |
| 12:L:7:ILE:O | 12:L:8:ASN:C | 2.52 | 0.48 |
| 13:M:121:LYS:N | 13:M:121:LYS:HD2 | 2.29 | 0.48 |
| 15:O:27:VAL:O | 15:O:31:LEU:HD12 | 2.14 | 0.48 |
| 15:O:87:ILE:O | 15:O:88:ARG:CB | 2.61 | 0.48 |
| 18:R:74:ARG:HB3 | 18:R:81:PHE:CZ | 2.48 | 0.48 |
| 19:S:62:ILE:HD12 | 19:S:66:MET:CG | 2.41 | 0.48 |
| 1:A:1102:C:OP2 | 9:I:9:ARG:NH2 | 2.46 | 0.47 |
| 1:A:1280:C:H1' | 1:A:1281:A:C6 | 2.49 | 0.47 |
| 1:A:1296:C:OP2 | 19:S:6:LYS:CD | 2.62 | 0.47 |
| 1:A:20:C:O2' | 1:A:21:U:H5' | 2.15 | 0.47 |
| 1:A:225:U:H2' | 1:A:226:G:H8 | 1.78 | 0.47 |
| 1:A:332:C:H2' | 1:A:333:C:C6 | 2.48 | 0.47 |
| 1:A:589:U:H2' | 1:A:590:G:C8 | 2.48 | 0.47 |
| 1:A:715:G:OP1 | 1:A:750:A:H1' | 2.14 | 0.47 |
| 1:A:982:G:N1 | 1:A:983:A:H1' | 2.29 | 0.47 |
| 2:B:187:LEU:HA | 2:B:201:ILE:HB | 1.96 | 0.47 |
| 3:C:152:ILE:HG22 | 3:C:153:VAL:N | 2.28 | 0.47 |
| 5:E:89:ILE:HD13 | 5:E:90:VAL:CA | 2.44 | 0.47 |
| 7:G:60:LYS:O | 7:G:61:VAL:C | 2.52 | 0.47 |
| 8:H:82:HIS:HD2 | 8:H:138:TRP:NE1 | 2.11 | 0.47 |
| 9:I:110:GLU:OE2 | 9:I:113:LYS:NZ | 2.45 | 0.47 |
| 9:I:114:TYR:CD1 | 9:I:114:TYR:C | 2.87 | 0.47 |
| 16:P:11:SER:O | 16:P:12:LYS:C | 2.51 | 0.47 |
| 16:P:6:LEU:N | 16:P:6:LEU:HD12 | 2.29 | 0.47 |
| 19:S:52:TYR:HA | 19:S:56:GLN:O | 2.14 | 0.47 |
| 20:T:53:LEU:O | 20:T:57:ARG:HD3 | 2.14 | 0.47 |
| 1:A:1055:G:H2' | 1:A:1056:U:C6 | 2.49 | 0.47 |
| 1:A:1186:A:H2' | 1:A:1187:U:H6 | 1.78 | 0.47 |
| 1:A:1204:G:C5' | 19:S:77:THR:HG21 | 2.44 | 0.47 |
| 1:A:1363:U:O2' | 1:A:1364:U:OP2 | 2.27 | 0.47 |
| 1:A:143:G:H2' | 1:A:144:A:H8 | 1.79 | 0.47 |
| 1:A:369:A:H1' | 1:A:466:G:H1' | 1.95 | 0.47 |
| 1:A:45:G:H2' | 1:A:46:U:H6 | 1.79 | 0.47 |
| 1:A:472:A:C2' | 1:A:473:C:H5' | 2.45 | 0.47 |
| 1:A:487:C:OP1 | 12:L:119:LYS:NZ | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:486:G:C4' | 1:A:534:G:H4' | 2.43 | 0.47 |
| 1:A:868:G:H2' | 1:A:884:G:O6 | 2.15 | 0.47 |
| 1:A:903:G:C2 | 1:A:905:G:C8 | 3.01 | 0.47 |
| 2:B:176:GLU:O | 2:B:180:LEU:HG | 2.14 | 0.47 |
| 2:B:54:THR:O | 2:B:57:PHE:N | 2.45 | 0.47 |
| 3:C:5:ILE:HD12 | 3:C:5:ILE:C | 2.34 | 0.47 |
| 5:E:105:VAL:HB | 5:E:106:PRO:CD | 2.44 | 0.47 |
| 5:E:9:LYS:HB2 | 5:E:112:LEU:HD11 | 1.96 | 0.47 |
| 6:F:78:GLU:HA | 6:F:81:ILE:CD1 | 2.44 | 0.47 |
| 7:G:65:ALA:O | 7:G:66:VAL:C | 2.52 | 0.47 |
| 9:I:89:ASN:HB3 | 9:I:92:TYR:CD1 | 2.49 | 0.47 |
| 17:Q:26:GLN:HG2 | 17:Q:37:LYS:HG3 | 1.96 | 0.47 |
| 6:F:97:PHE:HB2 | 18:R:32:ARG:HH21 | 1.79 | 0.47 |
| 18:R:36:ASN:O | 18:R:38:GLU:N | 2.47 | 0.47 |
| 19:S:33:THR:CG2 | 19:S:35:SER:H | 2.22 | 0.47 |
| 20:T:91:LEU:O | 20:T:93:GLU:N | 2.46 | 0.47 |
| 1:A:1163:G:O2' | 1:A:1164:G:O5' | 2.31 | 0.47 |
| 22:A:1523:KSG:O6 | 22:A:1523:KSG:H1 | 2.13 | 0.47 |
| 1:A:176:G:H4' | 1:A:177:U:C5' | 2.44 | 0.47 |
| 1:A:424:G:HO2' | 1:A:425:U:P | 2.37 | 0.47 |
| 1:A:682:G:H2' | 1:A:683:C:H6 | 1.78 | 0.47 |
| 1:A:765:A:H2' | 1:A:766:A:O4' | 2.14 | 0.47 |
| 1:A:776:A:O2' | 1:A:777:U:OP2 | 2.33 | 0.47 |
| 1:A:814:G:H4' | 2:B:23:ARG:HA | 1.95 | 0.47 |
| 1:A:943:A:C2 | 1:A:947:A:N1 | 2.82 | 0.47 |
| 5:E:12:LEU:C | 5:E:12:LEU:HD22 | 2.34 | 0.47 |
| 9:I:63:ILE:HG21 | 9:I:77:ILE:HG12 | 1.97 | 0.47 |
| 11:K:30:VAL:N | 11:K:43:SER:O | 2.48 | 0.47 |
| 15:O:32:LEU:O | 15:O:35:ARG:N | 2.47 | 0.47 |
| 18:R:29:PHE:HE1 | 18:R:31:LEU:HD21 | 1.80 | 0.47 |
| 19:S:41:VAL:HG23 | 19:S:43:GLU:HG2 | 1.97 | 0.47 |
| 20:T:78:ALA:O | 20:T:79:ARG:C | 2.52 | 0.47 |
| 1:A:1238:A:H2 | 1:A:1240:G:N1 | 2.13 | 0.47 |
| 1:A:1260:U:H5' | 1:A:1261:A:O4' | 2.13 | 0.47 |
| 1:A:275:A:OP2 | 17:Q:95:TYR:HE2 | 1.98 | 0.47 |
| 1:A:288:G:N7 | 1:A:289:G:H1' | 2.29 | 0.47 |
| 1:A:938:U:O2 | 1:A:938:U:H2' | 2.13 | 0.47 |
| 2:B:184:VAL:HG23 | 2:B:198:ASP:OD2 | 2.13 | 0.47 |
| 4:D:156:GLU:HG2 | 4:D:160:GLN:NE2 | 2.28 | 0.47 |
| 4:D:161:ASN:O | 4:D:163:GLU:N | 2.47 | 0.47 |
| 5:E:153:LYS:HD2 | 5:E:154:GLY:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:6:THR:O | 12:L:7:ILE:C | 2.53 | 0.47 |
| 13:M:125:ARG:C | 13:M:125:ARG:HD2 | 2.33 | 0.47 |
| 13:M:71:ARG:HG2 | 13:M:71:ARG:HH11 | 1.79 | 0.47 |
| 17:Q:57:VAL:HA | 17:Q:77:VAL:HG23 | 1.97 | 0.47 |
| 20:T:37:SER:O | 20:T:38:LYS:C | 2.53 | 0.47 |
| 1:A:1094:A:H61 | 3:C:177:THR:HA | 1.79 | 0.47 |
| 1:A:1104:U:O2' | 1:A:1105:U:H5' | 2.14 | 0.47 |
| 1:A:1351:G:H5'' | 9:I:112:LYS:O | 2.15 | 0.47 |
| 1:A:1476:U:O2' | 1:A:1477:A:P | 2.71 | 0.47 |
| 1:A:170:C:C2 | 1:A:171:C:C5 | 3.02 | 0.47 |
| 1:A:462:G:O2' | 1:A:463:A:H5' | 2.13 | 0.47 |
| 1:A:522:G:C4' | 12:L:114:LYS:HD3 | 2.44 | 0.47 |
| 1:A:736:G:C4' | 1:A:738:C:H5 | 2.27 | 0.47 |
| 1:A:971:G:O2' | 1:A:972:A:OP1 | 2.30 | 0.47 |
| 1:A:98:G:H4' | 1:A:169:C:O4' | 2.15 | 0.47 |
| 2:B:105:PHE:HE2 | 2:B:157:ARG:HA | 1.78 | 0.47 |
| 2:B:84:GLU:OE1 | 2:B:216:SER:HA | 2.14 | 0.47 |
| 3:C:29:TYR:C | 3:C:29:TYR:CD2 | 2.88 | 0.47 |
| 4:D:102:ASP:OD1 | 4:D:136:PRO:O | 2.31 | 0.47 |
| 5:E:137:GLU:O | 5:E:139:LEU:N | 2.47 | 0.47 |
| 22:A:1524:KSG:H5 | 7:G:82:GLY:HA3 | 1.96 | 0.47 |
| 8:H:41:ARG:HG2 | 8:H:41:ARG:O | 2.12 | 0.47 |
| 8:H:64:LYS:C | 8:H:65:TYR:CD1 | 2.87 | 0.47 |
| 8:H:86:ILE:HD12 | 8:H:133:LEU:HD21 | 1.92 | 0.47 |
| 8:H:91:ARG:HG2 | 12:L:7:ILE:HG21 | 1.97 | 0.47 |
| 10:J:3:LYS:O | 10:J:100:THR:HG23 | 2.14 | 0.47 |
| 11:K:72:ALA:HB1 | 11:K:77:MET:HG3 | 1.97 | 0.47 |
| 13:M:37:THR:HG21 | 13:M:39:ILE:HD11 | 1.97 | 0.47 |
| 13:M:89:GLY:O | 13:M:92:HIS:HB2 | 2.14 | 0.47 |
| 1:A:1213:G:O2' | 1:A:1214:U:H5' | 2.15 | 0.47 |
| 1:A:340:A:O2' | 1:A:341:C:P | 2.73 | 0.47 |
| 1:A:765:A:H2' | 1:A:766:A:C5' | 2.45 | 0.47 |
| 1:A:805:G:C6 | 1:A:858:C:N4 | 2.83 | 0.47 |
| 3:C:179:ARG:HG3 | 3:C:179:ARG:HH11 | 1.79 | 0.47 |
| 6:F:76:ALA:O | 6:F:77:ARG:C | 2.53 | 0.47 |
| 8:H:137:VAL:CG1 | 8:H:138:TRP:N | 2.77 | 0.47 |
| 10:J:56:HIS:HB2 | 10:J:59:SER:OG | 2.15 | 0.47 |
| 11:K:110:ASP:HB2 | 18:R:88:LYS:HD2 | 1.96 | 0.47 |
| 11:K:114:VAL:HG13 | 11:K:114:VAL:O | 2.14 | 0.47 |
| 11:K:93:GLN:NE2 | 11:K:96:ARG:NH2 | 2.63 | 0.47 |
| 12:L:55:VAL:CG1 | 12:L:56:ALA:N | 2.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:59:TYR:O | 13:M:60:VAL:O | 2.32 | 0.47 |
| 17:Q:29:HIS:O | 17:Q:29:HIS:ND1 | 2.47 | 0.47 |
| 17:Q:63:ARG:HG2 | 17:Q:64:PRO:O | 2.14 | 0.47 |
| 6:F:91:VAL:HG13 | 18:R:72:ARG:NH2 | 2.29 | 0.47 |
| 20:T:23:ARG:HG2 | 20:T:23:ARG:NH1 | 2.28 | 0.47 |
| 1:A:1099:C:C2' | 1:A:1100:G:H5' | 2.36 | 0.47 |
| 1:A:1239:U:O2' | 1:A:1240:G:OP2 | 2.28 | 0.47 |
| 1:A:1303:C:H2' | 1:A:1304:C:C5 | 2.50 | 0.47 |
| 1:A:172:C:O2' | 1:A:173:C:H5' | 2.15 | 0.47 |
| 1:A:470:G:O2' | 1:A:471:U:P | 2.73 | 0.47 |
| 1:A:492:C:H5'' | 1:A:493:A:OP1 | 2.15 | 0.47 |
| 1:A:574:C:N3 | 1:A:575:U:C5 | 2.83 | 0.47 |
| 1:A:768:C:H2' | 1:A:769:G:H8 | 1.80 | 0.47 |
| 2:B:157:ARG:HG3 | 2:B:157:ARG:HH11 | 1.80 | 0.47 |
| 2:B:212:GLN:C | 2:B:212:GLN:CD | 2.74 | 0.47 |
| 2:B:239:VAL:O | 2:B:239:VAL:HG12 | 2.15 | 0.47 |
| 3:C:56:ASP:O | 3:C:57:ILE:CG1 | 2.62 | 0.47 |
| 4:D:12:CYS:CA | 4:D:19:LEU:HD12 | 2.45 | 0.47 |
| 4:D:162:LEU:HD12 | 4:D:181:MET:CE | 2.44 | 0.47 |
| 4:D:76:ARG:HD3 | 4:D:207:TYR:CE2 | 2.49 | 0.47 |
| 6:F:9:VAL:HG22 | 6:F:60:PHE:CD2 | 2.50 | 0.47 |
| 7:G:107:ALA:O | 7:G:110:GLN:HB2 | 2.14 | 0.47 |
| 11:K:120:ARG:NH2 | 11:K:126:ARG:NH1 | 2.63 | 0.47 |
| 1:A:36:G:N2 | 12:L:118:SER:OG | 2.44 | 0.47 |
| 13:M:37:THR:O | 13:M:37:THR:HG22 | 2.15 | 0.47 |
| 19:S:12:ASP:H | 19:S:38:SER:CB | 2.24 | 0.47 |
| 20:T:33:ILE:O | 20:T:34:LYS:C | 2.52 | 0.47 |
| 1:A:1161:A:O2' | 1:A:1162:A:H5' | 2.15 | 0.47 |
| 1:A:1209:A:O3' | 13:M:115:LYS:HD3 | 2.14 | 0.47 |
| 1:A:1328:A:H4' | 1:A:1329:G:O5' | 2.14 | 0.47 |
| 1:A:1333:U:H2' | 1:A:1334:C:C6 | 2.46 | 0.47 |
| 1:A:251:G:O6 | 1:A:262:G:O6 | 2.33 | 0.47 |
| 1:A:437:C:H6 | 1:A:437:C:O5' | 1.97 | 0.47 |
| 1:A:505:G:O2' | 1:A:506:C:H5' | 2.14 | 0.47 |
| 1:A:665:C:H2' | 1:A:666:G:C8 | 2.50 | 0.47 |
| 1:A:674:G:O5' | 1:A:674:G:H8 | 1.97 | 0.47 |
| 1:A:765:A:H2' | 1:A:766:A:H5' | 1.96 | 0.47 |
| 2:B:149:LEU:C | 2:B:151:GLY:N | 2.68 | 0.47 |
| 4:D:103:ASN:O | 4:D:104:VAL:C | 2.50 | 0.47 |
| 8:H:16:ALA:HB1 | 8:H:21:LYS:HB2 | 1.97 | 0.47 |
| 12:L:33:ARG:CD | 12:L:62:SER:HB3 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:65:GLU:CD | 12:L:65:GLU:N | 2.68 | 0.47 |
| 13:M:84:ILE:C | 13:M:86:CYS:N | 2.66 | 0.47 |
| 14:N:33:VAL:O | 14:N:33:VAL:HG23 | 2.15 | 0.47 |
| 15:O:24:SER:HB2 | 15:O:27:VAL:HG23 | 1.96 | 0.47 |
| 15:O:81:LEU:O | 15:O:82:ILE:C | 2.51 | 0.47 |
| 1:A:1094:A:N6 | 3:C:177:THR:HA | 2.30 | 0.47 |
| 1:A:1221:A:H1' | 1:A:1223:G:C4 | 2.50 | 0.47 |
| 1:A:1230:A:H2' | 1:A:1231:C:H6 | 1.80 | 0.47 |
| 1:A:1246:C:H2' | 1:A:1247:G:H8 | 1.78 | 0.47 |
| 1:A:1318:C:H1' | 1:A:1319:G:C6 | 2.50 | 0.47 |
| 1:A:1467:G:H2' | 1:A:1468:C:C5' | 2.34 | 0.47 |
| 1:A:161:G:H2' | 1:A:162:G:H8 | 1.79 | 0.47 |
| 1:A:278:A:H3' | 1:A:279:C:C6 | 2.49 | 0.47 |
| 1:A:342:G:O2' | 1:A:343:G:H5' | 2.14 | 0.47 |
| 1:A:342:G:C2' | 1:A:343:G:H5' | 2.44 | 0.47 |
| 1:A:709:G:C4 | 1:A:710:C:C5 | 3.03 | 0.47 |
| 2:B:155:LEU:HA | 2:B:155:LEU:HD23 | 1.76 | 0.47 |
| 2:B:16:HIS:CE1 | 2:B:210:SER:HA | 2.50 | 0.47 |
| 2:B:203:GLY:O | 2:B:205:ASP:N | 2.47 | 0.47 |
| 3:C:182:ILE:HG22 | 3:C:183:ASP:O | 2.15 | 0.47 |
| 3:C:186:PHE:HA | 3:C:198:VAL:O | 2.14 | 0.47 |
| 1:A:526:G:P | 4:D:10:ARG:HH22 | 2.37 | 0.47 |
| 4:D:179:GLU:C | 4:D:181:MET:N | 2.68 | 0.47 |
| 5:E:13:ILE:HD12 | 5:E:51:VAL:CG1 | 2.45 | 0.47 |
| 5:E:91:LEU:HA | 5:E:91:LEU:HD23 | 1.60 | 0.47 |
| 10:J:11:PHE:CZ | 10:J:65:LEU:HD21 | 2.50 | 0.47 |
| 14:N:17:LYS:C | 14:N:17:LYS:HD3 | 2.35 | 0.47 |
| 15:O:25:THR:O | 15:O:29:VAL:HG23 | 2.15 | 0.47 |
| 15:O:36:ILE:HA | 15:O:59:MET:HE1 | 1.97 | 0.47 |
| 17:Q:9:VAL:CG2 | 17:Q:56:VAL:HG22 | 2.39 | 0.47 |
| 1:A:1203:G:O2' | 19:S:77:THR:HG23 | 2.15 | 0.47 |
| 1:A:1058:C:OP1 | 2:B:103:THR:HG21 | 2.14 | 0.47 |
| 1:A:1128:C:O2' | 1:A:1129:A:O5' | 2.32 | 0.47 |
| 1:A:1204:G:OP1 | 19:S:77:THR:HG21 | 2.13 | 0.47 |
| 1:A:1439:G:H2' | 1:A:1440:G:C8 | 2.48 | 0.47 |
| 1:A:1463:U:H2' | 1:A:1463:U:O2 | 2.14 | 0.47 |
| 22:A:1524:KSG:O2 | 22:A:1524:KSG:H8 | 2.15 | 0.47 |
| 1:A:339:U:H2' | 1:A:341:C:C5 | 2.49 | 0.47 |
| 1:A:400:U:C2 | 1:A:401:U:C5 | 3.02 | 0.47 |
| 1:A:524:G:H2' | 1:A:525:G:O4' | 2.15 | 0.47 |
| 1:A:706:A:C6 | 1:A:708:G:C5 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:950:C:OP1 | 10:J:57:LYS:NZ | 2.40 | 0.47 |
| 2:B:142:LEU:HD23 | 2:B:142:LEU:HA | 1.79 | 0.47 |
| 4:D:65:ARG:HD2 | 4:D:75:PHE:CB | 2.43 | 0.47 |
| 4:D:8:VAL:HG12 | 4:D:9:CYS:N | 2.29 | 0.47 |
| 6:F:19:LEU:HD23 | 6:F:23:LYS:HG3 | 1.97 | 0.47 |
| 6:F:64:GLN:O | 6:F:64:GLN:HG2 | 2.15 | 0.47 |
| 7:G:113:GLU:CG | 7:G:119:ARG:HG2 | 2.30 | 0.47 |
| 7:G:51:GLN:OE1 | 7:G:51:GLN:HA | 2.14 | 0.47 |
| 8:H:112:LEU:CA | 8:H:134:ILE:HD12 | 2.45 | 0.47 |
| 1:A:1329:G:C8 | 9:I:107:ARG:HB3 | 2.50 | 0.47 |
| 12:L:104:VAL:O | 12:L:105:TYR:HB2 | 2.14 | 0.47 |
| 12:L:43:VAL:HG12 | 12:L:44:THR:N | 2.30 | 0.47 |
| 14:N:47:LEU:O | 14:N:48:ALA:C | 2.53 | 0.47 |
| 1:A:458:A:C4' | 16:P:82:GLN:HE21 | 2.27 | 0.47 |
| 17:Q:19:VAL:O | 17:Q:19:VAL:HG23 | 2.15 | 0.47 |
| 19:S:70:LYS:O | 19:S:71:LEU:C | 2.53 | 0.47 |
| 1:A:1253:G:H8 | 1:A:1253:G:O5' | 1.98 | 0.47 |
| 1:A:1260:U:H5'' | 1:A:1261:A:C5' | 2.45 | 0.47 |
| 1:A:1363:U:O2' | 1:A:1364:U:P | 2.73 | 0.47 |
| 1:A:1485:A:H2' | 1:A:1486:G:H8 | 1.78 | 0.47 |
| 1:A:453:C:H2' | 1:A:454:G:O4' | 2.15 | 0.47 |
| 1:A:510:C:H2' | 1:A:511:G:O4' | 2.15 | 0.47 |
| 1:A:661:U:H3 | 1:A:697:G:N2 | 2.01 | 0.47 |
| 4:D:161:ASN:O | 4:D:164:ALA:N | 2.48 | 0.47 |
| 4:D:10:ARG:HH12 | 4:D:40:PRO:HB2 | 1.80 | 0.47 |
| 5:E:9:LYS:HG3 | 5:E:112:LEU:HD21 | 1.96 | 0.47 |
| 5:E:13:ILE:HG22 | 5:E:30:ALA:HA | 1.96 | 0.47 |
| 8:H:45:ILE:HD13 | 8:H:61:VAL:HG13 | 1.97 | 0.47 |
| 9:I:10:ARG:O | 9:I:11:LYS:C | 2.54 | 0.47 |
| 9:I:3:GLN:HG3 | 9:I:20:ARG:NE | 2.27 | 0.47 |
| 11:K:84:VAL:HG23 | 11:K:110:ASP:HA | 1.97 | 0.47 |
| 14:N:3:ARG:HD3 | 14:N:6:LEU:HD12 | 1.96 | 0.47 |
| 18:R:87:ARG:CG | 18:R:87:ARG:NH1 | 2.75 | 0.47 |
| 1:A:199:U:C1' | 20:T:103:GLY:HA2 | 2.45 | 0.47 |
| 20:T:59:ALA:C | 20:T:63:ILE:HD12 | 2.36 | 0.47 |
| 1:A:1032:U:H4' | 1:A:1033:G:OP2 | 2.14 | 0.46 |
| 1:A:1050:A:O2' | 1:A:1051:G:OP2 | 2.33 | 0.46 |
| 1:A:1149:G:H22 | 1:A:1151:A:H3' | 1.80 | 0.46 |
| 1:A:1140:A:C6 | 1:A:1162:A:C6 | 3.03 | 0.46 |
| 1:A:1280:C:O2 | 1:A:1280:C:C2' | 2.62 | 0.46 |
| 1:A:1352:C:H2' | 1:A:1353:G:H8 | 1.76 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:A:1523:KSG:O2 | 22:A:1523:KSG:H8 | 2.15 | 0.46 |
| 1:A:17:A:H4' | 5:E:17:ALA:H | 1.80 | 0.46 |
| 1:A:432:C:O2' | 1:A:433:U:H5' | 2.14 | 0.46 |
| 1:A:502:C:O2' | 1:A:503:C:OP2 | 2.26 | 0.46 |
| 1:A:609:G:C5 | 1:A:610:U:C4 | 3.02 | 0.46 |
| 1:A:850:A:C4 | 1:A:852:G:C8 | 3.03 | 0.46 |
| 1:A:951:G:H2' | 1:A:952:A:H8 | 1.79 | 0.46 |
| 2:B:134:GLU:O | 2:B:138:LEU:N | 2.41 | 0.46 |
| 2:B:119:GLU:OE2 | 2:B:153:ARG:NH2 | 2.47 | 0.46 |
| 2:B:212:GLN:NE2 | 2:B:216:SER:HB3 | 2.30 | 0.46 |
| 4:D:43:HIS:O | 4:D:44:GLY:C | 2.51 | 0.46 |
| 4:D:65:ARG:O | 4:D:69:GLY:N | 2.47 | 0.46 |
| 5:E:137:GLU:C | 5:E:139:LEU:N | 2.68 | 0.46 |
| 8:H:17:THR:OG1 | 8:H:18:ARG:N | 2.47 | 0.46 |
| 1:A:507:A:H61 | 12:L:53:ARG:NH1 | 2.14 | 0.46 |
| 12:L:65:GLU:N | 12:L:65:GLU:OE1 | 2.48 | 0.46 |
| 13:M:37:THR:HG22 | 13:M:39:ILE:HD11 | 1.97 | 0.46 |
| 15:O:9:GLN:O | 15:O:12:ILE:HB | 2.15 | 0.46 |
| 16:P:59:TRP:O | 16:P:60:LEU:C | 2.52 | 0.46 |
| 17:Q:45:HIS:HB2 | 17:Q:69:LYS:HE2 | 1.96 | 0.46 |
| 19:S:7:LYS:CG | 19:S:7:LYS:O | 2.63 | 0.46 |
| 1:A:1014:G:H2' | 1:A:1015:G:C8 | 2.39 | 0.46 |
| 1:A:1145:C:N3 | 1:A:1157:G:C2 | 2.83 | 0.46 |
| 1:A:1169:G:H3' | 1:A:1170:A:H8 | 1.80 | 0.46 |
| 1:A:1248:G:N2 | 1:A:1252:C:C2 | 2.84 | 0.46 |
| 1:A:803:A:N7 | 1:A:1507:G:C2 | 2.83 | 0.46 |
| 1:A:161:G:O2' | 1:A:162:G:H5' | 2.15 | 0.46 |
| 1:A:23:G:O2' | 1:A:24:C:H5' | 2.16 | 0.46 |
| 1:A:341:C:H1' | 1:A:342:G:N2 | 2.31 | 0.46 |
| 1:A:311:A:H1' | 1:A:349:A:C2 | 2.50 | 0.46 |
| 1:A:525:G:O2' | 1:A:526:G:H5' | 2.15 | 0.46 |
| 1:A:728:C:H2' | 1:A:729:C:C6 | 2.50 | 0.46 |
| 1:A:783:G:O2' | 1:A:784:G:H5' | 2.15 | 0.46 |
| 1:A:997:C:O5' | 1:A:997:C:H6 | 1.98 | 0.46 |
| 2:B:108:ILE:O | 2:B:111:ARG:N | 2.48 | 0.46 |
| 2:B:216:SER:OG | 2:B:217:ARG:N | 2.48 | 0.46 |
| 3:C:112:SER:CB | 3:C:115:LEU:HD12 | 2.45 | 0.46 |
| 3:C:174:PRO:HB2 | 3:C:177:THR:CG2 | 2.43 | 0.46 |
| 4:D:173:TRP:O | 4:D:186:LEU:HB2 | 2.14 | 0.46 |
| 5:E:115:VAL:CG1 | 5:E:116:THR:N | 2.75 | 0.46 |
| 5:E:31:LEU:HD23 | 5:E:44:GLY:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 6:F:69:GLU:HA | 6:F:72:VAL:CG2 | 2.45 | 0.46 |
| 7:G:50:ILE:HG12 | 7:G:125:MET:HE2 | 1.95 | 0.46 |
| 8:H:44:PHE:HD1 | 8:H:80:ILE:HG12 | 1.80 | 0.46 |
| 9:I:79:LEU:CD1 | 9:I:83:ARG:HD2 | 2.45 | 0.46 |
| 17:Q:90:ILE:O | 17:Q:93:GLN:CB | 2.61 | 0.46 |
| 18:R:65:ILE:C | 18:R:67:ALA:H | 2.17 | 0.46 |
| 20:T:42:GLN:NE2 | 20:T:46:GLU:OE2 | 2.48 | 0.46 |
| 20:T:79:ARG:O | 20:T:80:ARG:C | 2.52 | 0.46 |
| 1:A:1280:C:H3' | 7:G:114:ARG:HH22 | 1.79 | 0.46 |
| 1:A:1385:C:H2' | 1:A:1386:C:C6 | 2.50 | 0.46 |
| 1:A:1494:G:H2' | 1:A:1496:A:OP2 | 2.15 | 0.46 |
| 1:A:355:U:O2' | 1:A:356:A:H5' | 2.16 | 0.46 |
| 1:A:370:A:C6 | 1:A:371:U:C4 | 3.04 | 0.46 |
| 1:A:377:C:H2' | 1:A:378:A:O4' | 2.15 | 0.46 |
| 1:A:406:G:C2 | 1:A:425:U:C2 | 3.04 | 0.46 |
| 1:A:429:C:H2' | 1:A:430:U:H6 | 1.80 | 0.46 |
| 1:A:604:C:H2' | 1:A:605:A:O4' | 2.15 | 0.46 |
| 1:A:803:A:C4' | 1:A:804:U:OP2 | 2.63 | 0.46 |
| 1:A:873:G:C6 | 1:A:874:C:N4 | 2.82 | 0.46 |
| 2:B:90:MET:HB3 | 2:B:91:PRO:HD2 | 1.98 | 0.46 |
| 3:C:32:LEU:HD21 | 3:C:59:ARG:CD | 2.40 | 0.46 |
| 3:C:49:SER:O | 3:C:51:GLY:N | 2.49 | 0.46 |
| 7:G:87:VAL:HG22 | 7:G:154:TYR:HD1 | 1.79 | 0.46 |
| 8:H:18:ARG:HG3 | 8:H:18:ARG:NH1 | 2.31 | 0.46 |
| 9:I:10:ARG:HE | 9:I:11:LYS:HB2 | 1.80 | 0.46 |
| 9:I:111:ARG:HD3 | 9:I:112:LYS:C | 2.35 | 0.46 |
| 13:M:23:TYR:CD2 | 13:M:70:LEU:HB3 | 2.51 | 0.46 |
| 1:A:225:U:O2' | 16:P:23:ASP:OD2 | 2.33 | 0.46 |
| 17:Q:82:MET:O | 17:Q:83:ASP:C | 2.54 | 0.46 |
| 19:S:50:ALA:HA | 19:S:58:VAL:O | 2.15 | 0.46 |
| 20:T:96:GLY:O | 20:T:97:ALA:HB3 | 2.16 | 0.46 |
| 21:U:6:ARG:HD2 | 21:U:15:ARG:NH1 | 2.30 | 0.46 |
| 1:A:10:G:H5' | 5:E:122:GLU:OE2 | 2.14 | 0.46 |
| 1:A:1152:A:O5' | 1:A:1152:A:H8 | 1.97 | 0.46 |
| 1:A:1177:C:H2' | 1:A:1179:G:H5' | 1.97 | 0.46 |
| 1:A:1293:G:N7 | 19:S:2:PRO:HA | 2.30 | 0.46 |
| 1:A:1337:G:O2' | 1:A:1338:G:H5' | 2.16 | 0.46 |
| 1:A:1335:G:N2 | 1:A:1353:G:C4 | 2.84 | 0.46 |
| 1:A:198:G:O2' | 1:A:199:U:H5' | 2.15 | 0.46 |
| 1:A:424:G:C4 | 1:A:426:A:C6 | 3.04 | 0.46 |
| 1:A:458:A:H2' | 1:A:459:G:O4' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:626:A:H2' | 1:A:627:C:C6 | 2.50 | 0.46 |
| 1:A:757:G:C4 | 1:A:758:G:C8 | 3.04 | 0.46 |
| 2:B:125:PRO:O | 2:B:127:ILE:N | 2.48 | 0.46 |
| 4:D:11:LEU:C | 4:D:13:ARG:N | 2.66 | 0.46 |
| 4:D:203:VAL:O | 4:D:204:ILE:C | 2.54 | 0.46 |
| 4:D:53:ASP:O | 4:D:57:ARG:CD | 2.62 | 0.46 |
| 5:E:95:ALA:HB1 | 5:E:96:PRO:HD2 | 1.97 | 0.46 |
| 6:F:53:ALA:O | 6:F:55:ASP:N | 2.48 | 0.46 |
| 7:G:65:ALA:HB1 | 7:G:127:ALA:HB1 | 1.96 | 0.46 |
| 9:I:108:VAL:CG1 | 9:I:109:VAL:N | 2.74 | 0.46 |
| 1:A:1349:C:O2' | 10:J:60:ARG:NH2 | 2.48 | 0.46 |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:HD2 | 1.81 | 0.46 |
| 13:M:45:VAL:O | 13:M:48:LEU:HB2 | 2.15 | 0.46 |
| 15:O:51:HIS:ND1 | 15:O:51:HIS:N | 2.61 | 0.46 |
| 20:T:23:ARG:HH11 | 20:T:23:ARG:HG2 | 1.81 | 0.46 |
| 1:A:1283:U:HO2' | 1:A:1284:U:P | 2.38 | 0.46 |
| 1:A:32:G:N1 | 1:A:49:C:H5'' | 2.30 | 0.46 |
| 1:A:501:G:HO2' | 1:A:514:G:C4' | 2.26 | 0.46 |
| 1:A:62:G:H2' | 1:A:63:U:O4' | 2.15 | 0.46 |
| 1:A:936:A:C6 | 1:A:937:A:N1 | 2.84 | 0.46 |
| 2:B:69:LEU:HB3 | 2:B:162:ILE:HG12 | 1.98 | 0.46 |
| 4:D:100:ARG:HB3 | 4:D:102:ASP:OD1 | 2.15 | 0.46 |
| 4:D:57:ARG:NH2 | 5:E:107:ARG:HD3 | 2.30 | 0.46 |
| 7:G:103:TRP:CD1 | 7:G:137:LYS:HD3 | 2.50 | 0.46 |
| 7:G:23:VAL:O | 7:G:27:ILE:HG13 | 2.15 | 0.46 |
| 7:G:64:GLN:HG3 | 7:G:68:ASN:HD21 | 1.80 | 0.46 |
| 9:I:9:ARG:CG | 9:I:14:VAL:HG22 | 2.43 | 0.46 |
| 1:A:1160:G:P | 9:I:97:LYS:NZ | 2.88 | 0.46 |
| 10:J:29:ARG:HB2 | 10:J:84:GLN:NE2 | 2.26 | 0.46 |
| 10:J:15:THR:HG23 | 10:J:94:VAL:CG2 | 2.45 | 0.46 |
| 13:M:59:TYR:O | 13:M:63:THR:HB | 2.15 | 0.46 |
| 15:O:36:ILE:HG12 | 15:O:59:MET:HE3 | 1.98 | 0.46 |
| 15:O:75:PRO:HG2 | 15:O:76:GLU:H | 1.81 | 0.46 |
| 18:R:40:LEU:CB | 18:R:79:LEU:HD11 | 2.45 | 0.46 |
| 19:S:30:LEU:CD2 | 19:S:31:ILE:H | 2.29 | 0.46 |
| 1:A:1231:C:H2' | 1:A:1232:A:H5' | 1.97 | 0.46 |
| 1:A:1438:A:H2' | 1:A:1439:G:O4' | 2.15 | 0.46 |
| 1:A:1486:G:C4 | 1:A:1487:C:C5 | 3.03 | 0.46 |
| 1:A:198:G:C6 | 1:A:199:U:C4 | 3.04 | 0.46 |
| 1:A:542:G:H2' | 1:A:543:A:C2 | 2.51 | 0.46 |
| 1:A:609:G:C6 | 1:A:610:U:C4 | 3.04 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:676:U:H2' | 1:A:678:A:OP2 | 2.16 | 0.46 |
| 1:A:776:A:H4' | 1:A:777:U:C5' | 2.44 | 0.46 |
| 1:A:6:U:O2' | 1:A:7:G:N3 | 2.47 | 0.46 |
| 1:A:902:C:C6 | 1:A:902:C:H3' | 2.51 | 0.46 |
| 1:A:905:G:O2' | 1:A:906:G:H5' | 2.16 | 0.46 |
| 3:C:70:VAL:HG12 | 3:C:71:ALA:N | 2.31 | 0.46 |
| 3:C:76:VAL:O | 3:C:83:ARG:HB3 | 2.16 | 0.46 |
| 5:E:109:ILE:HD12 | 5:E:135:THR:CG2 | 2.44 | 0.46 |
| 5:E:59:GLY:O | 5:E:63:ARG:HB2 | 2.14 | 0.46 |
| 7:G:69:VAL:O | 7:G:69:VAL:HG12 | 2.15 | 0.46 |
| 9:I:43:ALA:O | 9:I:44:VAL:C | 2.53 | 0.46 |
| 1:A:691:C:H4' | 11:K:20:TYR:CD1 | 2.51 | 0.46 |
| 11:K:91:ARG:NH1 | 18:R:88:LYS:HE3 | 2.31 | 0.46 |
| 13:M:29:ARG:O | 13:M:32:GLU:N | 2.49 | 0.46 |
| 18:R:19:LYS:HD2 | 18:R:19:LYS:N | 2.31 | 0.46 |
| 19:S:19:VAL:O | 19:S:22:LEU:HB2 | 2.16 | 0.46 |
| 1:A:1004:U:H2' | 1:A:1005:G:C8 | 2.50 | 0.46 |
| 1:A:1169:G:C6 | 1:A:1170:A:C5 | 3.04 | 0.46 |
| 1:A:1282:G:O2' | 1:A:1283:U:O5' | 2.34 | 0.46 |
| 1:A:1438:A:C6 | 1:A:1439:G:C4 | 3.03 | 0.46 |
| 1:A:905:G:H4' | 1:A:1481:A:N7 | 2.30 | 0.46 |
| 1:A:441:G:H2' | 1:A:442:G:C5' | 2.46 | 0.46 |
| 2:B:101:MET:HG3 | 2:B:108:ILE:HD13 | 1.98 | 0.46 |
| 3:C:147:LYS:O | 3:C:203:PHE:HD2 | 1.99 | 0.46 |
| 4:D:18:LYS:HD3 | 4:D:20:TYR:HE2 | 1.81 | 0.46 |
| 5:E:147:ASP:N | 5:E:147:ASP:OD2 | 2.35 | 0.46 |
| 7:G:42:ILE:HG23 | 7:G:117:ALA:HA | 1.98 | 0.46 |
| 10:J:33:GLN:HG2 | 10:J:33:GLN:O | 2.16 | 0.46 |
| 10:J:61:GLU:OE1 | 10:J:63:PHE:CZ | 2.69 | 0.46 |
| 16:P:57:ARG:CZ | 16:P:79:VAL:O | 2.63 | 0.46 |
| 18:R:74:ARG:HA | 18:R:79:LEU:O | 2.15 | 0.46 |
| 1:A:100:C:C5 | 20:T:15:ARG:NH2 | 2.84 | 0.46 |
| 1:A:1199:C:H2' | 1:A:1200:C:O4' | 2.16 | 0.46 |
| 22:A:1524:KSG:H91 | 22:A:1524:KSG:C13 | 2.46 | 0.46 |
| 1:A:431:C:H2' | 1:A:432:C:H6 | 1.81 | 0.46 |
| 1:A:79:G:H3' | 1:A:80:U:C5' | 2.45 | 0.46 |
| 3:C:65:ALA:O | 3:C:66:VAL:HB | 2.16 | 0.46 |
| 3:C:72:LYS:C | 3:C:74:GLY:N | 2.68 | 0.46 |
| 4:D:105:VAL:HG13 | 4:D:110:PHE:HB2 | 1.98 | 0.46 |
| 7:G:23:VAL:CG1 | 7:G:43:PHE:CE2 | 2.99 | 0.46 |
| 1:A:1361:C:OP1 | 7:G:6:ARG:O | 2.34 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:4:ASP:OD2 | 8:H:89:PRO:HD3 | 2.16 | 0.46 |
| 11:K:48:ILE:HD11 | 11:K:64:ALA:CA | 2.46 | 0.46 |
| 1:A:523:A:OP1 | 12:L:114:LYS:HE2 | 2.15 | 0.46 |
| 13:M:52:GLU:O | 13:M:53:VAL:C | 2.54 | 0.46 |
| 1:A:1421:G:C2 | 1:A:1442:G:N3 | 2.84 | 0.46 |
| 1:A:179:G:H2' | 1:A:180:A:C8 | 2.44 | 0.46 |
| 1:A:435:A:C4 | 1:A:481:A:C2 | 3.03 | 0.46 |
| 1:A:495:C:HO2' | 1:A:496:U:P | 2.38 | 0.46 |
| 1:A:517:A:O2' | 1:A:518:U:P | 2.74 | 0.46 |
| 1:A:559:G:O2' | 1:A:560:G:P | 2.74 | 0.46 |
| 1:A:982:G:C5 | 1:A:983:A:N3 | 2.84 | 0.46 |
| 3:C:68:VAL:HG12 | 3:C:70:VAL:HG23 | 1.98 | 0.46 |
| 4:D:165:MET:HE2 | 4:D:176:LEU:HD11 | 1.98 | 0.46 |
| 4:D:63:LYS:HG2 | 4:D:64:LEU:N | 2.31 | 0.46 |
| 4:D:64:LEU:HB2 | 4:D:198:VAL:HG11 | 1.98 | 0.46 |
| 4:D:67:ILE:HG22 | 4:D:68:TYR:CD1 | 2.51 | 0.46 |
| 5:E:80:ILE:HD11 | 5:E:91:LEU:HB2 | 1.96 | 0.46 |
| 6:F:1:MET:HG2 | 6:F:68:PRO:HA | 1.97 | 0.46 |
| 8:H:58:TYR:O | 8:H:59:LEU:HD23 | 2.16 | 0.46 |
| 8:H:69:ARG:HB2 | 8:H:74:PRO:HA | 1.98 | 0.46 |
| 8:H:85:ARG:HD3 | 8:H:88:LYS:HG2 | 1.97 | 0.46 |
| 9:I:32:ASP:O | 9:I:34:ASN:N | 2.49 | 0.46 |
| 10:J:33:GLN:O | 10:J:34:VAL:O | 2.33 | 0.46 |
| 11:K:18:ARG:HB2 | 11:K:33:THR:CG2 | 2.46 | 0.46 |
| 12:L:59:ARG:CZ | 12:L:65:GLU:HG3 | 2.45 | 0.46 |
| 1:A:100:C:H2' | 1:A:101:G:H8 | 1.81 | 0.46 |
| 1:A:1291:G:C5 | 1:A:1311:A:C2 | 3.03 | 0.46 |
| 1:A:1319:G:H5'' | 1:A:1320:G:OP1 | 2.15 | 0.46 |
| 1:A:1501:G:O2' | 1:A:1502:C:H5' | 2.16 | 0.46 |
| 1:A:402:G:H1' | 1:A:480:A:N1 | 2.31 | 0.46 |
| 1:A:744:G:H2' | 1:A:745:G:C5' | 2.46 | 0.46 |
| 1:A:805:G:H2' | 1:A:806:C:C6 | 2.51 | 0.46 |
| 1:A:863:G:C2 | 1:A:864:G:C8 | 3.04 | 0.46 |
| 1:A:868:G:O2' | 1:A:869:U:P | 2.73 | 0.46 |
| 1:A:86:U:H2' | 1:A:87:C:C6 | 2.50 | 0.46 |
| 3:C:35:GLU:OE2 | 3:C:59:ARG:NH1 | 2.47 | 0.46 |
| 4:D:194:LEU:CD2 | 4:D:194:LEU:H | 2.28 | 0.46 |
| 4:D:64:LEU:HD12 | 4:D:75:PHE:HE1 | 1.80 | 0.46 |
| 8:H:111:ILE:C | 8:H:134:ILE:HD12 | 2.36 | 0.46 |
| 11:K:29:ILE:HA | 11:K:44:SER:HA | 1.98 | 0.46 |
| 1:A:859:G:P | 12:L:12:ARG:HH22 | 2.38 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:P:58:TYR:CD1 | 16:P:59:TRP:N | 2.84 | 0.46 |
| 18:R:53:ARG:HG2 | 18:R:63:GLN:CG | 2.44 | 0.46 |
| 18:R:75:ILE:O | 18:R:77:GLY:N | 2.44 | 0.46 |
| 19:S:17:GLU:HA | 19:S:20:LEU:HG | 1.98 | 0.46 |
| 19:S:17:GLU:O | 19:S:21:GLU:HG3 | 2.16 | 0.46 |
| 1:A:1302:C:N4 | 19:S:36:ARG:HG3 | 2.31 | 0.46 |
| 19:S:51:VAL:HG12 | 19:S:52:TYR:H | 1.80 | 0.46 |
| 20:T:61:SER:O | 20:T:62:LEU:C | 2.54 | 0.46 |
| 20:T:68:LYS:HA | 20:T:68:LYS:HD2 | 1.72 | 0.46 |
| 1:A:1055:G:C6 | 1:A:1087:G:C2 | 3.04 | 0.45 |
| 1:A:1107:G:C8 | 1:A:1128:C:C5 | 3.04 | 0.45 |
| 1:A:1315:A:C5 | 1:A:1316:G:C8 | 3.03 | 0.45 |
| 1:A:1424:G:H4' | 1:A:1425:G:N7 | 2.31 | 0.45 |
| 1:A:242:A:O3' | 1:A:243:G:H4' | 2.16 | 0.45 |
| 1:A:244:C:C2' | 1:A:245:U:H5' | 2.46 | 0.45 |
| 1:A:274:G:OP2 | 17:Q:41:LYS:NZ | 2.46 | 0.45 |
| 1:A:686:A:H5'' | 1:A:687:G:C8 | 2.51 | 0.45 |
| 1:A:685:C:O2' | 1:A:686:A:OP2 | 2.24 | 0.45 |
| 1:A:850:A:C4 | 1:A:852:G:N7 | 2.84 | 0.45 |
| 2:B:119:GLU:CD | 2:B:153:ARG:HH22 | 2.20 | 0.45 |
| 4:D:50:ARG:HA | 4:D:51:PRO:HD3 | 1.82 | 0.45 |
| 9:I:69:GLY:C | 9:I:73:GLN:HG3 | 2.36 | 0.45 |
| 10:J:38:ILE:CG1 | 10:J:71:LEU:HB3 | 2.46 | 0.45 |
| 15:O:45:VAL:HG12 | 15:O:46:HIS:N | 2.31 | 0.45 |
| 18:R:40:LEU:O | 18:R:43:PHE:N | 2.48 | 0.45 |
| 1:A:1302:C:H42 | 19:S:36:ARG:HG3 | 1.81 | 0.45 |
| 1:A:16:G:C2 | 1:A:17:A:C4 | 3.05 | 0.45 |
| 1:A:405:G:H2' | 1:A:406:G:O4' | 2.16 | 0.45 |
| 1:A:56:A:C2 | 1:A:57:U:C1' | 2.99 | 0.45 |
| 1:A:56:A:C2' | 1:A:57:U:H5' | 2.47 | 0.45 |
| 1:A:846:C:H5' | 1:A:851:A:N6 | 2.32 | 0.45 |
| 1:A:953:A:O2' | 1:A:954:G:P | 2.74 | 0.45 |
| 2:B:123:ALA:N | 2:B:127:ILE:HD11 | 2.31 | 0.45 |
| 3:C:165:THR:CG2 | 3:C:166:GLU:N | 2.79 | 0.45 |
| 4:D:209:ARG:NH1 | 4:D:209:ARG:HG2 | 2.30 | 0.45 |
| 5:E:101:ILE:HG22 | 5:E:101:ILE:O | 2.16 | 0.45 |
| 6:F:24:GLU:O | 6:F:25:ILE:C | 2.53 | 0.45 |
| 7:G:111:ARG:NH1 | 7:G:122:HIS:HB3 | 2.32 | 0.45 |
| 7:G:113:GLU:O | 7:G:119:ARG:NH1 | 2.45 | 0.45 |
| 7:G:122:HIS:HA | 7:G:125:MET:HE3 | 1.98 | 0.45 |
| 7:G:20:ASP:OD1 | 7:G:22:LEU:HB3 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:18:ARG:HG3 | 8:H:18:ARG:HH11 | 1.81 | 0.45 |
| 9:I:65:VAL:HG13 | 9:I:65:VAL:O | 2.15 | 0.45 |
| 10:J:61:GLU:CD | 14:N:45:ARG:NH1 | 2.69 | 0.45 |
| 12:L:68:ALA:HB1 | 12:L:100:ILE:HG13 | 1.98 | 0.45 |
| 18:R:48:GLY:HA3 | 18:R:82:THR:HA | 1.99 | 0.45 |
| 20:T:58:LYS:O | 20:T:62:LEU:HG | 2.15 | 0.45 |
| 1:A:1169:G:C6 | 1:A:1170:A:C6 | 3.04 | 0.45 |
| 1:A:1332:A:H2' | 1:A:1333:U:C6 | 2.52 | 0.45 |
| 1:A:1350:C:H5'' | 9:I:114:TYR:HB2 | 1.99 | 0.45 |
| 1:A:382:C:O2' | 1:A:383:U:H5' | 2.16 | 0.45 |
| 1:A:764:A:C2 | 1:A:787:G:C6 | 3.04 | 0.45 |
| 1:A:787:G:H2' | 1:A:788:U:O4' | 2.16 | 0.45 |
| 1:A:879:A:C5 | 1:A:880:G:H1' | 2.52 | 0.45 |
| 1:A:964:A:C6 | 1:A:1202:G:C6 | 3.04 | 0.45 |
| 4:D:23:GLY:HA3 | 4:D:112:VAL:HG12 | 1.97 | 0.45 |
| 4:D:176:LEU:HA | 4:D:183:GLY:HA2 | 1.96 | 0.45 |
| 5:E:115:VAL:HG11 | 5:E:118:ILE:CD1 | 2.46 | 0.45 |
| 5:E:89:ILE:HD13 | 5:E:90:VAL:C | 2.36 | 0.45 |
| 6:F:45:LEU:O | 6:F:46:ARG:HG2 | 2.16 | 0.45 |
| 7:G:31:MET:SD | 7:G:36:LYS:HB2 | 2.56 | 0.45 |
| 9:I:63:ILE:CD1 | 9:I:77:ILE:HG23 | 2.46 | 0.45 |
| 10:J:7:LYS:HG3 | 10:J:71:LEU:CD2 | 2.46 | 0.45 |
| 11:K:94:ALA:O | 11:K:97:ALA:HB3 | 2.16 | 0.45 |
| 12:L:37:CYS:HA | 12:L:57:LYS:O | 2.17 | 0.45 |
| 12:L:59:ARG:NE | 12:L:65:GLU:HG3 | 2.31 | 0.45 |
| 14:N:22:THR:O | 14:N:23:ARG:HB2 | 2.16 | 0.45 |
| 15:O:87:ILE:CG2 | 15:O:88:ARG:N | 2.77 | 0.45 |
| 16:P:20:VAL:HG23 | 16:P:35:LYS:HA | 1.99 | 0.45 |
| 19:S:17:GLU:HA | 19:S:20:LEU:CD2 | 2.47 | 0.45 |
| 19:S:42:PRO:O | 19:S:44:MET:N | 2.49 | 0.45 |
| 19:S:44:MET:O | 19:S:45:VAL:C | 2.54 | 0.45 |
| 1:A:1043:C:OP1 | 14:N:45:ARG:NH2 | 2.50 | 0.45 |
| 1:A:120:G:H2' | 1:A:121:G:O4' | 2.16 | 0.45 |
| 1:A:1356:G:H5'' | 7:G:36:LYS:HB3 | 1.98 | 0.45 |
| 1:A:1499:G:H2' | 1:A:1500:U:C6 | 2.51 | 0.45 |
| 1:A:241:C:C2 | 1:A:280:G:C2 | 3.04 | 0.45 |
| 1:A:626:A:H2' | 1:A:627:C:H6 | 1.82 | 0.45 |
| 1:A:718:G:H21 | 18:R:75:ILE:HD11 | 1.81 | 0.45 |
| 1:A:820:G:C6 | 1:A:829:G:C5 | 3.05 | 0.45 |
| 2:B:93:VAL:HG21 | 2:B:97:TRP:CD1 | 2.51 | 0.45 |
| 6:F:32:ASN:HD22 | 6:F:32:ASN:N | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 6:F:4:TYR:CZ | 6:F:72:VAL:HG21 | 2.51 | 0.45 |
| 7:G:42:ILE:CG2 | 7:G:117:ALA:HA | 2.47 | 0.45 |
| 1:A:1100:G:H4' | 9:I:104:ARG:NH1 | 2.32 | 0.45 |
| 1:A:1331:A:H5'' | 9:I:121:ARG:HB2 | 1.99 | 0.45 |
| 9:I:63:ILE:HG22 | 9:I:64:THR:N | 2.32 | 0.45 |
| 9:I:95:LYS:O | 9:I:98:PRO:HD2 | 2.17 | 0.45 |
| 10:J:24:VAL:HG12 | 10:J:28:ARG:HD2 | 1.98 | 0.45 |
| 1:A:891:A:O5' | 12:L:47:LYS:NZ | 2.50 | 0.45 |
| 12:L:6:THR:O | 12:L:9:GLN:HB2 | 2.16 | 0.45 |
| 13:M:10:PRO:HG2 | 13:M:10:PRO:O | 2.16 | 0.45 |
| 15:O:61:GLY:O | 15:O:64:ARG:HG2 | 2.16 | 0.45 |
| 1:A:1287:G:H5'' | 21:U:4:GLY:C | 2.36 | 0.45 |
| 1:A:1063:A:O3' | 5:E:16:THR:OG1 | 2.35 | 0.45 |
| 1:A:1127:G:N2 | 1:A:1129:A:N6 | 2.61 | 0.45 |
| 1:A:1301:A:P | 19:S:5:LEU:HD21 | 2.57 | 0.45 |
| 1:A:1379:A:H4' | 1:A:1380:C:H5'' | 1.98 | 0.45 |
| 1:A:1387:C:H2' | 1:A:1388:G:C8 | 2.52 | 0.45 |
| 1:A:1395:C:H2' | 1:A:1396:A:H8 | 1.80 | 0.45 |
| 1:A:237:C:O2' | 1:A:238:C:H5' | 2.16 | 0.45 |
| 1:A:281:G:C2' | 1:A:282:G:H5' | 2.45 | 0.45 |
| 1:A:398:G:C2' | 1:A:399:C:H5' | 2.47 | 0.45 |
| 1:A:441:G:O2' | 1:A:442:G:H5' | 2.17 | 0.45 |
| 1:A:453:C:H2' | 1:A:454:G:H8 | 1.81 | 0.45 |
| 1:A:491:C:H2' | 1:A:492:C:H5 | 1.81 | 0.45 |
| 1:A:503:C:H2' | 1:A:504:A:C8 | 2.51 | 0.45 |
| 1:A:58:G:C5 | 1:A:59:C:C4 | 3.05 | 0.45 |
| 1:A:641:G:N2 | 1:A:734:G:C8 | 2.85 | 0.45 |
| 1:A:744:G:C2 | 17:Q:103:GLY:O | 2.70 | 0.45 |
| 1:A:79:G:H2' | 1:A:80:U:H5'' | 1.99 | 0.45 |
| 2:B:114:ARG:O | 2:B:114:ARG:HD2 | 2.16 | 0.45 |
| 3:C:173:VAL:N | 3:C:174:PRO:CD | 2.80 | 0.45 |
| 5:E:16:THR:HG23 | 5:E:16:THR:O | 2.17 | 0.45 |
| 6:F:23:LYS:HE2 | 6:F:23:LYS:HB3 | 1.75 | 0.45 |
| 6:F:75:LEU:HD13 | 6:F:75:LEU:C | 2.36 | 0.45 |
| 11:K:106:LYS:HD3 | 11:K:106:LYS:HA | 1.84 | 0.45 |
| 13:M:84:ILE:HG13 | 13:M:86:CYS:CB | 2.46 | 0.45 |
| 15:O:61:GLY:O | 15:O:62:GLN:C | 2.54 | 0.45 |
| 17:Q:29:HIS:HB2 | 17:Q:36:ILE:CG2 | 2.47 | 0.45 |
| 20:T:38:LYS:O | 20:T:41:ILE:N | 2.49 | 0.45 |
| 1:A:985:C:O2 | 1:A:1003:G:H1' | 2.17 | 0.45 |
| 1:A:100:C:H2' | 1:A:101:G:C8 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1259:C:HO2' | 1:A:1261:A:H8 | 1.60 | 0.45 |
| 1:A:1284:U:O2' | 1:A:1285:C:OP1 | 2.30 | 0.45 |
| 1:A:1216:C:H5' | 1:A:1347:U:HO2' | 1.82 | 0.45 |
| 1:A:1410:U:H2' | 1:A:1411:A:C8 | 2.51 | 0.45 |
| 1:A:172:C:H2' | 1:A:173:C:H6 | 1.82 | 0.45 |
| 1:A:190:U:C5 | 17:Q:72:ARG:NH2 | 2.85 | 0.45 |
| 1:A:535:U:C2 | 1:A:536:U:C5 | 3.05 | 0.45 |
| 1:A:548:C:N1 | 17:Q:31:LEU:HD11 | 2.31 | 0.45 |
| 1:A:758:G:O2' | 1:A:759:G:H5' | 2.15 | 0.45 |
| 1:A:757:G:C6 | 1:A:791:A:C6 | 3.05 | 0.45 |
| 1:A:845:G:HO2' | 1:A:851:A:N6 | 2.15 | 0.45 |
| 2:B:206:ASP:O | 2:B:207:ALA:HB3 | 2.17 | 0.45 |
| 3:C:113:ALA:N | 3:C:114:PRO:CD | 2.79 | 0.45 |
| 3:C:160:ALA:C | 3:C:162:GLN:H | 2.19 | 0.45 |
| 4:D:173:TRP:CD1 | 4:D:174:LEU:HD21 | 2.52 | 0.45 |
| 4:D:68:TYR:CD2 | 4:D:97:LEU:HB3 | 2.51 | 0.45 |
| 5:E:74:GLY:HA3 | 5:E:116:THR:HG22 | 1.99 | 0.45 |
| 5:E:37:ARG:NH1 | 5:E:37:ARG:HG2 | 2.31 | 0.45 |
| 8:H:63:LEU:HD23 | 8:H:65:TYR:OH | 2.17 | 0.45 |
| 9:I:3:GLN:HB3 | 9:I:3:GLN:HE21 | 1.53 | 0.45 |
| 9:I:69:GLY:O | 9:I:70:LYS:C | 2.53 | 0.45 |
| 10:J:92:THR:O | 10:J:92:THR:CG2 | 2.65 | 0.45 |
| 11:K:66:LEU:O | 11:K:67:ASP:C | 2.54 | 0.45 |
| 13:M:18:ALA:O | 13:M:19:LEU:C | 2.54 | 0.45 |
| 17:Q:68:ARG:O | 17:Q:69:LYS:CB | 2.63 | 0.45 |
| 18:R:51:LEU:HA | 18:R:52:PRO:HD3 | 1.76 | 0.45 |
| 1:A:1178:U:H4' | 1:A:1179:G:OP2 | 2.16 | 0.45 |
| 1:A:1335:G:N2 | 1:A:1353:G:N3 | 2.65 | 0.45 |
| 1:A:411:A:H2' | 1:A:412:G:O4' | 2.17 | 0.45 |
| 1:A:428:A:C8 | 1:A:429:C:C5 | 3.04 | 0.45 |
| 1:A:293:G:H4' | 1:A:541:G:H4' | 1.99 | 0.45 |
| 1:A:802:G:H3' | 1:A:803:A:H5'' | 1.96 | 0.45 |
| 1:A:803:A:C5' | 1:A:804:U:OP2 | 2.64 | 0.45 |
| 1:A:816:C:H2' | 1:A:817:U:O4' | 2.17 | 0.45 |
| 1:A:971:G:H4' | 1:A:972:A:OP2 | 2.16 | 0.45 |
| 1:A:985:C:N3 | 1:A:1002:G:O6 | 2.50 | 0.45 |
| 3:C:152:ILE:CG2 | 3:C:153:VAL:N | 2.80 | 0.45 |
| 3:C:154:SER:OG | 3:C:197:GLY:N | 2.47 | 0.45 |
| 3:C:182:ILE:HA | 3:C:202:ILE:O | 2.15 | 0.45 |
| 3:C:39:ILE:C | 3:C:41:GLY:N | 2.69 | 0.45 |
| 4:D:71:SER:O | 4:D:72:GLU:C | 2.54 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:37:ASN:O | 7:G:40:ALA:N | 2.50 | 0.45 |
| 8:H:104:ARG:NH2 | 8:H:138:TRP:CZ3 | 2.84 | 0.45 |
| 1:A:702:G:C4' | 11:K:117:ASN:ND2 | 2.78 | 0.45 |
| 13:M:81:LEU:O | 13:M:86:CYS:HB3 | 2.17 | 0.45 |
| 15:O:10:LYS:CG | 15:O:11:VAL:N | 2.80 | 0.45 |
| 16:P:69:THR:O | 16:P:73:LEU:HG | 2.16 | 0.45 |
| 20:T:56:MET:O | 20:T:57:ARG:C | 2.55 | 0.45 |
| 1:A:1110:G:N2 | 1:A:1129:A:H62 | 2.15 | 0.45 |
| 1:A:1281:A:C5 | 1:A:1283:U:O2 | 2.70 | 0.45 |
| 1:A:1315:A:H2' | 1:A:1316:G:O4' | 2.16 | 0.45 |
| 1:A:1401:A:H3' | 1:A:1402:G:H8 | 1.82 | 0.45 |
| 1:A:317:A:H2' | 1:A:318:C:C6 | 2.51 | 0.45 |
| 1:A:360:A:H2' | 1:A:361:U:O2 | 2.16 | 0.45 |
| 1:A:410:A:OP2 | 1:A:424:G:N2 | 2.50 | 0.45 |
| 1:A:413:C:H6 | 1:A:413:C:O5' | 2.00 | 0.45 |
| 1:A:469:G:O2' | 1:A:470:G:P | 2.75 | 0.45 |
| 1:A:483:A:H4' | 1:A:484:G:H5' | 1.98 | 0.45 |
| 1:A:61:A:H1' | 1:A:62:G:O4' | 2.17 | 0.45 |
| 1:A:753:G:C2 | 1:A:754:C:C6 | 3.05 | 0.45 |
| 1:A:856:G:H5' | 8:H:89:PRO:HG2 | 1.98 | 0.45 |
| 1:A:805:G:C2 | 1:A:858:C:N3 | 2.85 | 0.45 |
| 2:B:148:TYR:HD2 | 2:B:148:TYR:N | 2.13 | 0.45 |
| 2:B:73:THR:CG2 | 2:B:96:ARG:CZ | 2.95 | 0.45 |
| 3:C:151:VAL:CG1 | 3:C:152:ILE:N | 2.80 | 0.45 |
| 5:E:115:VAL:HG13 | 5:E:116:THR:N | 2.32 | 0.45 |
| 1:A:1232:A:H5' | 9:I:68:GLY:O | 2.17 | 0.45 |
| 9:I:78:LYS:O | 9:I:79:LEU:C | 2.53 | 0.45 |
| 9:I:89:ASN:O | 9:I:92:TYR:HB2 | 2.17 | 0.45 |
| 10:J:29:ARG:C | 10:J:84:GLN:HE22 | 2.19 | 0.45 |
| 10:J:85:LEU:O | 10:J:86:MET:C | 2.55 | 0.45 |
| 13:M:71:ARG:O | 13:M:72:ALA:C | 2.55 | 0.45 |
| 13:M:86:CYS:SG | 13:M:88:ARG:HB3 | 2.57 | 0.45 |
| 13:M:96:LEU:HB3 | 13:M:97:PRO:CD | 2.40 | 0.45 |
| 1:A:459:G:OP2 | 16:P:75:ARG:NH1 | 2.50 | 0.45 |
| 17:Q:43:LEU:CD1 | 17:Q:68:ARG:HH12 | 2.28 | 0.45 |
| 19:S:40:ILE:HG23 | 19:S:44:MET:SD | 2.57 | 0.45 |
| 1:A:1174:C:H2' | 1:A:1175:G:O4' | 2.17 | 0.45 |
| 1:A:1239:U:H4' | 1:A:1240:G:O5' | 2.16 | 0.45 |
| 1:A:1273:G:H4' | 9:I:38:GLN:O | 2.17 | 0.45 |
| 1:A:1423:C:O2' | 1:A:1424:G:H5' | 2.17 | 0.45 |
| 1:A:1437:C:O2' | 1:A:1438:A:H5' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:168:U:H6 | 1:A:205:G:HO2' | 1.62 | 0.45 |
| 1:A:186:C:O2' | 1:A:187:C:H5' | 2.17 | 0.45 |
| 1:A:198:G:C5 | 1:A:199:U:C5 | 3.04 | 0.45 |
| 1:A:418:C:O2' | 1:A:419:G:H5'' | 2.17 | 0.45 |
| 1:A:502:C:H5'' | 1:A:503:C:C6 | 2.52 | 0.45 |
| 1:A:51:A:N6 | 1:A:357:G:C4' | 2.80 | 0.45 |
| 1:A:586:A:C2 | 1:A:587:U:C2 | 3.05 | 0.45 |
| 1:A:641:G:H2' | 1:A:642:G:H8 | 1.81 | 0.45 |
| 1:A:954:G:C8 | 1:A:1340:U:O2 | 2.70 | 0.45 |
| 2:B:89:GLY:N | 2:B:226:ARG:HH22 | 2.14 | 0.45 |
| 2:B:229:VAL:HG12 | 2:B:229:VAL:O | 2.16 | 0.45 |
| 3:C:108:ASN:ND2 | 3:C:111:LEU:HG | 2.31 | 0.45 |
| 3:C:51:GLY:O | 3:C:71:ALA:N | 2.42 | 0.45 |
| 3:C:92:ALA:C | 3:C:94:LEU:N | 2.70 | 0.45 |
| 6:F:37:VAL:HG12 | 6:F:39:LYS:H | 1.82 | 0.45 |
| 7:G:27:ILE:HG13 | 7:G:27:ILE:H | 1.64 | 0.45 |
| 12:L:42:THR:CG2 | 12:L:52:LEU:HB3 | 2.47 | 0.45 |
| 15:O:46:HIS:C | 15:O:48:LYS:H | 2.20 | 0.45 |
| 15:O:39:LEU:HD13 | 15:O:56:LEU:CA | 2.46 | 0.45 |
| 20:T:29:LYS:O | 20:T:32:ALA:HB3 | 2.17 | 0.45 |
| 21:U:5:ASP:O | 21:U:8:THR:HG23 | 2.16 | 0.45 |
| 1:A:1030:G:O2' | 1:A:1031:G:H5' | 2.17 | 0.45 |
| 1:A:1216:C:C2 | 1:A:1217:U:C5 | 3.05 | 0.45 |
| 1:A:1287:G:N2 | 1:A:1313:G:HO2' | 2.15 | 0.45 |
| 1:A:468:C:H2' | 1:A:469:G:N7 | 2.32 | 0.45 |
| 1:A:750:A:C8 | 1:A:798:A:C6 | 3.05 | 0.45 |
| 1:A:970:U:HO2' | 1:A:971:G:P | 2.38 | 0.45 |
| 2:B:108:ILE:C | 2:B:110:GLN:N | 2.70 | 0.45 |
| 2:B:115:LEU:O | 2:B:116:GLU:C | 2.55 | 0.45 |
| 2:B:135:GLN:O | 2:B:139:LYS:HB2 | 2.17 | 0.45 |
| 3:C:101:LEU:O | 3:C:101:LEU:HD22 | 2.17 | 0.45 |
| 4:D:173:TRP:CD2 | 4:D:189:PRO:HB3 | 2.52 | 0.45 |
| 6:F:38:GLU:O | 6:F:39:LYS:CB | 2.65 | 0.45 |
| 12:L:51:ALA:C | 12:L:52:LEU:HG | 2.37 | 0.45 |
| 13:M:57:ARG:CG | 13:M:61:GLU:OE2 | 2.59 | 0.45 |
| 14:N:29:ARG:HB3 | 14:N:40:CYS:HB3 | 1.98 | 0.45 |
| 15:O:17:ARG:NH1 | 15:O:17:ARG:HG3 | 2.27 | 0.45 |
| 15:O:32:LEU:HA | 15:O:32:LEU:HD23 | 1.69 | 0.45 |
| 17:Q:17:LYS:CA | 17:Q:46:ASP:O | 2.63 | 0.45 |
| 19:S:36:ARG:NH2 | 19:S:75:ALA:O | 2.50 | 0.45 |
| 1:A:1067:G:C5 | 1:A:1068:U:C4 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1122:G:HO2' | 1:A:1123:C:P | 2.40 | 0.44 |
| 1:A:1177:C:C3' | 1:A:1178:U:C5' | 2.87 | 0.44 |
| 1:A:1313:G:HO2' | 1:A:1314:A:P | 2.40 | 0.44 |
| 1:A:1484:U:OP1 | 22:A:1523:KSG:N3 | 2.50 | 0.44 |
| 1:A:447:A:C2 | 1:A:448:A:C4 | 3.05 | 0.44 |
| 1:A:499:G:C6 | 1:A:500:U:N3 | 2.85 | 0.44 |
| 1:A:561:G:C2 | 1:A:562:C:C6 | 3.05 | 0.44 |
| 1:A:653:U:H2' | 1:A:654:G:C8 | 2.52 | 0.44 |
| 1:A:726:G:H2' | 1:A:727:U:H5' | 1.98 | 0.44 |
| 1:A:951:G:H2' | 1:A:952:A:OP1 | 2.16 | 0.44 |
| 2:B:26:PRO:C | 2:B:28:PHE:N | 2.70 | 0.44 |
| 2:B:44:LEU:C | 2:B:46:LYS:N | 2.67 | 0.44 |
| 4:D:111:ALA:HB2 | 4:D:120:LEU:CD1 | 2.43 | 0.44 |
| 4:D:130:GLY:O | 4:D:131:ARG:C | 2.55 | 0.44 |
| 4:D:148:VAL:HG12 | 4:D:149:ALA:N | 2.31 | 0.44 |
| 4:D:10:ARG:NH1 | 4:D:40:PRO:CB | 2.79 | 0.44 |
| 1:A:10:G:OP2 | 5:E:121:LYS:HD2 | 2.16 | 0.44 |
| 5:E:93:PRO:HG3 | 8:H:105:ARG:HE | 1.80 | 0.44 |
| 6:F:40:VAL:HG22 | 6:F:41:GLU:H | 1.80 | 0.44 |
| 7:G:71:PRO:O | 7:G:96:GLN:HG2 | 2.17 | 0.44 |
| 10:J:25:GLU:O | 10:J:26:ALA:C | 2.54 | 0.44 |
| 10:J:49:VAL:CG1 | 10:J:50:ILE:N | 2.79 | 0.44 |
| 12:L:7:ILE:O | 12:L:11:VAL:HG23 | 2.17 | 0.44 |
| 13:M:70:LEU:O | 13:M:71:ARG:C | 2.56 | 0.44 |
| 18:R:19:LYS:H | 18:R:19:LYS:HD2 | 1.82 | 0.44 |
| 18:R:53:ARG:NH1 | 18:R:58:LEU:O | 2.50 | 0.44 |
| 1:A:1196:C:H4' | 1:A:1197:G:OP1 | 2.18 | 0.44 |
| 1:A:1401:A:H2' | 1:A:1402:G:O4' | 2.17 | 0.44 |
| 1:A:164:C:O2' | 1:A:165:U:H5' | 2.16 | 0.44 |
| 1:A:174:A:H2' | 1:A:175:U:C6 | 2.52 | 0.44 |
| 1:A:329:G:C6 | 1:A:330:C:N4 | 2.86 | 0.44 |
| 1:A:502:C:C5 | 1:A:514:G:C4 | 3.05 | 0.44 |
| 1:A:585:C:O2' | 1:A:586:A:H5' | 2.17 | 0.44 |
| 1:A:606:A:C8 | 1:A:607:C:C6 | 3.05 | 0.44 |
| 3:C:131:ARG:O | 3:C:134:ILE:HB | 2.17 | 0.44 |
| 3:C:154:SER:HB3 | 3:C:197:GLY:H | 1.81 | 0.44 |
| 4:D:158:ILE:HG22 | 4:D:159:ARG:N | 2.32 | 0.44 |
| 5:E:87:SER:HB3 | 5:E:131:ILE:HD13 | 1.99 | 0.44 |
| 6:F:17:SER:O | 6:F:18:GLN:C | 2.55 | 0.44 |
| 10:J:25:GLU:O | 10:J:28:ARG:N | 2.48 | 0.44 |
| 10:J:81:THR:O | 10:J:85:LEU:HG | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:36:ILE:HD12 | 15:O:63:ARG:HD3 | 1.98 | 0.44 |
| 1:A:548:C:O4' | 17:Q:32:TYR:CD2 | 2.70 | 0.44 |
| 17:Q:97:SER:C | 17:Q:98:LEU:HD12 | 2.37 | 0.44 |
| 18:R:53:ARG:HD3 | 18:R:63:GLN:CB | 2.47 | 0.44 |
| 20:T:49:ALA:O | 20:T:52:ALA:HB3 | 2.18 | 0.44 |
| 1:A:1308:C:H5'' | 21:U:12:LYS:HZ2 | 1.82 | 0.44 |
| 1:A:204:A:C5 | 1:A:217:C:H4' | 2.52 | 0.44 |
| 1:A:353:G:C2 | 1:A:354:U:C6 | 3.05 | 0.44 |
| 1:A:447:A:HO2' | 1:A:448:A:H8 | 1.61 | 0.44 |
| 1:A:490:G:C5 | 1:A:491:C:C4 | 3.05 | 0.44 |
| 1:A:563:G:H2' | 1:A:564:U:H6 | 1.83 | 0.44 |
| 1:A:891:A:H4' | 1:A:892:A:O5' | 2.16 | 0.44 |
| 3:C:82:GLU:HG3 | 3:C:83:ARG:N | 2.33 | 0.44 |
| 6:F:77:ARG:O | 6:F:81:ILE:HG13 | 2.16 | 0.44 |
| 8:H:44:PHE:CE2 | 8:H:109:ILE:HD13 | 2.51 | 0.44 |
| 12:L:54:LYS:C | 12:L:55:VAL:HG23 | 2.38 | 0.44 |
| 13:M:10:PRO:CB | 13:M:18:ALA:HB1 | 2.42 | 0.44 |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:NE1 | 2.31 | 0.44 |
| 20:T:60:GLU:CA | 20:T:63:ILE:HD12 | 2.47 | 0.44 |
| 1:A:1288:A:C2 | 1:A:1289:U:N1 | 2.86 | 0.44 |
| 1:A:1487:C:N3 | 1:A:1488:U:C4 | 2.85 | 0.44 |
| 1:A:1495:G:H2' | 1:A:1496:A:O4' | 2.17 | 0.44 |
| 1:A:373:G:C2 | 1:A:383:U:O2 | 2.70 | 0.44 |
| 1:A:48:C:H1' | 1:A:361:U:C4 | 2.52 | 0.44 |
| 1:A:550:G:C4' | 1:A:551:G:OP1 | 2.55 | 0.44 |
| 1:A:576:G:C2 | 1:A:577:G:C5 | 3.05 | 0.44 |
| 1:A:762:G:O2' | 1:A:763:C:H5' | 2.18 | 0.44 |
| 2:B:13:ALA:C | 2:B:15:VAL:H | 2.21 | 0.44 |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:CZ | 2.48 | 0.44 |
| 3:C:29:TYR:HD2 | 3:C:29:TYR:C | 2.20 | 0.44 |
| 3:C:50:ALA:O | 3:C:70:VAL:CG1 | 2.65 | 0.44 |
| 4:D:8:VAL:CG1 | 4:D:21:LEU:CB | 2.96 | 0.44 |
| 6:F:44:GLY:O | 6:F:59:TYR:HA | 2.17 | 0.44 |
| 7:G:20:ASP:OD1 | 7:G:22:LEU:N | 2.51 | 0.44 |
| 9:I:100:GLY:C | 9:I:102:LEU:H | 2.20 | 0.44 |
| 9:I:126:SER:OG | 9:I:127:LYS:N | 2.48 | 0.44 |
| 12:L:58:VAL:O | 12:L:65:GLU:HA | 2.17 | 0.44 |
| 16:P:43:LYS:HB3 | 16:P:48:TRP:CD1 | 2.51 | 0.44 |
| 18:R:45:SER:O | 18:R:47:THR:N | 2.51 | 0.44 |
| 1:A:1079:C:O5' | 1:A:1079:C:H6 | 2.01 | 0.44 |
| 1:A:1128:C:H1' | 1:A:1129:A:C8 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:125:A:H1' | 1:A:260:U:H5' | 1.99 | 0.44 |
| 1:A:1268:A:H2' | 1:A:1269:A:H4' | 1.99 | 0.44 |
| 1:A:1335:G:H2' | 1:A:1336:C:C6 | 2.48 | 0.44 |
| 1:A:1443:C:O2' | 1:A:1444:C:H5' | 2.17 | 0.44 |
| 1:A:176:G:N2 | 1:A:202:A:C4 | 2.86 | 0.44 |
| 1:A:221:C:H6 | 1:A:221:C:O5' | 2.00 | 0.44 |
| 1:A:299:A:C5 | 1:A:300:U:C5 | 3.06 | 0.44 |
| 1:A:341:C:H4' | 1:A:342:G:O5' | 2.18 | 0.44 |
| 1:A:636:U:O2' | 1:A:637:A:H5'' | 2.17 | 0.44 |
| 1:A:78:G:C2 | 1:A:87:C:C2 | 3.06 | 0.44 |
| 2:B:157:ARG:HG3 | 2:B:157:ARG:NH1 | 2.33 | 0.44 |
| 4:D:107:ARG:NH1 | 4:D:114:ARG:HH22 | 2.11 | 0.44 |
| 6:F:48:LEU:HD22 | 6:F:52:ILE:HD11 | 1.99 | 0.44 |
| 7:G:20:ASP:HB3 | 7:G:23:VAL:CG2 | 2.47 | 0.44 |
| 1:A:637:A:P | 8:H:56:LYS:NZ | 2.91 | 0.44 |
| 9:I:17:VAL:HG22 | 9:I:63:ILE:CD1 | 2.47 | 0.44 |
| 13:M:108:ARG:O | 13:M:109:THR:C | 2.54 | 0.44 |
| 13:M:67:GLU:O | 13:M:70:LEU:HB2 | 2.17 | 0.44 |
| 14:N:24:CYS:N | 14:N:29:ARG:O | 2.44 | 0.44 |
| 16:P:13:HIS:C | 16:P:15:PRO:CD | 2.85 | 0.44 |
| 16:P:20:VAL:CG2 | 16:P:32:TYR:CD2 | 3.01 | 0.44 |
| 16:P:45:THR:C | 16:P:47:ASP:N | 2.71 | 0.44 |
| 16:P:53:VAL:O | 16:P:54:GLU:C | 2.56 | 0.44 |
| 20:T:43:LEU:O | 20:T:46:GLU:N | 2.49 | 0.44 |
| 20:T:46:GLU:CB | 20:T:48:LYS:HZ2 | 2.28 | 0.44 |
| 20:T:43:LEU:CD1 | 20:T:52:ALA:HA | 2.46 | 0.44 |
| 1:A:1192:C:C4' | 1:A:1196:C:C4 | 3.00 | 0.44 |
| 1:A:1268:A:C8 | 1:A:1269:A:H4' | 2.53 | 0.44 |
| 1:A:1309:C:OP1 | 21:U:20:LYS:N | 2.50 | 0.44 |
| 1:A:1328:A:N1 | 1:A:1357:A:H5'' | 2.32 | 0.44 |
| 1:A:186:C:C2' | 1:A:187:C:H5' | 2.47 | 0.44 |
| 1:A:784:G:H2' | 1:A:785:U:C5 | 2.53 | 0.44 |
| 1:A:829:G:H2' | 1:A:830:G:H8 | 1.81 | 0.44 |
| 1:A:838:A:H3' | 1:A:839:G:H8 | 1.83 | 0.44 |
| 1:A:901:A:H1' | 1:A:1381:A:C2 | 2.53 | 0.44 |
| 1:A:938:U:HO2' | 1:A:939:U:P | 2.40 | 0.44 |
| 1:A:972:A:C2 | 1:A:973:C:C6 | 3.05 | 0.44 |
| 2:B:153:ARG:O | 2:B:155:LEU:N | 2.50 | 0.44 |
| 2:B:8:LYS:HD3 | 2:B:9:GLU:H | 1.82 | 0.44 |
| 3:C:120:VAL:HG12 | 3:C:124:ILE:HD11 | 2.00 | 0.44 |
| 3:C:120:VAL:O | 3:C:123:GLN:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:61:LYS:HD2 | 4:D:207:TYR:HH | 1.82 | 0.44 |
| 5:E:89:ILE:CD1 | 5:E:91:LEU:HG | 2.47 | 0.44 |
| 6:F:65:VAL:HG23 | 6:F:66:GLU:N | 2.31 | 0.44 |
| 9:I:17:VAL:HG11 | 9:I:81:ILE:HG12 | 2.00 | 0.44 |
| 11:K:79:SER:OG | 11:K:106:LYS:HG2 | 2.18 | 0.44 |
| 13:M:88:ARG:HG3 | 13:M:98:VAL:HG13 | 2.00 | 0.44 |
| 13:M:8:GLU:C | 13:M:9:ILE:HG13 | 2.38 | 0.44 |
| 15:O:54:ARG:HG2 | 15:O:58:MET:HE2 | 1.99 | 0.44 |
| 19:S:51:VAL:O | 19:S:58:VAL:N | 2.50 | 0.44 |
| 19:S:40:ILE:O | 19:S:67:VAL:HG12 | 2.18 | 0.44 |
| 1:A:1051:G:C2 | 1:A:1052:C:C6 | 3.06 | 0.44 |
| 1:A:1168:G:N2 | 1:A:1169:G:H1' | 2.33 | 0.44 |
| 1:A:1240:G:O2' | 1:A:1241:C:H5' | 2.18 | 0.44 |
| 1:A:227:G:H2' | 1:A:228:G:H8 | 1.81 | 0.44 |
| 1:A:240:U:H5' | 1:A:241:C:OP1 | 2.18 | 0.44 |
| 1:A:276:C:H1' | 17:Q:38:ARG:HG3 | 2.00 | 0.44 |
| 1:A:308:C:O2' | 1:A:309:A:H5' | 2.17 | 0.44 |
| 1:A:447:A:O2' | 1:A:448:A:H8 | 2.00 | 0.44 |
| 1:A:664:C:O2 | 1:A:695:G:C2 | 2.70 | 0.44 |
| 1:A:741:U:H2' | 1:A:742:G:O4' | 2.17 | 0.44 |
| 1:A:745:G:H4' | 17:Q:102:GLY:HA3 | 1.98 | 0.44 |
| 1:A:794:C:O2' | 1:A:795:C:H5' | 2.18 | 0.44 |
| 1:A:14:U:O2 | 1:A:892:A:H3' | 2.18 | 0.44 |
| 1:A:972:A:H2' | 1:A:972:A:N3 | 2.32 | 0.44 |
| 1:A:982:G:C6 | 1:A:983:A:H1' | 2.52 | 0.44 |
| 2:B:104:ASN:OD1 | 2:B:107:THR:CB | 2.65 | 0.44 |
| 3:C:162:GLN:O | 3:C:163:ALA:O | 2.36 | 0.44 |
| 4:D:148:VAL:CG1 | 4:D:149:ALA:N | 2.81 | 0.44 |
| 4:D:55:ALA:O | 4:D:58:LEU:N | 2.51 | 0.44 |
| 5:E:53:LEU:O | 5:E:56:GLN:HB2 | 2.18 | 0.44 |
| 7:G:76:ARG:HD2 | 7:G:89:MET:SD | 2.58 | 0.44 |
| 10:J:27:ALA:C | 10:J:29:ARG:H | 2.20 | 0.44 |
| 10:J:49:VAL:HG13 | 14:N:41:ARG:HB2 | 1.98 | 0.44 |
| 10:J:32:ALA:HB2 | 10:J:76:ASN:HD22 | 1.82 | 0.44 |
| 11:K:26:ASN:O | 11:K:27:ASN:HB2 | 2.17 | 0.44 |
| 11:K:99:GLN:HA | 11:K:105:VAL:CG2 | 2.48 | 0.44 |
| 12:L:102:ARG:O | 12:L:121:GLY:HA3 | 2.18 | 0.44 |
| 13:M:73:GLU:O | 13:M:76:ALA:HB3 | 2.17 | 0.44 |
| 14:N:25:VAL:O | 14:N:25:VAL:HG22 | 2.18 | 0.44 |
| 17:Q:20:THR:HA | 17:Q:43:LEU:CD2 | 2.48 | 0.44 |
| 18:R:21:LYS:O | 18:R:22:VAL:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:97:PHE:HB2 | 18:R:32:ARG:NH2 | 2.33 | 0.44 |
| 19:S:44:MET:O | 19:S:47:HIS:HB2 | 2.17 | 0.44 |
| 1:A:1140:A:N6 | 1:A:1160:G:H1' | 2.32 | 0.44 |
| 1:A:1274:U:OP1 | 7:G:41:ARG:NH2 | 2.51 | 0.44 |
| 1:A:1330:U:H2' | 1:A:1331:A:H8 | 1.83 | 0.44 |
| 1:A:1388:G:O2' | 1:A:1389:U:H5' | 2.18 | 0.44 |
| 1:A:158:C:O2' | 1:A:159:U:H5' | 2.18 | 0.44 |
| 1:A:240:U:O4 | 1:A:884:G:H1' | 2.18 | 0.44 |
| 1:A:441:G:C2' | 1:A:442:G:H5' | 2.48 | 0.44 |
| 1:A:491:C:C4 | 1:A:492:C:C4 | 3.06 | 0.44 |
| 1:A:631:C:O2' | 1:A:632:A:H5' | 2.18 | 0.44 |
| 1:A:943:A:O2' | 1:A:944:G:C5' | 2.64 | 0.44 |
| 1:A:947:A:N6 | 13:M:126:LYS:HD2 | 2.33 | 0.44 |
| 3:C:165:THR:HG22 | 3:C:166:GLU:N | 2.33 | 0.44 |
| 3:C:174:PRO:O | 3:C:175:LEU:C | 2.56 | 0.44 |
| 3:C:175:LEU:HD23 | 3:C:182:ILE:CD1 | 2.48 | 0.44 |
| 3:C:3:ASN:HD22 | 3:C:3:ASN:H | 1.58 | 0.44 |
| 3:C:74:GLY:O | 3:C:75:VAL:C | 2.56 | 0.44 |
| 4:D:92:VAL:O | 4:D:96:LEU:HD13 | 2.17 | 0.44 |
| 5:E:11:ILE:CG2 | 5:E:31:LEU:HB3 | 2.48 | 0.44 |
| 7:G:23:VAL:HG12 | 7:G:27:ILE:HD11 | 1.99 | 0.44 |
| 8:H:82:HIS:HB3 | 8:H:138:TRP:CD2 | 2.52 | 0.44 |
| 1:A:853:C:O2' | 8:H:14:ARG:HD2 | 2.17 | 0.44 |
| 12:L:110:VAL:O | 12:L:122:THR:CG2 | 2.66 | 0.44 |
| 1:A:486:G:OP1 | 12:L:118:SER:N | 2.50 | 0.44 |
| 14:N:5:ALA:O | 14:N:7:ILE:N | 2.51 | 0.44 |
| 1:A:1168:G:H21 | 14:N:61:TRP:C | 2.20 | 0.44 |
| 15:O:11:VAL:O | 15:O:15:PHE:HD1 | 2.01 | 0.44 |
| 18:R:35:ARG:O | 18:R:37:VAL:N | 2.46 | 0.44 |
| 19:S:25:LYS:N | 19:S:25:LYS:HD2 | 2.25 | 0.44 |
| 1:A:180:A:N3 | 20:T:81:LYS:NZ | 2.63 | 0.44 |
| 1:A:1140:A:C2 | 1:A:1163:G:C4 | 3.06 | 0.44 |
| 1:A:1194:U:OP2 | 1:A:1194:U:O4' | 2.36 | 0.44 |
| 1:A:1212:C:O2' | 1:A:1213:G:H5' | 2.18 | 0.44 |
| 1:A:1313:G:O2' | 1:A:1314:A:P | 2.76 | 0.44 |
| 1:A:27:A:N6 | 1:A:542:G:O2' | 2.41 | 0.44 |
| 1:A:928:U:H2' | 1:A:929:G:C8 | 2.52 | 0.44 |
| 2:B:149:LEU:C | 2:B:151:GLY:H | 2.21 | 0.44 |
| 3:C:89:GLU:O | 3:C:92:ALA:N | 2.48 | 0.44 |
| 7:G:66:VAL:HG12 | 7:G:67:GLU:N | 2.33 | 0.44 |
| 9:I:70:LYS:O | 9:I:74:ILE:HG13 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:27:ALA:HB2 | 10:J:85:LEU:HD21 | 2.00 | 0.44 |
| 10:J:6:ILE:O | 10:J:71:LEU:HD13 | 2.17 | 0.44 |
| 10:J:9:ARG:HB3 | 10:J:9:ARG:NH1 | 2.33 | 0.44 |
| 13:M:23:TYR:HB2 | 13:M:67:GLU:OE2 | 2.17 | 0.44 |
| 14:N:14:PRO:O | 14:N:16:PHE:N | 2.50 | 0.44 |
| 17:Q:9:VAL:HG12 | 17:Q:10:VAL:N | 2.32 | 0.44 |
| 1:A:1220:A:C4 | 1:A:1285:C:O2' | 2.71 | 0.43 |
| 1:A:137:G:H2' | 1:A:138:A:H8 | 1.82 | 0.43 |
| 1:A:1503:G:O2' | 1:A:1504:G:H5' | 2.17 | 0.43 |
| 1:A:440:G:C2 | 1:A:475:G:C2 | 3.06 | 0.43 |
| 1:A:566:U:H2' | 1:A:567:A:C8 | 2.53 | 0.43 |
| 1:A:641:G:C2 | 1:A:734:G:C5 | 3.05 | 0.43 |
| 1:A:989:G:O2' | 1:A:990:G:H5' | 2.18 | 0.43 |
| 1:A:989:G:H2' | 1:A:990:G:H8 | 1.83 | 0.43 |
| 3:C:121:ALA:O | 3:C:122:GLU:C | 2.56 | 0.43 |
| 3:C:179:ARG:O | 3:C:180:ALA:C | 2.56 | 0.43 |
| 3:C:34:LEU:CD2 | 3:C:34:LEU:C | 2.87 | 0.43 |
| 5:E:105:VAL:O | 5:E:106:PRO:C | 2.54 | 0.43 |
| 5:E:9:LYS:CB | 5:E:112:LEU:HD11 | 2.48 | 0.43 |
| 5:E:74:GLY:CA | 5:E:116:THR:HG22 | 2.48 | 0.43 |
| 6:F:30:LEU:CD2 | 6:F:75:LEU:HD21 | 2.36 | 0.43 |
| 9:I:32:ASP:O | 9:I:33:PHE:C | 2.56 | 0.43 |
| 12:L:113:ARG:NH2 | 12:L:120:TYR:CE1 | 2.86 | 0.43 |
| 13:M:5:ALA:O | 13:M:8:GLU:N | 2.50 | 0.43 |
| 13:M:91:ARG:HB3 | 13:M:97:PRO:O | 2.18 | 0.43 |
| 14:N:17:LYS:HD3 | 14:N:17:LYS:O | 2.17 | 0.43 |
| 10:J:45:ARG:NH2 | 14:N:36:PHE:HD2 | 2.15 | 0.43 |
| 15:O:18:PHE:CE1 | 15:O:21:ASP:HB2 | 2.53 | 0.43 |
| 19:S:30:LEU:HD23 | 19:S:31:ILE:H | 1.83 | 0.43 |
| 20:T:16:HIS:O | 20:T:17:ARG:C | 2.55 | 0.43 |
| 1:A:1140:A:N3 | 1:A:1163:G:C2 | 2.86 | 0.43 |
| 1:A:137:G:O2' | 1:A:138:A:H5' | 2.18 | 0.43 |
| 1:A:1414:C:C2 | 1:A:1448:G:C2 | 3.06 | 0.43 |
| 1:A:249:U:H2' | 1:A:250:G:H8 | 1.84 | 0.43 |
| 1:A:519:A:H5'' | 1:A:520:C:OP2 | 2.18 | 0.43 |
| 1:A:635:C:N4 | 1:A:636:U:O4 | 2.51 | 0.43 |
| 1:A:736:G:H1' | 1:A:738:C:H41 | 1.82 | 0.43 |
| 2:B:16:HIS:NE2 | 2:B:214:ILE:HG12 | 2.34 | 0.43 |
| 3:C:139:GLN:CA | 3:C:139:GLN:NE2 | 2.80 | 0.43 |
| 3:C:3:ASN:O | 3:C:4:LYS:O | 2.36 | 0.43 |
| 4:D:3:ARG:O | 4:D:5:ILE:HG13 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:69:VAL:HG22 | 7:G:135:VAL:HG22 | 1.99 | 0.43 |
| 10:J:31:GLY:O | 10:J:32:ALA:O | 2.35 | 0.43 |
| 11:K:26:ASN:O | 11:K:27:ASN:CB | 2.65 | 0.43 |
| 11:K:33:THR:OG1 | 11:K:38:ASN:N | 2.52 | 0.43 |
| 1:A:891:A:P | 12:L:47:LYS:NZ | 2.90 | 0.43 |
| 13:M:105:THR:HB | 13:M:106:ASN:H | 1.47 | 0.43 |
| 13:M:28:ALA:O | 13:M:29:ARG:C | 2.55 | 0.43 |
| 13:M:46:LYS:HG3 | 13:M:47:ASP:H | 1.83 | 0.43 |
| 13:M:54:VAL:HG12 | 13:M:58:GLU:HG2 | 2.00 | 0.43 |
| 15:O:15:PHE:O | 15:O:16:ALA:C | 2.57 | 0.43 |
| 19:S:19:VAL:HG13 | 19:S:20:LEU:N | 2.33 | 0.43 |
| 1:A:1301:A:H5' | 19:S:70:LYS:NZ | 2.33 | 0.43 |
| 20:T:101:GLY:O | 20:T:102:GLY:O | 2.35 | 0.43 |
| 20:T:15:ARG:O | 20:T:16:HIS:C | 2.56 | 0.43 |
| 20:T:57:ARG:CB | 20:T:57:ARG:HH11 | 2.31 | 0.43 |
| 1:A:1169:G:C4 | 1:A:1170:A:C8 | 3.06 | 0.43 |
| 1:A:1276:G:O2' | 1:A:1277:G:H5' | 2.18 | 0.43 |
| 1:A:1302:C:C4 | 1:A:1303:C:C4 | 3.06 | 0.43 |
| 1:A:1329:G:H22 | 1:A:1356:G:H2' | 1.83 | 0.43 |
| 1:A:125:A:OP2 | 1:A:190:U:H2' | 2.18 | 0.43 |
| 1:A:248:U:H2' | 1:A:249:U:C6 | 2.54 | 0.43 |
| 1:A:393:A:N7 | 1:A:531:A:O2' | 2.47 | 0.43 |
| 1:A:56:A:O2' | 1:A:57:U:H5' | 2.17 | 0.43 |
| 1:A:932:G:H21 | 1:A:1209:A:N6 | 2.10 | 0.43 |
| 3:C:5:ILE:C | 3:C:5:ILE:CD1 | 2.87 | 0.43 |
| 4:D:98:GLU:HG2 | 4:D:194:LEU:HD11 | 1.99 | 0.43 |
| 1:A:1063:A:H5' | 5:E:14:ARG:NH2 | 2.33 | 0.43 |
| 5:E:31:LEU:HA | 5:E:31:LEU:HD23 | 1.78 | 0.43 |
| 6:F:35:ALA:HA | 6:F:67:MET:HB3 | 2.00 | 0.43 |
| 6:F:78:GLU:CD | 6:F:81:ILE:HD12 | 2.39 | 0.43 |
| 8:H:24:THR:CG2 | 8:H:24:THR:O | 2.66 | 0.43 |
| 9:I:10:ARG:HD2 | 9:I:11:LYS:H | 1.82 | 0.43 |
| 9:I:24:GLY:CA | 9:I:60:ASP:HA | 2.48 | 0.43 |
| 9:I:7:THR:CG2 | 9:I:8:GLY:H | 2.21 | 0.43 |
| 11:K:111:ASP:CG | 11:K:111:ASP:O | 2.57 | 0.43 |
| 12:L:45:PRO:HG2 | 12:L:50:SER:CA | 2.48 | 0.43 |
| 13:M:66:LEU:C | 13:M:70:LEU:HB2 | 2.37 | 0.43 |
| 16:P:74:LEU:O | 16:P:79:VAL:CG2 | 2.65 | 0.43 |
| 17:Q:19:VAL:CG2 | 17:Q:44:ALA:HB3 | 2.48 | 0.43 |
| 17:Q:58:GLU:HG3 | 17:Q:75:ARG:HG2 | 2.00 | 0.43 |
| 18:R:46:GLU:CD | 18:R:46:GLU:H | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:1077:G:OP2 | 1:A:1078:U:C5 | 2.71 | 0.43 |
| 1:A:1251:A:C2 | 1:A:1295:U:C1' | 3.02 | 0.43 |
| 1:A:1334:C:H2' | 1:A:1335:G:C8 | 2.54 | 0.43 |
| 1:A:1347:U:HO2' | 1:A:1348:G:P | 2.33 | 0.43 |
| 1:A:194:G:H2' | 1:A:195:U:O4' | 2.17 | 0.43 |
| 1:A:274:G:H1' | 1:A:278:A:H1' | 2.01 | 0.43 |
| 1:A:155:A:H1' | 1:A:340:A:C5 | 2.54 | 0.43 |
| 1:A:435:A:H5'' | 1:A:478:G:H22 | 1.83 | 0.43 |
| 1:A:690:A:N3 | 11:K:31:THR:OG1 | 2.49 | 0.43 |
| 2:B:117:GLU:HG2 | 2:B:117:GLU:O | 2.19 | 0.43 |
| 2:B:168:THR:OG1 | 2:B:192:SER:HB3 | 2.18 | 0.43 |
| 2:B:46:LYS:C | 2:B:48:MET:N | 2.70 | 0.43 |
| 3:C:23:TYR:CG | 3:C:24:ALA:N | 2.87 | 0.43 |
| 4:D:178:VAL:O | 4:D:179:GLU:C | 2.57 | 0.43 |
| 5:E:65:ASN:O | 5:E:65:ASN:OD1 | 2.36 | 0.43 |
| 1:A:1328:A:C4 | 7:G:10:ARG:NH2 | 2.87 | 0.43 |
| 5:E:78:HIS:HD2 | 8:H:107:LEU:HD12 | 1.82 | 0.43 |
| 9:I:44:VAL:O | 9:I:45:ALA:C | 2.57 | 0.43 |
| 11:K:108:ILE:O | 11:K:109:VAL:HG23 | 2.18 | 0.43 |
| 11:K:24:SER:HB3 | 11:K:27:ASN:O | 2.19 | 0.43 |
| 13:M:87:TYR:O | 13:M:90:LEU:N | 2.51 | 0.43 |
| 13:M:90:LEU:O | 13:M:93:ARG:N | 2.51 | 0.43 |
| 15:O:14:GLU:HA | 15:O:14:GLU:OE2 | 2.18 | 0.43 |
| 15:O:55:GLY:O | 15:O:56:LEU:C | 2.56 | 0.43 |
| 16:P:39:TYR:CZ | 16:P:41:PRO:HA | 2.53 | 0.43 |
| 17:Q:63:ARG:HG2 | 17:Q:64:PRO:N | 2.33 | 0.43 |
| 1:A:1208:C:H5' | 13:M:96:LEU:HD13 | 2.00 | 0.43 |
| 1:A:1409:C:H2' | 1:A:1410:U:C6 | 2.53 | 0.43 |
| 1:A:172:C:H2' | 1:A:173:C:C6 | 2.53 | 0.43 |
| 1:A:173:C:H2' | 1:A:174:A:H8 | 1.83 | 0.43 |
| 1:A:646:G:O2' | 1:A:647:A:H5' | 2.18 | 0.43 |
| 1:A:674:G:C6 | 1:A:675:G:N1 | 2.86 | 0.43 |
| 1:A:8:G:O2' | 1:A:9:A:OP1 | 2.32 | 0.43 |
| 4:D:115:ARG:O | 4:D:116:GLN:C | 2.56 | 0.43 |
| 4:D:200:GLU:O | 4:D:203:VAL:HB | 2.18 | 0.43 |
| 4:D:30:LYS:C | 4:D:32:ALA:N | 2.71 | 0.43 |
| 6:F:11:ASN:C | 6:F:11:ASN:OD1 | 2.56 | 0.43 |
| 6:F:27:GLN:HE21 | 6:F:27:GLN:HA | 1.83 | 0.43 |
| 6:F:2:ARG:NE | 6:F:69:GLU:HG2 | 2.33 | 0.43 |
| 8:H:20:TYR:CD1 | 8:H:65:TYR:CD2 | 3.06 | 0.43 |
| 1:A:1136:C:P | 10:J:13:HIS:HE2 | 2.41 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:22:LYS:HE2 | 10:J:90:LEU:HD12 | 2.00 | 0.43 |
| 13:M:5:ALA:O | 13:M:6:GLY:C | 2.56 | 0.43 |
| 14:N:53:LEU:HB3 | 14:N:56:VAL:HG21 | 1.99 | 0.43 |
| 15:O:87:ILE:CG2 | 15:O:88:ARG:H | 2.30 | 0.43 |
| 17:Q:97:SER:CB | 17:Q:103:GLY:N | 2.82 | 0.43 |
| 17:Q:81:ARG:HB2 | 17:Q:81:ARG:HE | 1.68 | 0.43 |
| 18:R:75:ILE:C | 18:R:77:GLY:H | 2.21 | 0.43 |
| 19:S:46:GLY:N | 19:S:62:ILE:HG23 | 2.33 | 0.43 |
| 1:A:1180:G:H2' | 1:A:1181:U:O4' | 2.18 | 0.43 |
| 1:A:1331:A:P | 9:I:118:LYS:NZ | 2.92 | 0.43 |
| 1:A:258:A:H5' | 20:T:74:LYS:HG3 | 2.01 | 0.43 |
| 1:A:282:G:O2' | 1:A:283:U:H5' | 2.18 | 0.43 |
| 1:A:340:A:HO2' | 1:A:341:C:P | 2.41 | 0.43 |
| 1:A:36:G:H2' | 1:A:37:C:H6 | 1.84 | 0.43 |
| 1:A:662:U:H2' | 1:A:663:C:O4' | 2.19 | 0.43 |
| 1:A:764:A:P | 11:K:122:LYS:HB2 | 2.59 | 0.43 |
| 1:A:802:G:H2' | 1:A:803:A:H5'' | 2.01 | 0.43 |
| 1:A:79:G:C2' | 1:A:80:U:H5'' | 2.49 | 0.43 |
| 1:A:902:C:C6 | 1:A:902:C:C3' | 3.01 | 0.43 |
| 1:A:912:C:C4 | 1:A:1327:U:C5 | 3.07 | 0.43 |
| 1:A:934:U:O2' | 1:A:935:U:H5' | 2.18 | 0.43 |
| 1:A:939:U:H2' | 1:A:940:C:H5' | 2.00 | 0.43 |
| 2:B:132:LYS:HG2 | 2:B:135:GLN:OE1 | 2.19 | 0.43 |
| 1:A:1086:C:H5'' | 2:B:98:LEU:HD22 | 1.99 | 0.43 |
| 3:C:12:LEU:O | 3:C:16:ARG:O | 2.36 | 0.43 |
| 3:C:11:ARG:HG2 | 3:C:15:THR:OG1 | 2.19 | 0.43 |
| 3:C:179:ARG:HG3 | 3:C:179:ARG:NH1 | 2.34 | 0.43 |
| 3:C:35:GLU:O | 3:C:36:ASP:C | 2.55 | 0.43 |
| 4:D:104:VAL:HG12 | 4:D:108:LEU:CD1 | 2.35 | 0.43 |
| 1:A:400:U:H5' | 4:D:122:ARG:HD2 | 1.99 | 0.43 |
| 6:F:74:ASP:O | 6:F:75:LEU:C | 2.56 | 0.43 |
| 7:G:118:VAL:O | 7:G:121:ALA:N | 2.51 | 0.43 |
| 9:I:47:LEU:C | 9:I:49:PRO:CD | 2.84 | 0.43 |
| 10:J:48:THR:OG1 | 10:J:62:HIS:CD2 | 2.71 | 0.43 |
| 13:M:79:LYS:CD | 13:M:83:ASP:OD2 | 2.66 | 0.43 |
| 15:O:27:VAL:CG1 | 15:O:31:LEU:HD11 | 2.48 | 0.43 |
| 15:O:82:ILE:O | 15:O:83:GLU:C | 2.55 | 0.43 |
| 17:Q:56:VAL:O | 17:Q:77:VAL:HB | 2.18 | 0.43 |
| 18:R:62:GLU:O | 18:R:64:ARG:N | 2.52 | 0.43 |
| 20:T:50:GLU:HG3 | 20:T:99:LEU:CD1 | 2.48 | 0.43 |
| 20:T:54:LYS:HG3 | 20:T:100:ILE:CD1 | 2.45 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:A:O2' | 1:A:114:A:OP2 | 2.28 | 0.43 |
| 1:A:1184:G:C4 | 14:N:42:ILE:HD13 | 2.53 | 0.43 |
| 1:A:1287:G:C2 | 1:A:1313:G:N3 | 2.87 | 0.43 |
| 1:A:1507:G:C5' | 1:A:1508:G:OP2 | 2.64 | 0.43 |
| 1:A:458:A:C6 | 1:A:459:G:C4 | 3.07 | 0.43 |
| 1:A:648:G:OP1 | 18:R:64:ARG:HD2 | 2.19 | 0.43 |
| 1:A:676:U:H5' | 1:A:781:C:C5' | 2.49 | 0.43 |
| 1:A:762:G:H2' | 1:A:763:C:H5' | 2.00 | 0.43 |
| 1:A:741:U:H4' | 1:A:806:C:O2 | 2.19 | 0.43 |
| 1:A:902:C:H3' | 1:A:902:C:H6 | 1.84 | 0.43 |
| 1:A:945:C:OP1 | 1:A:947:A:H5' | 2.18 | 0.43 |
| 2:B:113:HIS:O | 2:B:114:ARG:C | 2.56 | 0.43 |
| 2:B:26:PRO:C | 2:B:28:PHE:H | 2.22 | 0.43 |
| 2:B:51:LEU:O | 2:B:55:PHE:N | 2.45 | 0.43 |
| 2:B:84:GLU:HB3 | 2:B:219:VAL:CG2 | 2.44 | 0.43 |
| 3:C:122:GLU:O | 3:C:125:GLU:N | 2.51 | 0.43 |
| 3:C:142:MET:HE1 | 3:C:146:ALA:O | 2.19 | 0.43 |
| 3:C:70:VAL:C | 3:C:106:VAL:HG23 | 2.39 | 0.43 |
| 3:C:72:LYS:C | 3:C:74:GLY:H | 2.22 | 0.43 |
| 4:D:78:LEU:HA | 4:D:78:LEU:HD23 | 1.75 | 0.43 |
| 5:E:11:ILE:CG2 | 5:E:31:LEU:CB | 2.96 | 0.43 |
| 9:I:84:ALA:O | 9:I:87:GLN:N | 2.52 | 0.43 |
| 10:J:78:ASN:O | 10:J:79:ARG:C | 2.57 | 0.43 |
| 10:J:91:PRO:HB2 | 10:J:94:VAL:HG23 | 2.01 | 0.43 |
| 13:M:108:ARG:O | 13:M:111:LYS:N | 2.50 | 0.43 |
| 13:M:15:VAL:O | 13:M:16:ASP:C | 2.57 | 0.43 |
| 13:M:67:GLU:O | 13:M:70:LEU:N | 2.50 | 0.43 |
| 15:O:12:ILE:O | 15:O:13:GLN:C | 2.56 | 0.43 |
| 15:O:51:HIS:O | 15:O:52:SER:C | 2.56 | 0.43 |
| 16:P:51:VAL:O | 16:P:52:ASP:HB3 | 2.19 | 0.43 |
| 19:S:39:THR:HG22 | 19:S:40:ILE:H | 1.84 | 0.43 |
| 19:S:63:THR:O | 19:S:66:MET:HG2 | 2.18 | 0.43 |
| 20:T:11:SER:HA | 20:T:13:LEU:CD1 | 2.49 | 0.43 |
| 1:A:1024:A:H2' | 1:A:1025:G:C8 | 2.54 | 0.43 |
| 1:A:1100:G:N1 | 1:A:1166:G:C6 | 2.87 | 0.43 |
| 1:A:1113:A:C2 | 1:A:1129:A:C4 | 3.07 | 0.43 |
| 1:A:1137:G:H2' | 1:A:1138:G:H8 | 1.82 | 0.43 |
| 1:A:1239:U:O2' | 1:A:1240:G:P | 2.76 | 0.43 |
| 1:A:1254:G:C4 | 1:A:1255:G:C8 | 3.07 | 0.43 |
| 1:A:393:A:N6 | 1:A:532:G:C5 | 2.87 | 0.43 |
| 1:A:419:G:N3 | 1:A:419:G:H3' | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:419:G:C2' | 1:A:420:G:H5' | 2.49 | 0.43 |
| 1:A:441:G:H2' | 1:A:442:G:H5' | 2.00 | 0.43 |
| 1:A:574:C:H2' | 1:A:575:U:H6 | 1.84 | 0.43 |
| 1:A:630:U:H2' | 1:A:631:C:C6 | 2.54 | 0.43 |
| 1:A:878:A:N1 | 1:A:879:A:C2 | 2.87 | 0.43 |
| 1:A:556:A:N3 | 1:A:895:G:H1' | 2.34 | 0.43 |
| 2:B:95:GLN:O | 2:B:96:ARG:HD2 | 2.18 | 0.43 |
| 3:C:117:ALA:O | 3:C:118:GLN:C | 2.56 | 0.43 |
| 3:C:33:LEU:O | 3:C:36:ASP:N | 2.52 | 0.43 |
| 3:C:64:VAL:HB | 3:C:99:VAL:CG2 | 2.48 | 0.43 |
| 5:E:135:THR:HG22 | 5:E:136:MET:N | 2.34 | 0.43 |
| 6:F:94:GLN:O | 6:F:95:GLU:C | 2.54 | 0.43 |
| 7:G:146:GLU:CA | 7:G:149:ARG:HB2 | 2.45 | 0.43 |
| 7:G:23:VAL:HG13 | 7:G:43:PHE:CZ | 2.54 | 0.43 |
| 7:G:62:PHE:O | 7:G:63:LYS:C | 2.56 | 0.43 |
| 8:H:4:ASP:OD2 | 8:H:89:PRO:CD | 2.67 | 0.43 |
| 9:I:14:VAL:O | 9:I:65:VAL:HA | 2.18 | 0.43 |
| 12:L:41:ARG:HB2 | 12:L:41:ARG:NH1 | 2.34 | 0.43 |
| 13:M:58:GLU:O | 13:M:62:ASN:CB | 2.67 | 0.43 |
| 15:O:39:LEU:O | 15:O:40:SER:C | 2.57 | 0.43 |
| 16:P:14:ASN:N | 16:P:15:PRO:CD | 2.81 | 0.43 |
| 17:Q:81:ARG:HG3 | 17:Q:84:LEU:HD12 | 2.00 | 0.43 |
| 1:A:1050:A:H1' | 1:A:1051:G:C1' | 2.49 | 0.43 |
| 1:A:1184:G:C2 | 14:N:42:ILE:CG2 | 3.01 | 0.43 |
| 1:A:1222:U:C4' | 1:A:1223:G:OP2 | 2.62 | 0.43 |
| 1:A:1267:A:O2' | 1:A:1268:A:OP2 | 2.34 | 0.43 |
| 1:A:277:G:C2' | 1:A:278:A:OP2 | 2.67 | 0.43 |
| 1:A:476:G:O2' | 1:A:477:G:H5' | 2.19 | 0.43 |
| 1:A:56:A:C2 | 1:A:57:U:N1 | 2.87 | 0.43 |
| 1:A:698:G:H1' | 1:A:761:A:C8 | 2.54 | 0.43 |
| 1:A:758:G:C2 | 1:A:790:C:N3 | 2.87 | 0.43 |
| 1:A:844:C:C5 | 1:A:845:G:H1' | 2.53 | 0.43 |
| 1:A:868:G:C2' | 1:A:869:U:OP2 | 2.66 | 0.43 |
| 1:A:947:A:H2' | 1:A:948:C:H5' | 1.99 | 0.43 |
| 1:A:98:G:O2' | 1:A:169:C:H5' | 2.18 | 0.43 |
| 2:B:124:SER:HB2 | 2:B:125:PRO:CD | 2.43 | 0.43 |
| 2:B:126:GLU:HA | 2:B:129:GLU:OE1 | 2.19 | 0.43 |
| 2:B:97:TRP:CH2 | 2:B:176:GLU:OE2 | 2.71 | 0.43 |
| 3:C:71:ALA:HA | 3:C:106:VAL:HB | 2.00 | 0.43 |
| 3:C:33:LEU:CD2 | 3:C:34:LEU:N | 2.81 | 0.43 |
| 4:D:61:LYS:NZ | 4:D:72:GLU:OE2 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:12:LEU:HD13 | 5:E:31:LEU:HB2 | 1.99 | 0.43 |
| 7:G:24:THR:C | 7:G:28:ASN:ND2 | 2.73 | 0.43 |
| 2:B:179:LYS:HA | 8:H:72:PRO:HD3 | 2.01 | 0.43 |
| 9:I:126:SER:O | 9:I:128:ARG:N | 2.40 | 0.43 |
| 9:I:63:ILE:HD13 | 9:I:77:ILE:HG23 | 2.01 | 0.43 |
| 10:J:34:VAL:C | 10:J:36:GLY:H | 2.21 | 0.43 |
| 11:K:87:THR:HA | 11:K:91:ARG:NH2 | 2.31 | 0.43 |
| 12:L:85:ILE:HG23 | 12:L:98:TYR:HB3 | 1.99 | 0.43 |
| 13:M:64:TRP:CB | 13:M:66:LEU:HD21 | 2.49 | 0.43 |
| 18:R:28:GLU:H | 18:R:28:GLU:CD | 2.21 | 0.43 |
| 18:R:53:ARG:NH1 | 18:R:59:SER:CA | 2.75 | 0.43 |
| 18:R:47:THR:HG23 | 18:R:83:GLU:H | 1.83 | 0.43 |
| 20:T:53:LEU:O | 20:T:54:LYS:C | 2.57 | 0.43 |
| 1:A:109:G:H4' | 1:A:110:A:O5' | 2.19 | 0.43 |
| 1:A:1111:C:H2' | 1:A:1112:C:C5' | 2.48 | 0.43 |
| 1:A:1208:C:O2' | 1:A:1209:A:P | 2.77 | 0.43 |
| 1:A:1293:G:N2 | 1:A:1309:C:C2 | 2.87 | 0.43 |
| 1:A:1328:A:N9 | 7:G:10:ARG:NH2 | 2.67 | 0.43 |
| 1:A:292:U:O2' | 1:A:293:G:H5' | 2.19 | 0.43 |
| 1:A:814:G:H2' | 1:A:815:U:O4' | 2.19 | 0.43 |
| 1:A:845:G:HO2' | 1:A:851:A:H61 | 1.65 | 0.43 |
| 1:A:960:U:H1' | 1:A:961:A:C6 | 2.53 | 0.43 |
| 2:B:144:ARG:HG3 | 2:B:145:LEU:N | 2.33 | 0.43 |
| 2:B:44:LEU:O | 2:B:46:LYS:N | 2.51 | 0.43 |
| 4:D:142:PRO:HA | 4:D:185:PHE:HD2 | 1.84 | 0.43 |
| 4:D:23:GLY:O | 4:D:26:CYS:HB2 | 2.19 | 0.43 |
| 4:D:78:LEU:HD22 | 4:D:96:LEU:HD23 | 2.00 | 0.43 |
| 6:F:85:VAL:O | 6:F:85:VAL:HG12 | 2.18 | 0.43 |
| 7:G:21:VAL:CG2 | 7:G:22:LEU:N | 2.81 | 0.43 |
| 9:I:42:ARG:O | 9:I:44:VAL:N | 2.52 | 0.43 |
| 12:L:59:ARG:HE | 12:L:59:ARG:HB2 | 1.52 | 0.43 |
| 15:O:54:ARG:O | 15:O:55:GLY:C | 2.56 | 0.43 |
| 16:P:20:VAL:HG22 | 16:P:34:GLU:O | 2.19 | 0.43 |
| 18:R:29:PHE:CE1 | 18:R:31:LEU:CD2 | 2.97 | 0.43 |
| 1:A:1425:G:C2' | 1:A:1425:G:N3 | 2.82 | 0.42 |
| 1:A:1421:G:N2 | 1:A:1442:G:H1' | 2.34 | 0.42 |
| 1:A:299:A:C6 | 1:A:300:U:C4 | 3.07 | 0.42 |
| 1:A:426:A:OP2 | 4:D:7:PRO:HA | 2.19 | 0.42 |
| 1:A:526:G:O2' | 1:A:527:C:H5' | 2.19 | 0.42 |
| 1:A:676:U:OP1 | 11:K:124:LYS:HE3 | 2.18 | 0.42 |
| 1:A:751:A:C4 | 1:A:752:A:C8 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:813:G:N2 | 1:A:814:G:C4 | 2.87 | 0.42 |
| 1:A:914:C:O2' | 1:A:915:A:H5' | 2.18 | 0.42 |
| 2:B:187:LEU:CD1 | 2:B:205:ASP:HA | 2.48 | 0.42 |
| 2:B:207:ALA:O | 2:B:208:ILE:C | 2.56 | 0.42 |
| 3:C:19:GLU:HB3 | 3:C:40:ARG:HH21 | 1.83 | 0.42 |
| 3:C:50:ALA:HB1 | 3:C:70:VAL:CG1 | 2.47 | 0.42 |
| 1:A:493:A:O4' | 4:D:58:LEU:HD12 | 2.19 | 0.42 |
| 5:E:12:LEU:C | 5:E:12:LEU:HD13 | 2.38 | 0.42 |
| 7:G:126:ASP:HB3 | 7:G:131:LYS:HG3 | 2.01 | 0.42 |
| 10:J:79:ARG:C | 10:J:81:THR:N | 2.71 | 0.42 |
| 11:K:21:ILE:CB | 11:K:84:VAL:HG12 | 2.42 | 0.42 |
| 13:M:65:LYS:HE2 | 13:M:73:GLU:HB2 | 2.00 | 0.42 |
| 1:A:1208:C:H5' | 13:M:96:LEU:CD1 | 2.49 | 0.42 |
| 14:N:31:ARG:HA | 14:N:31:ARG:HD2 | 1.72 | 0.42 |
| 14:N:26:ARG:HD3 | 14:N:43:CYS:SG | 2.59 | 0.42 |
| 17:Q:78:GLU:HG3 | 17:Q:78:GLU:O | 2.18 | 0.42 |
| 1:A:1145:C:H2' | 1:A:1146:C:C6 | 2.54 | 0.42 |
| 1:A:1255:G:C2 | 1:A:1256:G:H1' | 2.54 | 0.42 |
| 1:A:1335:G:C4 | 1:A:1336:C:C5 | 3.07 | 0.42 |
| 1:A:1498:G:C4 | 1:A:1499:G:N7 | 2.87 | 0.42 |
| 1:A:43:G:C6 | 1:A:44:C:N4 | 2.87 | 0.42 |
| 1:A:483:A:C1' | 1:A:531:A:N6 | 2.81 | 0.42 |
| 1:A:635:C:C4 | 1:A:636:U:O4 | 2.72 | 0.42 |
| 1:A:672:G:C5 | 1:A:684:G:C2 | 3.07 | 0.42 |
| 3:C:101:LEU:CD2 | 3:C:101:LEU:C | 2.87 | 0.42 |
| 4:D:8:VAL:HG11 | 4:D:21:LEU:HB2 | 2.00 | 0.42 |
| 3:C:23:TYR:OH | 10:J:9:ARG:HD3 | 2.18 | 0.42 |
| 11:K:123:LYS:O | 11:K:124:LYS:C | 2.57 | 0.42 |
| 13:M:63:THR:CG2 | 13:M:64:TRP:N | 2.82 | 0.42 |
| 17:Q:68:ARG:HH11 | 17:Q:68:ARG:HG2 | 1.84 | 0.42 |
| 20:T:38:LYS:O | 20:T:40:ALA:N | 2.52 | 0.42 |
| 1:A:1048:U:O5' | 1:A:1172:G:N2 | 2.51 | 0.42 |
| 1:A:107:G:H1' | 1:A:350:G:H5'' | 2.01 | 0.42 |
| 1:A:109:G:H1' | 1:A:110:A:N7 | 2.34 | 0.42 |
| 1:A:1101:C:OP1 | 9:I:104:ARG:HD2 | 2.19 | 0.42 |
| 1:A:10:G:C2 | 1:A:11:A:C4 | 3.07 | 0.42 |
| 1:A:1218:A:C2 | 1:A:1219:C:N3 | 2.87 | 0.42 |
| 1:A:1260:U:H5'' | 1:A:1261:A:H5' | 2.01 | 0.42 |
| 1:A:1318:C:O2' | 1:A:1319:G:C5 | 2.66 | 0.42 |
| 1:A:122:G:C2 | 1:A:230:C:C2 | 3.07 | 0.42 |
| 1:A:60:A:C3' | 1:A:327:G:H22 | 2.31 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:446:A:N6 | 1:A:466:G:N9 | 2.68 | 0.42 |
| 1:A:934:U:H2' | 1:A:935:U:O4' | 2.18 | 0.42 |
| 3:C:40:ARG:HG2 | 3:C:55:VAL:HG11 | 2.00 | 0.42 |
| 3:C:95:THR:C | 3:C:97:LYS:N | 2.71 | 0.42 |
| 5:E:118:ILE:HG22 | 5:E:119:LEU:N | 2.34 | 0.42 |
| 8:H:8:ASP:O | 8:H:9:MET:C | 2.56 | 0.42 |
| 9:I:7:THR:HB | 9:I:83:ARG:HH11 | 1.84 | 0.42 |
| 11:K:52:GLY:HA2 | 11:K:55:LYS:HE2 | 2.01 | 0.42 |
| 11:K:73:MET:SD | 11:K:103:LEU:HD23 | 2.59 | 0.42 |
| 11:K:91:ARG:CZ | 18:R:88:LYS:CE | 2.97 | 0.42 |
| 12:L:64:TYR:N | 12:L:64:TYR:CD1 | 2.87 | 0.42 |
| 13:M:101:GLN:OE1 | 13:M:101:GLN:N | 2.51 | 0.42 |
| 1:A:947:A:H62 | 13:M:126:LYS:HD2 | 1.84 | 0.42 |
| 13:M:64:TRP:O | 13:M:66:LEU:HG | 2.19 | 0.42 |
| 13:M:67:GLU:HB3 | 13:M:68:GLY:H | 1.51 | 0.42 |
| 13:M:94:ARG:NH1 | 19:S:81:ARG:HD3 | 2.32 | 0.42 |
| 20:T:57:ARG:O | 20:T:60:GLU:N | 2.52 | 0.42 |
| 21:U:2:GLY:C | 21:U:4:GLY:N | 2.72 | 0.42 |
| 1:A:1274:U:O2' | 1:A:1275:G:H5' | 2.19 | 0.42 |
| 1:A:1287:G:C8 | 1:A:1287:G:OP2 | 2.72 | 0.42 |
| 1:A:1476:U:O2' | 1:A:1477:A:N7 | 2.52 | 0.42 |
| 1:A:266:A:H2' | 1:A:267:C:H6 | 1.81 | 0.42 |
| 1:A:486:G:H1' | 1:A:534:G:H5' | 2.01 | 0.42 |
| 1:A:495:C:O2' | 1:A:496:U:C5' | 2.67 | 0.42 |
| 1:A:661:U:O2' | 1:A:662:U:H5' | 2.19 | 0.42 |
| 1:A:699:A:H5'' | 1:A:789:C:H1' | 2.01 | 0.42 |
| 1:A:706:A:O3' | 1:A:707:U:C6 | 2.72 | 0.42 |
| 1:A:833:G:H8 | 1:A:849:U:O4 | 2.03 | 0.42 |
| 1:A:896:A:C2 | 1:A:897:A:C4 | 3.08 | 0.42 |
| 2:B:13:ALA:O | 2:B:15:VAL:N | 2.52 | 0.42 |
| 1:A:1094:A:N1 | 3:C:177:THR:CB | 2.82 | 0.42 |
| 3:C:204:LEU:O | 3:C:205:GLY:C | 2.58 | 0.42 |
| 3:C:28:GLN:O | 3:C:29:TYR:C | 2.57 | 0.42 |
| 3:C:70:VAL:HG12 | 3:C:72:LYS:H | 1.84 | 0.42 |
| 4:D:142:PRO:HG2 | 4:D:187:ARG:HH11 | 1.84 | 0.42 |
| 4:D:32:ALA:C | 4:D:34:GLU:H | 2.21 | 0.42 |
| 4:D:78:LEU:O | 4:D:81:GLU:HB3 | 2.19 | 0.42 |
| 8:H:26:VAL:O | 8:H:58:TYR:HD2 | 2.03 | 0.42 |
| 9:I:111:ARG:O | 9:I:119:ALA:HB2 | 2.19 | 0.42 |
| 9:I:31:GLN:HB3 | 9:I:35:GLU:HB3 | 2.00 | 0.42 |
| 10:J:23:ILE:N | 10:J:23:ILE:HD12 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:K:73:MET:SD | 11:K:103:LEU:CD2 | 3.07 | 0.42 |
| 12:L:27:LEU:HG | 12:L:28:LYS:H | 1.84 | 0.42 |
| 12:L:41:ARG:HH11 | 12:L:41:ARG:CB | 2.32 | 0.42 |
| 1:A:1284:U:OP2 | 13:M:17:VAL:HG13 | 2.19 | 0.42 |
| 16:P:32:TYR:HE2 | 16:P:35:LYS:HB2 | 1.83 | 0.42 |
| 16:P:38:TYR:HE2 | 16:P:50:LYS:HD3 | 1.84 | 0.42 |
| 17:Q:56:VAL:CG1 | 17:Q:77:VAL:HB | 2.47 | 0.42 |
| 1:A:1041:G:C6 | 1:A:1042:C:N3 | 2.87 | 0.42 |
| 1:A:1468:C:C6 | 1:A:1468:C:H5' | 2.41 | 0.42 |
| 1:A:184:G:O2' | 1:A:185:C:H5' | 2.19 | 0.42 |
| 1:A:209:U:H4' | 1:A:210:U:OP2 | 2.19 | 0.42 |
| 1:A:213:C:O2' | 1:A:214:C:H5' | 2.20 | 0.42 |
| 1:A:390:G:C4 | 1:A:391:C:C5 | 3.08 | 0.42 |
| 1:A:869:U:H2' | 1:A:870:A:H8 | 1.84 | 0.42 |
| 1:A:898:U:O2 | 1:A:899:U:C2 | 2.73 | 0.42 |
| 1:A:939:U:C2 | 1:A:961:A:C5 | 3.07 | 0.42 |
| 2:B:126:GLU:HA | 2:B:129:GLU:CG | 2.50 | 0.42 |
| 3:C:188:LEU:O | 3:C:189:ALA:CB | 2.63 | 0.42 |
| 3:C:190:ARG:HB3 | 3:C:190:ARG:CZ | 2.49 | 0.42 |
| 4:D:8:VAL:HG23 | 4:D:115:ARG:NH1 | 2.34 | 0.42 |
| 5:E:118:ILE:CG2 | 5:E:119:LEU:N | 2.83 | 0.42 |
| 5:E:136:MET:O | 5:E:137:GLU:C | 2.56 | 0.42 |
| 5:E:52:PRO:O | 5:E:53:LEU:C | 2.56 | 0.42 |
| 5:E:72:GLN:O | 5:E:73:ASN:CB | 2.67 | 0.42 |
| 6:F:37:VAL:HG12 | 6:F:38:GLU:N | 2.35 | 0.42 |
| 6:F:2:ARG:CD | 6:F:69:GLU:HG2 | 2.50 | 0.42 |
| 7:G:12:LEU:CD1 | 7:G:12:LEU:N | 2.82 | 0.42 |
| 8:H:45:ILE:O | 8:H:45:ILE:HG13 | 2.19 | 0.42 |
| 8:H:92:ARG:HB3 | 8:H:94:TYR:CE1 | 2.55 | 0.42 |
| 9:I:126:SER:C | 9:I:128:ARG:N | 2.73 | 0.42 |
| 9:I:47:LEU:O | 9:I:48:GLU:C | 2.58 | 0.42 |
| 12:L:71:PRO:HB2 | 12:L:120:TYR:HE2 | 1.84 | 0.42 |
| 12:L:8:ASN:O | 12:L:9:GLN:C | 2.58 | 0.42 |
| 12:L:97:ARG:HB2 | 12:L:98:TYR:CE1 | 2.55 | 0.42 |
| 12:L:87:GLY:HA2 | 12:L:98:TYR:HA | 2.01 | 0.42 |
| 16:P:7:ALA:HB3 | 16:P:18:ARG:HB3 | 2.02 | 0.42 |
| 11:K:84:VAL:HG21 | 18:R:88:LYS:HD3 | 2.01 | 0.42 |
| 20:T:83:ARG:O | 20:T:87:LYS:HG3 | 2.19 | 0.42 |
| 1:A:1288:A:C2 | 1:A:1289:U:C2 | 3.08 | 0.42 |
| 1:A:1492:C:O2' | 1:A:1493:C:H5' | 2.20 | 0.42 |
| 1:A:246:A:H2 | 1:A:270:A:C6 | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:440:G:N1 | 1:A:475:G:C6 | 2.87 | 0.42 |
| 1:A:571:G:O2' | 1:A:572:G:H5' | 2.19 | 0.42 |
| 1:A:598:A:C2 | 1:A:611:G:C2 | 3.08 | 0.42 |
| 1:A:648:G:H2' | 1:A:650:G:OP1 | 2.19 | 0.42 |
| 1:A:671:A:HO2' | 1:A:672:G:P | 2.42 | 0.42 |
| 1:A:832:G:H3' | 1:A:849:U:C4 | 2.55 | 0.42 |
| 2:B:67:THR:N | 2:B:160:ASP:OD2 | 2.53 | 0.42 |
| 2:B:77:ALA:O | 2:B:79:ASP:N | 2.52 | 0.42 |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:CG1 | 2.50 | 0.42 |
| 3:C:139:GLN:CA | 3:C:139:GLN:HE21 | 2.32 | 0.42 |
| 3:C:58:GLU:HB2 | 3:C:65:ALA:CB | 2.50 | 0.42 |
| 3:C:98:ASN:OD1 | 3:C:98:ASN:O | 2.36 | 0.42 |
| 4:D:117:ALA:O | 4:D:118:ARG:C | 2.58 | 0.42 |
| 4:D:96:LEU:O | 4:D:97:LEU:C | 2.57 | 0.42 |
| 6:F:2:ARG:O | 6:F:4:TYR:CE2 | 2.72 | 0.42 |
| 8:H:114:THR:C | 8:H:116:LYS:N | 2.72 | 0.42 |
| 8:H:17:THR:O | 8:H:20:TYR:N | 2.39 | 0.42 |
| 8:H:60:ARG:HG3 | 8:H:60:ARG:NH1 | 2.35 | 0.42 |
| 9:I:40:LEU:O | 9:I:43:ALA:HB2 | 2.20 | 0.42 |
| 11:K:33:THR:OG1 | 11:K:38:ASN:C | 2.58 | 0.42 |
| 12:L:75:HIS:CD2 | 12:L:77:LEU:H | 2.37 | 0.42 |
| 14:N:57:ARG:HG2 | 14:N:58:LYS:N | 2.34 | 0.42 |
| 15:O:71:GLN:O | 15:O:72:ARG:C | 2.56 | 0.42 |
| 18:R:17:SER:OG | 18:R:55:ARG:HD3 | 2.19 | 0.42 |
| 20:T:32:ALA:O | 20:T:33:ILE:C | 2.57 | 0.42 |
| 1:A:1179:G:OP1 | 1:A:1180:G:OP2 | 2.37 | 0.42 |
| 1:A:1217:U:O2' | 1:A:1218:A:H5' | 2.20 | 0.42 |
| 1:A:1237:G:C2 | 1:A:1265:G:C2 | 3.07 | 0.42 |
| 1:A:1332:A:O2' | 1:A:1333:U:H5' | 2.19 | 0.42 |
| 1:A:1412:C:H2' | 1:A:1413:C:C6 | 2.54 | 0.42 |
| 1:A:242:A:C4 | 1:A:275:A:C6 | 3.08 | 0.42 |
| 1:A:282:G:H2' | 1:A:283:U:H6 | 1.85 | 0.42 |
| 1:A:332:C:O2' | 1:A:333:C:H5' | 2.20 | 0.42 |
| 1:A:409:G:H22 | 1:A:424:G:H1' | 1.85 | 0.42 |
| 1:A:558:A:N3 | 1:A:861:C:H1' | 2.34 | 0.42 |
| 1:A:610:U:H2' | 1:A:611:G:H8 | 1.84 | 0.42 |
| 1:A:882:C:H2' | 1:A:883:U:O4' | 2.20 | 0.42 |
| 2:B:43:ASP:OD1 | 2:B:45:GLN:N | 2.53 | 0.42 |
| 6:F:14:LEU:HA | 6:F:18:GLN:NE2 | 2.34 | 0.42 |
| 7:G:75:VAL:CG2 | 7:G:144:MET:HB3 | 2.42 | 0.42 |
| 7:G:16:LEU:HD22 | 7:G:16:LEU:N | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:76:ARG:O | 7:G:156:TRP:CZ3 | 2.71 | 0.42 |
| 8:H:51:VAL:CG1 | 8:H:52:ASP:N | 2.83 | 0.42 |
| 9:I:97:LYS:N | 9:I:98:PRO:CD | 2.83 | 0.42 |
| 12:L:89:ARG:HG2 | 12:L:97:ARG:CA | 2.45 | 0.42 |
| 1:A:1208:C:N4 | 13:M:104:ARG:HG3 | 2.35 | 0.42 |
| 1:A:931:G:H1' | 13:M:125:ARG:CB | 2.50 | 0.42 |
| 18:R:85:LEU:HD12 | 18:R:86:VAL:H | 1.85 | 0.42 |
| 1:A:1482:G:H4' | 1:A:1483:G:C5' | 2.50 | 0.42 |
| 1:A:337:C:H6 | 1:A:337:C:O5' | 2.03 | 0.42 |
| 1:A:745:G:C5 | 1:A:746:C:C5 | 3.08 | 0.42 |
| 2:B:123:ALA:CA | 2:B:127:ILE:HD11 | 2.50 | 0.42 |
| 3:C:139:GLN:HE21 | 3:C:143:GLU:HB2 | 1.83 | 0.42 |
| 3:C:188:LEU:CD1 | 3:C:195:VAL:HG22 | 2.49 | 0.42 |
| 3:C:73:PRO:O | 3:C:74:GLY:O | 2.38 | 0.42 |
| 5:E:13:ILE:HG22 | 5:E:30:ALA:CA | 2.50 | 0.42 |
| 5:E:8:GLU:OE2 | 5:E:63:ARG:NH2 | 2.52 | 0.42 |
| 1:A:1274:U:C5' | 9:I:38:GLN:NE2 | 2.73 | 0.42 |
| 10:J:61:GLU:CD | 14:N:45:ARG:HH12 | 2.23 | 0.42 |
| 10:J:27:ALA:CB | 10:J:74:ILE:HD13 | 2.49 | 0.42 |
| 12:L:73:GLU:OE2 | 12:L:73:GLU:HA | 2.20 | 0.42 |
| 13:M:8:GLU:HG3 | 13:M:22:ILE:HG12 | 2.02 | 0.42 |
| 14:N:58:LYS:HE3 | 14:N:58:LYS:HB3 | 1.81 | 0.42 |
| 17:Q:29:HIS:HE1 | 17:Q:31:LEU:HB3 | 1.84 | 0.42 |
| 18:R:55:ARG:HB3 | 18:R:55:ARG:NH1 | 2.27 | 0.42 |
| 1:A:10:G:OP1 | 5:E:122:GLU:HG3 | 2.20 | 0.42 |
| 1:A:1103:G:C8 | 1:A:1103:G:O5' | 2.69 | 0.42 |
| 1:A:1207:A:N3 | 1:A:1207:A:H2' | 2.35 | 0.42 |
| 1:A:1432:A:O2' | 1:A:1433:C:P | 2.77 | 0.42 |
| 1:A:144:A:H2' | 1:A:145:C:H6 | 1.84 | 0.42 |
| 1:A:1477:A:O2' | 1:A:1478:A:H5' | 2.20 | 0.42 |
| 1:A:1506:U:O2' | 1:A:1507:G:P | 2.77 | 0.42 |
| 1:A:486:G:C1' | 1:A:534:G:H5' | 2.50 | 0.42 |
| 1:A:691:C:H4' | 11:K:20:TYR:CE1 | 2.54 | 0.42 |
| 1:A:762:G:H2' | 1:A:763:C:C5' | 2.50 | 0.42 |
| 1:A:569:G:O2' | 1:A:857:C:OP1 | 2.30 | 0.42 |
| 1:A:951:G:H2' | 1:A:952:A:C8 | 2.55 | 0.42 |
| 2:B:108:ILE:O | 2:B:110:GLN:N | 2.52 | 0.42 |
| 2:B:73:THR:CG2 | 2:B:169:LYS:HE3 | 2.50 | 0.42 |
| 2:B:231:GLU:HB2 | 2:B:232:PRO:HD2 | 2.00 | 0.42 |
| 2:B:7:VAL:C | 2:B:8:LYS:HG3 | 2.40 | 0.42 |
| 1:A:403:G:O2' | 4:D:116:GLN:HG3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:7:G:C5 | 5:E:119:LEU:HD11 | 2.55 | 0.42 |
| 6:F:21:LEU:O | 6:F:24:GLU:HB3 | 2.20 | 0.42 |
| 6:F:78:GLU:OE2 | 6:F:81:ILE:HD12 | 2.20 | 0.42 |
| 11:K:29:ILE:HB | 11:K:44:SER:CB | 2.50 | 0.42 |
| 12:L:46:LYS:HG2 | 12:L:47:LYS:HG3 | 2.02 | 0.42 |
| 12:L:84:LEU:HA | 12:L:84:LEU:HD12 | 1.87 | 0.42 |
| 14:N:41:ARG:O | 14:N:41:ARG:HD2 | 2.20 | 0.42 |
| 14:N:42:ILE:O | 14:N:46:GLU:HG3 | 2.20 | 0.42 |
| 20:T:103:GLY:O | 20:T:104:LEU:HG | 2.19 | 0.42 |
| 20:T:94:ALA:O | 20:T:95:ALA:HB3 | 2.19 | 0.42 |
| 1:A:1056:U:O2' | 1:A:1057:G:H5' | 2.20 | 0.42 |
| 1:A:1111:C:C2 | 1:A:1127:G:N2 | 2.87 | 0.42 |
| 1:A:1341:C:H6 | 1:A:1341:C:O5' | 2.03 | 0.42 |
| 1:A:1398:G:C4 | 1:A:1399:G:C8 | 3.08 | 0.42 |
| 1:A:157:A:H8 | 1:A:157:A:O5' | 2.03 | 0.42 |
| 1:A:255:G:H2' | 1:A:256:G:O4' | 2.19 | 0.42 |
| 1:A:261:G:H2' | 1:A:263:C:H5 | 1.85 | 0.42 |
| 1:A:324:C:HO2' | 1:A:325:A:P | 2.43 | 0.42 |
| 1:A:477:G:H2' | 1:A:478:G:C8 | 2.55 | 0.42 |
| 1:A:533:C:C2 | 1:A:534:G:C8 | 3.08 | 0.42 |
| 1:A:576:G:N2 | 1:A:577:G:C4 | 2.88 | 0.42 |
| 1:A:606:A:N7 | 1:A:607:C:C6 | 2.88 | 0.42 |
| 1:A:610:U:H2' | 1:A:611:G:C8 | 2.55 | 0.42 |
| 1:A:691:C:H2' | 1:A:692:C:C6 | 2.55 | 0.42 |
| 1:A:720:C:O2' | 1:A:721:A:H5' | 2.20 | 0.42 |
| 1:A:745:G:H2' | 1:A:746:C:H6 | 1.83 | 0.42 |
| 2:B:140:HIS:O | 2:B:143:GLU:N | 2.53 | 0.42 |
| 2:B:215:LEU:O | 2:B:216:SER:C | 2.58 | 0.42 |
| 3:C:108:ASN:C | 3:C:110:ASN:H | 2.24 | 0.42 |
| 3:C:116:VAL:O | 3:C:119:ARG:HB3 | 2.20 | 0.42 |
| 5:E:137:GLU:O | 5:E:140:ARG:N | 2.53 | 0.42 |
| 7:G:42:ILE:HG23 | 7:G:117:ALA:CA | 2.50 | 0.42 |
| 8:H:19:VAL:CG2 | 8:H:21:LYS:HG2 | 2.42 | 0.42 |
| 1:A:1101:C:P | 9:I:104:ARG:HH11 | 2.40 | 0.42 |
| 9:I:25:LYS:O | 9:I:60:ASP:OD1 | 2.38 | 0.42 |
| 10:J:46:ARG:NH1 | 10:J:64:GLU:OE2 | 2.52 | 0.42 |
| 11:K:58:PRO:HB2 | 11:K:93:GLN:CG | 2.43 | 0.42 |
| 13:M:9:ILE:HD12 | 13:M:9:ILE:H | 1.84 | 0.42 |
| 13:M:3:ARG:HA | 13:M:9:ILE:HG23 | 2.01 | 0.42 |
| 20:T:30:LYS:O | 20:T:34:LYS:HG3 | 2.20 | 0.42 |
| 21:U:10:ARG:HA | 21:U:13:ILE:HB | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1032:U:H1' | 1:A:1183:A:C8 | 2.55 | 0.41 |
| 1:A:103:A:H4' | 1:A:104:C:OP2 | 2.20 | 0.41 |
| 1:A:1188:G:C5 | 1:A:1189:G:N7 | 2.88 | 0.41 |
| 1:A:1216:C:C4' | 1:A:1347:U:H1' | 2.50 | 0.41 |
| 1:A:1368:G:H2' | 1:A:1369:G:O4' | 2.20 | 0.41 |
| 1:A:1382:C:H4' | 1:A:1383:C:H5'' | 2.01 | 0.41 |
| 1:A:1387:C:O5' | 1:A:1387:C:H6 | 2.03 | 0.41 |
| 1:A:171:C:H2' | 1:A:172:C:C6 | 2.55 | 0.41 |
| 1:A:298:G:O2' | 1:A:299:A:H5' | 2.20 | 0.41 |
| 1:A:372:G:O3' | 16:P:5:ARG:NH1 | 2.50 | 0.41 |
| 1:A:415:C:C2 | 1:A:421:G:C2 | 3.08 | 0.41 |
| 1:A:458:A:O2' | 1:A:459:G:H5' | 2.20 | 0.41 |
| 1:A:769:G:C6 | 1:A:782:G:O6 | 2.73 | 0.41 |
| 2:B:121:LEU:HD23 | 2:B:121:LEU:H | 1.85 | 0.41 |
| 2:B:172:ILE:O | 2:B:173:ALA:C | 2.58 | 0.41 |
| 2:B:222:ILE:O | 2:B:225:ALA:HB3 | 2.20 | 0.41 |
| 3:C:190:ARG:NH1 | 3:C:190:ARG:HB3 | 2.35 | 0.41 |
| 3:C:70:VAL:HG12 | 3:C:72:LYS:N | 2.35 | 0.41 |
| 4:D:138:TYR:CD2 | 4:D:138:TYR:C | 2.94 | 0.41 |
| 5:E:57:LYS:O | 5:E:58:ALA:C | 2.57 | 0.41 |
| 6:F:22:GLU:O | 6:F:24:GLU:N | 2.53 | 0.41 |
| 7:G:37:ASN:O | 7:G:38:LEU:C | 2.58 | 0.41 |
| 7:G:62:PHE:HD1 | 7:G:124:LEU:HD22 | 1.84 | 0.41 |
| 8:H:84:ARG:HD2 | 8:H:85:ARG:O | 2.20 | 0.41 |
| 9:I:100:GLY:O | 9:I:101:PHE:C | 2.57 | 0.41 |
| 10:J:89:ASP:O | 10:J:90:LEU:HD23 | 2.20 | 0.41 |
| 12:L:26:ALA:O | 12:L:27:LEU:O | 2.37 | 0.41 |
| 12:L:54:LYS:C | 12:L:55:VAL:CG2 | 2.89 | 0.41 |
| 13:M:15:VAL:CB | 13:M:34:LEU:HD11 | 2.50 | 0.41 |
| 16:P:2:VAL:HA | 16:P:23:ASP:HA | 2.01 | 0.41 |
| 1:A:1030:G:C2' | 1:A:1031:G:H5' | 2.50 | 0.41 |
| 1:A:107:G:H2' | 1:A:108:U:O4' | 2.20 | 0.41 |
| 1:A:1175:G:N2 | 1:A:1176:U:C2 | 2.88 | 0.41 |
| 1:A:1207:A:C2' | 1:A:1207:A:N3 | 2.84 | 0.41 |
| 1:A:1475:G:H1' | 1:A:1496:A:C2 | 2.54 | 0.41 |
| 1:A:18:U:C4 | 1:A:19:C:N4 | 2.88 | 0.41 |
| 1:A:201:C:H2' | 1:A:202:A:H5'' | 2.01 | 0.41 |
| 1:A:340:A:OP2 | 1:A:341:C:N4 | 2.43 | 0.41 |
| 1:A:661:U:O2 | 1:A:761:A:O2' | 2.32 | 0.41 |
| 1:A:904:G:C6 | 1:A:1483:G:C5 | 3.08 | 0.41 |
| 2:B:53:ARG:HG3 | 2:B:56:ARG:NH1 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:99:VAL:HG23 | 3:C:100:ALA:N | 2.35 | 0.41 |
| 4:D:132:ARG:C | 4:D:133:VAL:HG23 | 2.39 | 0.41 |
| 4:D:134:ASP:C | 4:D:135:LEU:HD23 | 2.39 | 0.41 |
| 5:E:33:VAL:HG11 | 5:E:109:ILE:HA | 2.02 | 0.41 |
| 1:A:9:A:H5' | 5:E:120:THR:O | 2.20 | 0.41 |
| 5:E:31:LEU:HG | 5:E:45:PHE:HD1 | 1.85 | 0.41 |
| 7:G:25:ALA:CA | 7:G:28:ASN:ND2 | 2.79 | 0.41 |
| 8:H:20:TYR:HA | 8:H:65:TYR:HE2 | 1.82 | 0.41 |
| 11:K:116:HIS:O | 11:K:117:ASN:HB2 | 2.20 | 0.41 |
| 13:M:87:TYR:C | 13:M:89:GLY:N | 2.73 | 0.41 |
| 17:Q:29:HIS:HA | 17:Q:30:PRO:HD2 | 1.63 | 0.41 |
| 17:Q:90:ILE:O | 17:Q:93:GLN:N | 2.53 | 0.41 |
| 1:A:1287:G:H8 | 1:A:1287:G:OP2 | 2.03 | 0.41 |
| 1:A:1369:G:H2' | 1:A:1370:G:H8 | 1.85 | 0.41 |
| 1:A:1462:C:H2' | 1:A:1463:U:C6 | 2.39 | 0.41 |
| 1:A:1465:G:H2' | 1:A:1466:G:O4' | 2.20 | 0.41 |
| 1:A:1486:G:C4 | 1:A:1487:C:C6 | 3.09 | 0.41 |
| 1:A:157:A:H2' | 1:A:158:C:H5' | 2.02 | 0.41 |
| 1:A:204:A:H1' | 1:A:205:G:O4' | 2.20 | 0.41 |
| 1:A:249:U:H2' | 1:A:250:G:C8 | 2.55 | 0.41 |
| 1:A:303:C:C5 | 1:A:304:C:H5 | 2.38 | 0.41 |
| 1:A:451:C:H2' | 1:A:452:C:C6 | 2.55 | 0.41 |
| 1:A:524:G:O2' | 1:A:525:G:H5' | 2.19 | 0.41 |
| 2:B:18:GLY:HA2 | 2:B:42:ILE:H | 1.84 | 0.41 |
| 3:C:34:LEU:O | 3:C:35:GLU:C | 2.59 | 0.41 |
| 3:C:2:GLY:C | 3:C:3:ASN:ND2 | 2.73 | 0.41 |
| 4:D:70:ILE:HG21 | 4:D:74:GLN:HB2 | 2.03 | 0.41 |
| 7:G:145:ALA:O | 7:G:146:GLU:HB2 | 2.20 | 0.41 |
| 7:G:151:TYR:C | 7:G:153:HIS:H | 2.22 | 0.41 |
| 7:G:44:TYR:O | 7:G:47:CYS:N | 2.54 | 0.41 |
| 8:H:53:VAL:CB | 8:H:58:TYR:CD1 | 2.96 | 0.41 |
| 9:I:7:THR:O | 9:I:80:GLY:HA2 | 2.21 | 0.41 |
| 10:J:16:LEU:O | 10:J:17:ASP:C | 2.58 | 0.41 |
| 11:K:21:ILE:HB | 11:K:84:VAL:CG1 | 2.44 | 0.41 |
| 12:L:54:LYS:CD | 12:L:54:LYS:N | 2.82 | 0.41 |
| 16:P:65:GLN:HA | 16:P:66:PRO:HD2 | 1.84 | 0.41 |
| 17:Q:56:VAL:HG12 | 17:Q:77:VAL:CB | 2.49 | 0.41 |
| 19:S:28:LYS:CG | 19:S:29:ARG:N | 2.63 | 0.41 |
| 21:U:6:ARG:O | 21:U:12:LYS:HE2 | 2.20 | 0.41 |
| 1:A:106:G:C2 | 1:A:107:G:C8 | 3.08 | 0.41 |
| 1:A:1355:U:H5'' | 9:I:71:SER:CB | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:777:U:O4 | 1:A:1495:G:H5' | 2.19 | 0.41 |
| 1:A:22:G:N2 | 1:A:23:G:C2 | 2.89 | 0.41 |
| 1:A:324:C:H2' | 1:A:324:C:O2 | 2.21 | 0.41 |
| 1:A:494:A:O2' | 1:A:526:G:H1' | 2.21 | 0.41 |
| 1:A:777:U:O4 | 1:A:1495:G:H8 | 2.03 | 0.41 |
| 2:B:124:SER:CB | 2:B:125:PRO:CD | 2.98 | 0.41 |
| 2:B:211:ILE:O | 2:B:212:GLN:C | 2.58 | 0.41 |
| 3:C:82:GLU:CG | 3:C:83:ARG:N | 2.83 | 0.41 |
| 4:D:64:LEU:HD23 | 4:D:198:VAL:HG21 | 2.00 | 0.41 |
| 4:D:76:ARG:HG2 | 4:D:76:ARG:NH1 | 2.35 | 0.41 |
| 5:E:80:ILE:HD12 | 5:E:91:LEU:HB2 | 2.03 | 0.41 |
| 13:M:50:GLU:O | 13:M:53:VAL:HB | 2.21 | 0.41 |
| 15:O:39:LEU:HD22 | 15:O:43:LEU:HD11 | 2.02 | 0.41 |
| 15:O:65:ARG:O | 15:O:66:LEU:C | 2.57 | 0.41 |
| 20:T:13:LEU:C | 20:T:15:ARG:N | 2.72 | 0.41 |
| 20:T:51:GLU:HA | 20:T:54:LYS:HE3 | 2.02 | 0.41 |
| 1:A:1083:C:O2' | 1:A:1084:A:H5' | 2.21 | 0.41 |
| 1:A:938:U:HO2' | 1:A:1205:C:H4' | 1.84 | 0.41 |
| 1:A:1327:U:O2 | 1:A:1360:A:C6 | 2.73 | 0.41 |
| 1:A:1446:A:H2' | 1:A:1447:G:H5' | 2.03 | 0.41 |
| 1:A:1500:U:H2' | 1:A:1501:G:H8 | 1.85 | 0.41 |
| 1:A:199:U:C2 | 1:A:200:C:C5 | 3.08 | 0.41 |
| 1:A:374:G:H2' | 1:A:375:C:C6 | 2.55 | 0.41 |
| 1:A:801:C:C4 | 1:A:803:A:H1' | 2.56 | 0.41 |
| 1:A:985:C:O2' | 1:A:986:C:H5' | 2.20 | 0.41 |
| 3:C:22:TRP:CH2 | 3:C:32:LEU:HB3 | 2.55 | 0.41 |
| 4:D:64:LEU:CD2 | 4:D:198:VAL:HG21 | 2.51 | 0.41 |
| 4:D:43:HIS:O | 4:D:46:LYS:HB2 | 2.21 | 0.41 |
| 5:E:144:THR:C | 5:E:146:ALA:H | 2.23 | 0.41 |
| 5:E:34:VAL:O | 5:E:41:VAL:HA | 2.20 | 0.41 |
| 5:E:79:GLU:N | 5:E:79:GLU:OE1 | 2.46 | 0.41 |
| 9:I:25:LYS:O | 9:I:61:ALA:N | 2.48 | 0.41 |
| 10:J:3:LYS:HG2 | 10:J:75:ILE:CG2 | 2.42 | 0.41 |
| 10:J:3:LYS:CG | 10:J:75:ILE:HG23 | 2.42 | 0.41 |
| 11:K:38:ASN:HA | 11:K:39:PRO:HD2 | 1.89 | 0.41 |
| 1:A:502:C:HO2' | 12:L:50:SER:HB3 | 1.81 | 0.41 |
| 13:M:6:GLY:O | 13:M:67:GLU:HG3 | 2.20 | 0.41 |
| 13:M:78:ILE:HA | 13:M:81:LEU:HD21 | 2.03 | 0.41 |
| 13:M:81:LEU:CD2 | 13:M:81:LEU:H | 2.33 | 0.41 |
| 14:N:8:GLU:O | 14:N:11:LYS:HB2 | 2.20 | 0.41 |
| 14:N:36:PHE:C | 14:N:36:PHE:CD1 | 2.94 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:36:ILE:HG22 | 15:O:37:ASN:N | 2.36 | 0.41 |
| 15:O:3:ILE:N | 15:O:3:ILE:CD1 | 2.81 | 0.41 |
| 15:O:70:LEU:HD12 | 15:O:78:TYR:CA | 2.51 | 0.41 |
| 17:Q:104:LYS:HB3 | 17:Q:105:ALA:H | 1.44 | 0.41 |
| 20:T:97:ALA:O | 20:T:99:LEU:HD23 | 2.20 | 0.41 |
| 1:A:62:G:C5 | 1:A:101:G:N2 | 2.89 | 0.41 |
| 1:A:118:G:H2' | 1:A:119:U:C6 | 2.56 | 0.41 |
| 1:A:137:G:H2' | 1:A:138:A:C8 | 2.55 | 0.41 |
| 1:A:1397:U:H2' | 1:A:1398:G:C8 | 2.54 | 0.41 |
| 1:A:1414:C:H2' | 1:A:1415:G:O4' | 2.21 | 0.41 |
| 1:A:1441:C:O2' | 1:A:1442:G:H5' | 2.20 | 0.41 |
| 1:A:1448:G:O2' | 1:A:1449:G:H5' | 2.20 | 0.41 |
| 1:A:496:U:OP1 | 4:D:46:LYS:NZ | 2.51 | 0.41 |
| 1:A:542:G:C4 | 1:A:543:A:H2 | 2.38 | 0.41 |
| 1:A:552:G:N7 | 12:L:5:PRO:HD3 | 2.36 | 0.41 |
| 1:A:577:G:C6 | 1:A:578:G:C5 | 3.08 | 0.41 |
| 1:A:591:A:H2' | 1:A:592:A:H5' | 2.01 | 0.41 |
| 1:A:758:G:N2 | 1:A:759:G:H1' | 2.34 | 0.41 |
| 2:B:51:LEU:O | 2:B:52:GLU:C | 2.58 | 0.41 |
| 4:D:17:VAL:O | 4:D:19:LEU:HG | 2.21 | 0.41 |
| 6:F:47:ARG:HH11 | 6:F:57:GLN:HG2 | 1.84 | 0.41 |
| 1:A:917:G:C5' | 7:G:102:ARG:HH22 | 2.08 | 0.41 |
| 13:M:46:LYS:HG3 | 13:M:47:ASP:N | 2.36 | 0.41 |
| 13:M:64:TRP:HB2 | 13:M:66:LEU:HD21 | 2.01 | 0.41 |
| 14:N:27:CYS:HB3 | 14:N:43:CYS:SG | 2.60 | 0.41 |
| 15:O:17:ARG:O | 15:O:18:PHE:HB3 | 2.19 | 0.41 |
| 15:O:5:LYS:HB2 | 15:O:6:GLU:OE2 | 2.20 | 0.41 |
| 15:O:6:GLU:CD | 15:O:6:GLU:H | 2.23 | 0.41 |
| 16:P:51:VAL:HG21 | 16:P:77:ALA:HB2 | 2.02 | 0.41 |
| 16:P:58:TYR:HE1 | 16:P:59:TRP:CZ3 | 2.38 | 0.41 |
| 16:P:6:LEU:HD23 | 16:P:17:TYR:CD1 | 2.56 | 0.41 |
| 17:Q:81:ARG:HB2 | 17:Q:83:ASP:OD1 | 2.20 | 0.41 |
| 19:S:20:LEU:C | 19:S:20:LEU:HD12 | 2.41 | 0.41 |
| 19:S:39:THR:HG22 | 19:S:40:ILE:N | 2.36 | 0.41 |
| 1:A:1135:A:H5'' | 10:J:13:HIS:CG | 2.51 | 0.41 |
| 1:A:1215:G:H2' | 1:A:1216:C:C6 | 2.56 | 0.41 |
| 1:A:1239:U:H4' | 1:A:1240:G:C5' | 2.51 | 0.41 |
| 1:A:1290:U:H2' | 1:A:1291:G:C8 | 2.53 | 0.41 |
| 1:A:1303:C:H2' | 1:A:1304:C:C6 | 2.56 | 0.41 |
| 1:A:1313:G:O2' | 1:A:1314:A:H8 | 2.02 | 0.41 |
| 1:A:418:C:H4' | 1:A:419:G:C5 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:419:G:H2' | 1:A:420:G:H5' | 2.02 | 0.41 |
| 1:A:430:U:H2' | 1:A:431:C:C6 | 2.55 | 0.41 |
| 1:A:446:A:N6 | 1:A:466:G:C1' | 2.84 | 0.41 |
| 1:A:53:G:H2' | 1:A:54:A:O4' | 2.21 | 0.41 |
| 1:A:58:G:C6 | 1:A:59:C:N4 | 2.89 | 0.41 |
| 1:A:764:A:N6 | 1:A:785:U:OP2 | 2.51 | 0.41 |
| 1:A:552:G:C2 | 1:A:861:C:N3 | 2.89 | 0.41 |
| 1:A:76:G:C4 | 1:A:89:G:N2 | 2.89 | 0.41 |
| 2:B:8:LYS:HD3 | 2:B:9:GLU:N | 2.36 | 0.41 |
| 1:A:1095:C:O2 | 3:C:179:ARG:HB3 | 2.19 | 0.41 |
| 3:C:154:SER:OG | 3:C:196:LEU:HA | 2.20 | 0.41 |
| 4:D:202:LEU:HA | 4:D:202:LEU:HD23 | 1.86 | 0.41 |
| 5:E:43:LEU:C | 5:E:62:ALA:HB2 | 2.40 | 0.41 |
| 8:H:30:ARG:O | 8:H:33:GLU:HB3 | 2.21 | 0.41 |
| 9:I:111:ARG:O | 9:I:113:LYS:HD2 | 2.20 | 0.41 |
| 10:J:94:VAL:HG12 | 10:J:95:GLU:H | 1.84 | 0.41 |
| 11:K:30:VAL:HG12 | 11:K:31:THR:N | 2.34 | 0.41 |
| 11:K:70:LYS:O | 11:K:71:LYS:C | 2.59 | 0.41 |
| 15:O:81:LEU:C | 15:O:81:LEU:CD2 | 2.89 | 0.41 |
| 18:R:33:ASP:OD2 | 18:R:36:ASN:HB2 | 2.20 | 0.41 |
| 1:A:110:A:H2' | 1:A:111:G:O4' | 2.20 | 0.41 |
| 1:A:1131:U:H2' | 1:A:1132:C:O4' | 2.21 | 0.41 |
| 1:A:1238:A:O2' | 1:A:1239:U:P | 2.79 | 0.41 |
| 1:A:1334:C:C1' | 1:A:1354:G:N2 | 2.84 | 0.41 |
| 1:A:1369:G:O2' | 1:A:1370:G:H5' | 2.21 | 0.41 |
| 1:A:1476:U:H1' | 1:A:1477:A:N7 | 2.36 | 0.41 |
| 1:A:275:A:H5'' | 1:A:276:C:H3' | 2.02 | 0.41 |
| 1:A:412:G:C6 | 1:A:413:C:N3 | 2.89 | 0.41 |
| 1:A:443:A:H2' | 1:A:444:C:H6 | 1.84 | 0.41 |
| 1:A:768:C:H2' | 1:A:769:G:C8 | 2.56 | 0.41 |
| 1:A:873:G:H2' | 1:A:874:C:C6 | 2.55 | 0.41 |
| 1:A:923:G:N3 | 1:A:923:G:H2' | 2.36 | 0.41 |
| 1:A:93:U:N3 | 1:A:94:C:C5 | 2.88 | 0.41 |
| 2:B:81:VAL:O | 2:B:82:ARG:C | 2.58 | 0.41 |
| 3:C:49:SER:C | 3:C:51:GLY:H | 2.23 | 0.41 |
| 4:D:20:TYR:N | 4:D:20:TYR:CD2 | 2.87 | 0.41 |
| 5:E:137:GLU:O | 5:E:138:ALA:C | 2.59 | 0.41 |
| 6:F:37:VAL:HG12 | 6:F:39:LYS:N | 2.36 | 0.41 |
| 10:J:51:ARG:H | 10:J:59:SER:CB | 2.34 | 0.41 |
| 11:K:32:ILE:CG2 | 11:K:77:MET:HE2 | 2.50 | 0.41 |
| 12:L:87:GLY:H | 12:L:99:HIS:H | 1.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:122:LYS:O | 13:M:123:ALA:HB2 | 2.20 | 0.41 |
| 16:P:39:TYR:CD1 | 16:P:40:ASP:N | 2.89 | 0.41 |
| 16:P:53:VAL:HG23 | 16:P:54:GLU:H | 1.83 | 0.41 |
| 17:Q:66:SER:OG | 17:Q:69:LYS:HD3 | 2.20 | 0.41 |
| 20:T:14:LYS:O | 20:T:17:ARG:HB3 | 2.21 | 0.41 |
| 20:T:81:LYS:C | 20:T:83:ARG:H | 2.24 | 0.41 |
| 21:U:10:ARG:O | 21:U:11:GLY:C | 2.57 | 0.41 |
| 1:A:1036:G:N7 | 1:A:1181:U:H2' | 2.36 | 0.41 |
| 1:A:1282:G:C2' | 1:A:1283:U:OP2 | 2.68 | 0.41 |
| 1:A:1497:A:H2' | 1:A:1498:G:H5' | 2.02 | 0.41 |
| 1:A:362:C:HO2' | 1:A:363:U:P | 2.44 | 0.41 |
| 1:A:677:G:H1' | 22:A:1524:KSG:C6 | 2.50 | 0.41 |
| 1:A:67:G:H4' | 1:A:168:U:C4 | 2.56 | 0.41 |
| 1:A:754:C:H1' | 1:A:877:C:H42 | 1.86 | 0.41 |
| 1:A:939:U:H2' | 1:A:940:C:O4' | 2.21 | 0.41 |
| 3:C:154:SER:OG | 3:C:196:LEU:CA | 2.69 | 0.41 |
| 3:C:64:VAL:HG12 | 3:C:66:VAL:HG23 | 2.02 | 0.41 |
| 3:C:65:ALA:O | 3:C:66:VAL:O | 2.38 | 0.41 |
| 3:C:79:ARG:O | 3:C:81:GLY:N | 2.54 | 0.41 |
| 4:D:64:LEU:CD2 | 4:D:198:VAL:HG11 | 2.41 | 0.41 |
| 6:F:74:ASP:O | 6:F:76:ALA:N | 2.54 | 0.41 |
| 7:G:76:ARG:HD2 | 7:G:89:MET:CE | 2.51 | 0.41 |
| 9:I:106:ALA:O | 9:I:108:VAL:HG23 | 2.21 | 0.41 |
| 12:L:11:VAL:HG13 | 17:Q:29:HIS:HD2 | 1.86 | 0.41 |
| 12:L:27:LEU:HG | 12:L:28:LYS:N | 2.36 | 0.41 |
| 13:M:66:LEU:O | 13:M:70:LEU:N | 2.54 | 0.41 |
| 16:P:1:MET:O | 16:P:24:ALA:CB | 2.65 | 0.41 |
| 16:P:56:ALA:O | 16:P:58:TYR:N | 2.54 | 0.41 |
| 19:S:5:LEU:HA | 19:S:5:LEU:HD23 | 1.80 | 0.41 |
| 20:T:42:GLN:HE22 | 20:T:46:GLU:CG | 2.34 | 0.41 |
| 1:A:1023:U:H2' | 1:A:1024:A:C8 | 2.56 | 0.41 |
| 1:A:1047:G:H4' | 1:A:1048:U:OP1 | 2.20 | 0.41 |
| 1:A:115:C:H5' | 1:A:116:G:OP1 | 2.21 | 0.41 |
| 1:A:137:G:C2 | 1:A:218:U:C2 | 3.09 | 0.41 |
| 1:A:168:U:H1' | 1:A:204:A:C6 | 2.56 | 0.41 |
| 1:A:216:G:O2' | 1:A:217:C:H5' | 2.21 | 0.41 |
| 1:A:248:U:C2 | 1:A:249:U:C5 | 3.08 | 0.41 |
| 1:A:261:G:H4' | 17:Q:65:ILE:O | 2.21 | 0.41 |
| 1:A:395:G:H2' | 1:A:396:C:C6 | 2.55 | 0.41 |
| 1:A:53:G:H2' | 1:A:54:A:C8 | 2.56 | 0.41 |
| 1:A:732:C:H4' | 1:A:733:C:O5' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:982:G:H8 | 1:A:982:G:O5' | 2.03 | 0.41 |
| 2:B:189:ASP:HB3 | 2:B:203:GLY:O | 2.21 | 0.41 |
| 8:H:44:PHE:CD1 | 8:H:80:ILE:HG12 | 2.56 | 0.41 |
| 10:J:62:HIS:HB3 | 14:N:59:ALA:HB3 | 2.03 | 0.41 |
| 11:K:124:LYS:HB3 | 11:K:125:PHE:HD1 | 1.85 | 0.41 |
| 1:A:1289:U:H5' | 13:M:109:THR:HG21 | 2.03 | 0.41 |
| 14:N:12:ARG:O | 14:N:14:PRO:HD3 | 2.21 | 0.41 |
| 15:O:82:ILE:HG22 | 15:O:83:GLU:N | 2.36 | 0.41 |
| 17:Q:86:GLU:O | 17:Q:87:LYS:O | 2.39 | 0.41 |
| 17:Q:91:ARG:O | 17:Q:93:GLN:N | 2.54 | 0.41 |
| 18:R:36:ASN:HD22 | 18:R:38:GLU:HG2 | 1.82 | 0.41 |
| 1:A:1092:C:H2' | 1:A:1093:A:O4' | 2.21 | 0.41 |
| 1:A:1135:A:C4' | 10:J:13:HIS:HD2 | 2.34 | 0.41 |
| 1:A:1140:A:H4' | 1:A:1141:C:O5' | 2.21 | 0.41 |
| 1:A:1179:G:C2' | 1:A:1180:G:H5' | 2.51 | 0.41 |
| 1:A:1228:C:H2' | 1:A:1229:U:C6 | 2.53 | 0.41 |
| 1:A:466:G:H2' | 1:A:467:A:N7 | 2.36 | 0.41 |
| 1:A:512:C:H41 | 12:L:49:ASN:CG | 2.24 | 0.41 |
| 1:A:606:A:C8 | 1:A:607:C:C5 | 3.08 | 0.41 |
| 1:A:639:A:C2 | 1:A:738:C:C4 | 3.09 | 0.41 |
| 1:A:80:U:O2 | 1:A:83:U:H5 | 2.04 | 0.41 |
| 1:A:905:G:N3 | 1:A:906:G:C8 | 2.89 | 0.41 |
| 2:B:12:GLU:OE1 | 2:B:12:GLU:CA | 2.67 | 0.41 |
| 2:B:236:TYR:HD2 | 2:B:239:VAL:HG21 | 1.86 | 0.41 |
| 2:B:57:PHE:CE1 | 2:B:199:TYR:CE1 | 3.09 | 0.41 |
| 3:C:121:ALA:O | 3:C:124:ILE:N | 2.54 | 0.41 |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:CG2 | 2.49 | 0.41 |
| 5:E:33:VAL:HG21 | 5:E:108:ALA:HB1 | 2.03 | 0.41 |
| 5:E:78:HIS:CD2 | 5:E:143:ARG:O | 2.74 | 0.41 |
| 5:E:144:THR:CB | 5:E:146:ALA:H | 2.34 | 0.41 |
| 5:E:148:VAL:O | 5:E:151:LEU:N | 2.45 | 0.41 |
| 6:F:55:ASP:HA | 6:F:56:PRO:HD2 | 1.83 | 0.41 |
| 1:A:626:A:C5 | 8:H:115:SER:HA | 2.56 | 0.41 |
| 8:H:20:TYR:N | 8:H:20:TYR:CD2 | 2.89 | 0.41 |
| 9:I:127:LYS:CD | 9:I:127:LYS:N | 2.84 | 0.41 |
| 16:P:56:ALA:O | 16:P:57:ARG:C | 2.60 | 0.41 |
| 16:P:64:ALA:O | 16:P:66:PRO:HD3 | 2.20 | 0.41 |
| 1:A:372:G:OP2 | 16:P:67:THR:HG21 | 2.21 | 0.41 |
| 17:Q:8:GLY:CA | 17:Q:22:LEU:O | 2.69 | 0.41 |
| 17:Q:68:ARG:H | 17:Q:70:ARG:NH1 | 2.19 | 0.41 |
| 17:Q:97:SER:O | 17:Q:98:LEU:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:100:C:O2 | 1:A:375:C:H4' | 2.21 | 0.40 |
| 1:A:1091:G:H5'' | 3:C:176:HIS:CE1 | 2.56 | 0.40 |
| 1:A:1174:C:H2' | 1:A:1175:G:O5' | 2.21 | 0.40 |
| 1:A:1327:U:OP1 | 9:I:120:ARG:HD3 | 2.22 | 0.40 |
| 22:A:1524:KSG:C9 | 22:A:1524:KSG:N3 | 2.84 | 0.40 |
| 1:A:152:G:H2' | 1:A:153:G:H8 | 1.85 | 0.40 |
| 1:A:331:C:H2' | 1:A:332:C:H6 | 1.81 | 0.40 |
| 1:A:470:G:O2' | 1:A:471:U:H6 | 2.04 | 0.40 |
| 1:A:28:G:C5 | 1:A:541:G:C2 | 3.09 | 0.40 |
| 1:A:692:C:O2' | 1:A:693:G:H5' | 2.21 | 0.40 |
| 1:A:70:G:H2' | 1:A:71:G:C8 | 2.54 | 0.40 |
| 1:A:855:C:O2 | 8:H:3:THR:CG2 | 2.69 | 0.40 |
| 1:A:878:A:C6 | 1:A:879:A:C6 | 3.09 | 0.40 |
| 1:A:907:G:O2' | 1:A:908:C:H5' | 2.22 | 0.40 |
| 1:A:917:G:N3 | 1:A:1358:A:H2 | 2.20 | 0.40 |
| 1:A:932:G:H2' | 1:A:933:U:H6 | 1.87 | 0.40 |
| 1:A:961:A:N3 | 1:A:961:A:H3' | 2.35 | 0.40 |
| 2:B:132:LYS:HA | 2:B:135:GLN:CB | 2.51 | 0.40 |
| 2:B:170:GLU:O | 2:B:173:ALA:N | 2.54 | 0.40 |
| 2:B:231:GLU:HB2 | 2:B:232:PRO:CD | 2.51 | 0.40 |
| 2:B:25:ASN:O | 2:B:26:PRO:C | 2.59 | 0.40 |
| 3:C:174:PRO:CB | 3:C:177:THR:HG22 | 2.47 | 0.40 |
| 3:C:188:LEU:HD22 | 3:C:188:LEU:HA | 1.91 | 0.40 |
| 3:C:70:VAL:HG11 | 3:C:76:VAL:CG2 | 2.51 | 0.40 |
| 4:D:173:TRP:CD1 | 4:D:174:LEU:CD2 | 3.04 | 0.40 |
| 4:D:200:GLU:O | 4:D:203:VAL:N | 2.54 | 0.40 |
| 5:E:12:LEU:HD22 | 5:E:13:ILE:N | 2.35 | 0.40 |
| 9:I:121:ARG:O | 9:I:121:ARG:HD3 | 2.21 | 0.40 |
| 10:J:54:PHE:CD2 | 10:J:55:LYS:HG2 | 2.51 | 0.40 |
| 10:J:56:HIS:O | 10:J:58:ASP:N | 2.54 | 0.40 |
| 11:K:125:PHE:CD1 | 11:K:125:PHE:N | 2.88 | 0.40 |
| 12:L:38:THR:HB | 12:L:57:LYS:HB2 | 2.03 | 0.40 |
| 1:A:1212:C:O2 | 13:M:126:LYS:O | 2.39 | 0.40 |
| 13:M:13:LYS:O | 13:M:14:ARG:O | 2.39 | 0.40 |
| 13:M:53:VAL:O | 13:M:56:LEU:HB2 | 2.21 | 0.40 |
| 18:R:47:THR:CG2 | 18:R:48:GLY:N | 2.84 | 0.40 |
| 18:R:47:THR:OG1 | 18:R:49:LYS:HE3 | 2.20 | 0.40 |
| 20:T:89:ARG:HE | 20:T:104:LEU:HD22 | 1.86 | 0.40 |
| 20:T:91:LEU:C | 20:T:93:GLU:N | 2.72 | 0.40 |
| 1:A:1200:C:H2' | 1:A:1201:U:C5 | 2.54 | 0.40 |
| 1:A:964:A:N1 | 1:A:1202:G:C6 | 2.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1213:G:C5 | 1:A:1214:U:C5 | 3.09 | 0.40 |
| 1:A:1432:A:O2' | 1:A:1433:C:OP1 | 2.32 | 0.40 |
| 1:A:1482:G:O2' | 1:A:1483:G:P | 2.79 | 0.40 |
| 1:A:316:C:H2' | 1:A:317:A:C8 | 2.56 | 0.40 |
| 1:A:319:U:OP1 | 20:T:26:ASN:ND2 | 2.48 | 0.40 |
| 1:A:549:U:C5 | 1:A:550:G:H2' | 2.55 | 0.40 |
| 1:A:709:G:N3 | 1:A:710:C:C6 | 2.89 | 0.40 |
| 1:A:776:A:O2' | 1:A:777:U:O5' | 2.39 | 0.40 |
| 1:A:898:U:O2' | 1:A:899:U:H5' | 2.21 | 0.40 |
| 2:B:204:ASN:C | 2:B:206:ASP:H | 2.24 | 0.40 |
| 3:C:186:PHE:HE1 | 3:C:198:VAL:H | 1.68 | 0.40 |
| 7:G:15:ASP:OD1 | 7:G:17:VAL:N | 2.39 | 0.40 |
| 7:G:75:VAL:CG1 | 7:G:86:GLN:HB3 | 2.45 | 0.40 |
| 8:H:104:ARG:NH1 | 8:H:138:TRP:CH2 | 2.89 | 0.40 |
| 10:J:80:LYS:HA | 10:J:83:GLU:HB2 | 2.03 | 0.40 |
| 17:Q:61:GLU:HA | 17:Q:71:PHE:CE1 | 2.56 | 0.40 |
| 19:S:22:LEU:CD2 | 19:S:28:LYS:HD2 | 2.50 | 0.40 |
| 1:A:1081:C:O2' | 1:A:1082:G:H5' | 2.22 | 0.40 |
| 1:A:1111:C:C4 | 1:A:1122:G:C6 | 3.08 | 0.40 |
| 1:A:1132:C:C2 | 1:A:1133:U:C5 | 3.09 | 0.40 |
| 1:A:117:C:H6 | 1:A:117:C:O5' | 2.04 | 0.40 |
| 1:A:1228:C:O2' | 1:A:1229:U:H5' | 2.21 | 0.40 |
| 1:A:1287:G:C5' | 21:U:4:GLY:CA | 2.99 | 0.40 |
| 1:A:147:A:C6 | 1:A:165:U:O2 | 2.74 | 0.40 |
| 1:A:268:C:C2' | 1:A:269:A:H5' | 2.51 | 0.40 |
| 1:A:325:A:H4' | 1:A:326:C:OP1 | 2.21 | 0.40 |
| 1:A:352:A:C2 | 1:A:353:G:H1' | 2.56 | 0.40 |
| 1:A:504:A:N1 | 1:A:520:C:H1' | 2.36 | 0.40 |
| 1:A:598:A:H2' | 1:A:599:C:O4' | 2.21 | 0.40 |
| 1:A:756:U:C4 | 1:A:757:G:N7 | 2.90 | 0.40 |
| 1:A:791:A:C5 | 1:A:792:C:C5 | 3.09 | 0.40 |
| 1:A:901:A:C6 | 1:A:902:C:N3 | 2.89 | 0.40 |
| 1:A:901:A:N6 | 1:A:1375:G:O6 | 2.54 | 0.40 |
| 2:B:118:LEU:HA | 2:B:118:LEU:HD23 | 1.92 | 0.40 |
| 2:B:92:TYR:N | 2:B:92:TYR:CD2 | 2.89 | 0.40 |
| 3:C:125:GLU:HG3 | 3:C:189:ALA:HB1 | 2.04 | 0.40 |
| 3:C:190:ARG:NH1 | 3:C:190:ARG:CB | 2.85 | 0.40 |
| 4:D:19:LEU:O | 4:D:21:LEU:N | 2.52 | 0.40 |
| 4:D:64:LEU:C | 4:D:64:LEU:HD13 | 2.41 | 0.40 |
| 5:E:71:LEU:HD21 | 5:E:115:VAL:N | 2.36 | 0.40 |
| 8:H:44:PHE:HB3 | 8:H:80:ILE:CG1 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:51:VAL:HG12 | 8:H:52:ASP:N | 2.36 | 0.40 |
| 8:H:96:GLY:O | 8:H:97:VAL:C | 2.59 | 0.40 |
| 9:I:24:GLY:HA2 | 9:I:60:ASP:HA | 2.02 | 0.40 |
| 9:I:93:ARG:O | 9:I:95:LYS:N | 2.55 | 0.40 |
| 10:J:12:ASP:OD1 | 10:J:14:LYS:HB2 | 2.21 | 0.40 |
| 10:J:49:VAL:O | 10:J:61:GLU:N | 2.54 | 0.40 |
| 11:K:16:SER:HA | 11:K:79:SER:HB3 | 2.03 | 0.40 |
| 15:O:6:GLU:O | 15:O:8:LYS:N | 2.54 | 0.40 |
| 17:Q:29:HIS:O | 17:Q:31:LEU:N | 2.55 | 0.40 |
| 1:A:276:C:C2 | 17:Q:38:ARG:HG3 | 2.56 | 0.40 |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:HB3 | 2.03 | 0.40 |
| 21:U:24:ARG:O | 21:U:25:LYS:CB | 2.69 | 0.40 |
| 1:A:1192:C:C5' | 1:A:1196:C:N4 | 2.85 | 0.40 |
| 1:A:1342:A:O2' | 1:A:1343:G:H5' | 2.22 | 0.40 |
| 1:A:271:G:H5' | 17:Q:14:LYS:CD | 2.47 | 0.40 |
| 1:A:242:A:H62 | 1:A:277:G:H1' | 1.83 | 0.40 |
| 1:A:348:C:N3 | 1:A:352:A:N6 | 2.69 | 0.40 |
| 1:A:393:A:H5'' | 1:A:393:A:N3 | 2.37 | 0.40 |
| 1:A:65:G:H4' | 1:A:66:U:O5' | 2.21 | 0.40 |
| 1:A:732:C:O2' | 1:A:733:C:P | 2.79 | 0.40 |
| 1:A:761:A:C2 | 1:A:762:G:H1' | 2.57 | 0.40 |
| 1:A:858:C:OP1 | 12:L:8:ASN:ND2 | 2.54 | 0.40 |
| 1:A:964:A:C6 | 1:A:965:G:C6 | 3.08 | 0.40 |
| 1:A:974:A:H2' | 1:A:975:U:C6 | 2.56 | 0.40 |
| 1:A:981:G:H8 | 1:A:981:G:O5' | 2.04 | 0.40 |
| 1:A:983:A:H3' | 1:A:1004:U:O4 | 2.22 | 0.40 |
| 2:B:111:ARG:O | 2:B:114:ARG:HB3 | 2.21 | 0.40 |
| 2:B:141:GLU:O | 2:B:142:LEU:C | 2.57 | 0.40 |
| 3:C:28:GLN:HA | 3:C:31:HIS:HD2 | 1.85 | 0.40 |
| 4:D:32:ALA:O | 4:D:34:GLU:N | 2.54 | 0.40 |
| 1:A:421:G:H4' | 4:D:45:GLN:HE22 | 1.87 | 0.40 |
| 7:G:68:ASN:HD21 | 7:G:128:ALA:HA | 1.85 | 0.40 |
| 7:G:136:LYS:O | 7:G:140:ASP:N | 2.39 | 0.40 |
| 9:I:11:LYS:O | 9:I:11:LYS:HG2 | 2.22 | 0.40 |
| 10:J:87:THR:O | 10:J:88:LEU:HD23 | 2.21 | 0.40 |
| 11:K:87:THR:HG23 | 11:K:91:ARG:NH2 | 2.36 | 0.40 |
| 13:M:65:LYS:CG | 13:M:69:GLU:HG2 | 2.52 | 0.40 |
| 10:J:47:PHE:CZ | 14:N:37:PHE:CE1 | 3.10 | 0.40 |
| 15:O:74:ASP:HA | 15:O:75:PRO:HD2 | 1.85 | 0.40 |
| 15:O:5:LYS:O | 15:O:8:LYS:HB3 | 2.21 | 0.40 |
| 16:P:4:ILE:HA | 16:P:20:VAL:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:3:LYS:HB3 | 17:Q:61:GLU:HB3 | 2.04 | 0.40 |
| 17:Q:90:ILE:O | 17:Q:91:ARG:C | 2.59 | 0.40 |
| 1:A:275:A:C6 | 17:Q:98:LEU:HD13 | 2.56 | 0.40 |
| 20:T:22:ARG:O | 20:T:23:ARG:C | 2.59 | 0.40 |
| 1:A:1308:C:OP2 | 21:U:6:ARG:NH1 | 2.55 | 0.40 |
| 1:A:1074:U:C2 | 1:A:1078:U:C4 | 3.10 | 0.40 |
| 1:A:11:A:H2' | 1:A:12:G:C8 | 2.42 | 0.40 |
| 1:A:1255:G:N2 | 1:A:1256:G:H1' | 2.37 | 0.40 |
| 1:A:1296:C:H2' | 1:A:1297:U:C6 | 2.57 | 0.40 |
| 1:A:1421:G:C5 | 1:A:1422:C:C4 | 3.09 | 0.40 |
| 1:A:1435:G:H5' | 20:T:36:LEU:HD21 | 2.03 | 0.40 |
| 1:A:1481:A:O2' | 1:A:1482:G:P | 2.80 | 0.40 |
| 1:A:208:C:N4 | 1:A:212:G:H1 | 2.19 | 0.40 |
| 1:A:458:A:C2' | 1:A:459:G:H5' | 2.51 | 0.40 |
| 1:A:547:A:C8 | 1:A:551:G:O4' | 2.75 | 0.40 |
| 1:A:559:G:C6 | 1:A:805:G:N7 | 2.89 | 0.40 |
| 1:A:694:G:H2' | 1:A:695:G:O4' | 2.21 | 0.40 |
| 1:A:757:G:H2' | 1:A:758:G:H8 | 1.87 | 0.40 |
| 1:A:802:G:C3' | 1:A:803:A:H5'' | 2.49 | 0.40 |
| 1:A:939:U:N3 | 1:A:961:A:C5 | 2.90 | 0.40 |
| 3:C:11:ARG:O | 3:C:13:GLY:N | 2.54 | 0.40 |
| 4:D:178:VAL:O | 4:D:179:GLU:O | 2.39 | 0.40 |
| 4:D:98:GLU:OE2 | 4:D:107:ARG:NE | 2.55 | 0.40 |
| 5:E:144:THR:C | 5:E:146:ALA:N | 2.72 | 0.40 |
| 5:E:56:GLN:O | 5:E:57:LYS:C | 2.60 | 0.40 |
| 7:G:114:ARG:HG2 | 7:G:114:ARG:NH1 | 2.35 | 0.40 |
| 9:I:7:THR:CG2 | 9:I:8:GLY:N | 2.71 | 0.40 |
| 11:K:30:VAL:CG1 | 11:K:31:THR:N | 2.85 | 0.40 |
| 11:K:49:GLY:O | 11:K:50:TYR:C | 2.60 | 0.40 |
| 12:L:11:VAL:HG13 | 17:Q:29:HIS:CD2 | 2.57 | 0.40 |
| 12:L:40:VAL:HA | 12:L:55:VAL:O | 2.22 | 0.40 |
| 16:P:33:ILE:H | 16:P:33:ILE:HG13 | 1.73 | 0.40 |
| 16:P:43:LYS:HA | 16:P:48:TRP:HB3 | 2.03 | 0.40 |
| 18:R:78:LEU:HD23 | 18:R:78:LEU:HA | 1.64 | 0.40 |
| 1:A:993:A:C2 | 19:S:34:TRP:CE2 | 3.10 | 0.40 |
| 21:U:9:ARG:HD2 | 21:U:9:ARG:HA | 1.79 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 2 | B | 232/256 (91%) | 134 (58%) | 57 (25%) | 41 (18%) | 0 | 1 |
| 3 | C | 204/239 (85%) | 114 (56%) | 55 (27%) | 35 (17%) | 0 | 1 |
| 4 | D | 206/209 (99%) | 131 (64%) | 49 (24%) | 26 (13%) | 0 | 2 |
| 5 | E | 148/162 (91%) | 99 (67%) | 38 (26%) | 11 (7%) | 1 | 7 |
| 6 | F | 99/101 (98%) | 73 (74%) | 22 (22%) | 4 (4%) | 3 | 20 |
| 7 | G | 153/156 (98%) | 103 (67%) | 37 (24%) | 13 (8%) | 1 | 5 |
| 8 | H | 136/138 (99%) | 108 (79%) | 19 (14%) | 9 (7%) | 1 | 9 |
| 9 | I | 125/128 (98%) | 80 (64%) | 29 (23%) | 16 (13%) | 0 | 2 |
| 10 | J | 96/105 (91%) | 56 (58%) | 20 (21%) | 20 (21%) | 0 | 0 |
| 11 | K | 117/129 (91%) | 78 (67%) | 29 (25%) | 10 (8%) | 1 | 5 |
| 12 | L | 122/135 (90%) | 89 (73%) | 20 (16%) | 13 (11%) | 0 | 3 |
| 13 | M | 123/126 (98%) | 69 (56%) | 33 (27%) | 21 (17%) | 0 | 1 |
| 14 | N | 58/61 (95%) | 35 (60%) | 14 (24%) | 9 (16%) | 0 | 1 |
| 15 | O | 86/89 (97%) | 47 (55%) | 28 (33%) | 11 (13%) | 0 | 2 |
| 16 | P | 81/88 (92%) | 57 (70%) | 20 (25%) | 4 (5%) | 2 | 15 |
| 17 | Q | 102/105 (97%) | 73 (72%) | 15 (15%) | 14 (14%) | 0 | 1 |
| 18 | R | 71/88 (81%) | 46 (65%) | 16 (22%) | 9 (13%) | 0 | 2 |
| 19 | S | 78/93 (84%) | 50 (64%) | 18 (23%) | 10 (13%) | 0 | 2 |
| 20 | T | 97/106 (92%) | 44 (45%) | 38 (39%) | 15 (16%) | 0 | 1 |
| 21 | U | 22/27 (82%) | 18 (82%) | 2 (9%) | 2 (9%) | 1 | 4 |
| All | All | 2356/2541 (93%) | 1504 (64%) | 559 (24%) | 293 (12%) | 0 | 2 |

All (293) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 8 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 17 | PHE |
| 2 | B | 23 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 29 | ALA |
| 2 | B | 30 | ARG |
| 2 | B | 78 | GLN |
| 2 | B | 171 | ALA |
| 2 | B | 211 | ILE |
| 3 | C | 4 | LYS |
| 3 | C | 12 | LEU |
| 3 | C | 75 | VAL |
| 3 | C | 101 | LEU |
| 3 | C | 168 | ALA |
| 3 | C | 178 | LEU |
| 3 | C | 179 | ARG |
| 3 | C | 181 | ASN |
| 3 | C | 189 | ALA |
| 4 | D | 9 | CYS |
| 4 | D | 29 | PRO |
| 4 | D | 36 | ARG |
| 4 | D | 110 | PHE |
| 4 | D | 178 | VAL |
| 4 | D | 179 | GLU |
| 4 | D | 191 | ARG |
| 5 | E | 16 | THR |
| 5 | E | 37 | ARG |
| 7 | G | 155 | ARG |
| 8 | H | 91 | ARG |
| 9 | I | 7 | THR |
| 9 | I | 43 | ALA |
| 9 | I | 44 | VAL |
| 9 | I | 45 | ALA |
| 9 | I | 101 | PHE |
| 10 | J | 32 | ALA |
| 10 | J | 34 | VAL |
| 10 | J | 39 | PRO |
| 10 | J | 40 | LEU |
| 10 | J | 54 | PHE |
| 10 | J | 79 | ARG |
| 10 | J | 82 | ILE |
| 10 | J | 86 | MET |
| 11 | K | 50 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | K | 57 | THR |
| 11 | K | 126 | ARG |
| 12 | L | 45 | PRO |
| 12 | L | 47 | LYS |
| 12 | L | 116 | SER |
| 12 | L | 121 | GLY |
| 13 | M | 5 | ALA |
| 13 | M | 27 | LYS |
| 13 | M | 28 | ALA |
| 13 | M | 60 | VAL |
| 13 | M | 63 | THR |
| 13 | M | 67 | GLU |
| 13 | M | 106 | ASN |
| 13 | M | 123 | ALA |
| 13 | M | 124 | PRO |
| 14 | N | 12 | ARG |
| 14 | N | 22 | THR |
| 15 | O | 88 | ARG |
| 17 | Q | 69 | LYS |
| 17 | Q | 80 | GLY |
| 17 | Q | 83 | ASP |
| 17 | Q | 97 | SER |
| 17 | Q | 98 | LEU |
| 17 | Q | 104 | LYS |
| 18 | R | 49 | LYS |
| 18 | R | 58 | LEU |
| 18 | R | 77 | GLY |
| 18 | R | 87 | ARG |
| 19 | S | 3 | ARG |
| 19 | S | 6 | LYS |
| 20 | T | 11 | SER |
| 20 | T | 49 | ALA |
| 20 | T | 50 | GLU |
| 20 | T | 94 | ALA |
| 20 | T | 95 | ALA |
| 2 | B | 14 | GLY |
| 2 | B | 16 | HIS |
| 2 | B | 18 | GLY |
| 2 | B | 20 | GLU |
| 2 | B | 27 | LYS |
| 2 | B | 49 | GLU |
| 2 | B | 83 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 101 | MET |
| 2 | B | 121 | LEU |
| 2 | B | 143 | GLU |
| 2 | B | 150 | SER |
| 2 | B | 154 | LEU |
| 2 | B | 204 | ASN |
| 2 | B | 208 | ILE |
| 3 | C | 15 | THR |
| 3 | C | 16 | ARG |
| 3 | C | 50 | ALA |
| 3 | C | 53 | ALA |
| 3 | C | 57 | ILE |
| 3 | C | 66 | VAL |
| 3 | C | 74 | GLY |
| 3 | C | 100 | ALA |
| 3 | C | 128 | PHE |
| 3 | C | 130 | VAL |
| 3 | C | 163 | ALA |
| 3 | C | 180 | ALA |
| 3 | C | 205 | GLY |
| 4 | D | 3 | ARG |
| 4 | D | 72 | GLU |
| 5 | E | 96 | PRO |
| 5 | E | 142 | LEU |
| 5 | E | 153 | LYS |
| 6 | F | 35 | ALA |
| 6 | F | 39 | LYS |
| 6 | F | 65 | VAL |
| 7 | G | 7 | ALA |
| 7 | G | 42 | ILE |
| 7 | G | 90 | GLU |
| 7 | G | 149 | ARG |
| 8 | H | 29 | SER |
| 9 | I | 33 | PHE |
| 9 | I | 85 | LEU |
| 9 | I | 88 | TYR |
| 9 | I | 121 | ARG |
| 10 | J | 57 | LYS |
| 10 | J | 60 | ARG |
| 10 | J | 73 | ASP |
| 11 | K | 27 | ASN |
| 11 | K | 89 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | K | 124 | LYS |
| 12 | L | 27 | LEU |
| 12 | L | 28 | LYS |
| 12 | L | 51 | ALA |
| 12 | L | 118 | SER |
| 12 | L | 126 | LYS |
| 13 | M | 4 | ILE |
| 13 | M | 6 | GLY |
| 13 | M | 14 | ARG |
| 13 | M | 18 | ALA |
| 13 | M | 19 | LEU |
| 13 | M | 53 | VAL |
| 13 | M | 61 | GLU |
| 13 | M | 74 | VAL |
| 13 | M | 85 | GLY |
| 14 | N | 6 | LEU |
| 14 | N | 13 | THR |
| 14 | N | 17 | LYS |
| 14 | N | 19 | ARG |
| 14 | N | 36 | PHE |
| 15 | O | 32 | LEU |
| 16 | P | 24 | ALA |
| 17 | Q | 30 | PRO |
| 17 | Q | 87 | LYS |
| 18 | R | 20 | ALA |
| 18 | R | 37 | VAL |
| 18 | R | 62 | GLU |
| 19 | S | 17 | GLU |
| 19 | S | 35 | SER |
| 19 | S | 43 | GLU |
| 19 | S | 45 | VAL |
| 20 | T | 39 | LYS |
| 20 | T | 63 | ILE |
| 20 | T | 92 | LEU |
| 20 | T | 96 | GLY |
| 20 | T | 102 | GLY |
| 21 | U | 3 | LYS |
| 21 | U | 9 | ARG |
| 2 | B | 15 | VAL |
| 2 | B | 60 | ASP |
| 2 | B | 66 | GLY |
| 2 | B | 74 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 135 | GLN |
| 2 | B | 214 | ILE |
| 3 | C | 47 | LEU |
| 3 | C | 61 | ALA |
| 3 | C | 121 | ALA |
| 3 | C | 139 | GLN |
| 3 | C | 206 | GLU |
| 4 | D | 4 | TYR |
| 4 | D | 92 | VAL |
| 4 | D | 180 | GLY |
| 5 | E | 71 | LEU |
| 5 | E | 138 | ALA |
| 7 | G | 66 | VAL |
| 7 | G | 96 | GLN |
| 7 | G | 146 | GLU |
| 8 | H | 76 | PRO |
| 8 | H | 121 | ASP |
| 9 | I | 60 | ASP |
| 9 | I | 71 | SER |
| 9 | I | 78 | LYS |
| 9 | I | 94 | ALA |
| 10 | J | 26 | ALA |
| 10 | J | 35 | SER |
| 10 | J | 59 | SER |
| 10 | J | 90 | LEU |
| 11 | K | 15 | ALA |
| 11 | K | 35 | PRO |
| 11 | K | 48 | ILE |
| 12 | L | 14 | GLY |
| 14 | N | 11 | LYS |
| 15 | O | 30 | ALA |
| 15 | O | 33 | THR |
| 15 | O | 71 | GLN |
| 17 | Q | 47 | PRO |
| 17 | Q | 88 | TYR |
| 18 | R | 34 | TYR |
| 18 | R | 63 | GLN |
| 19 | S | 68 | GLY |
| 19 | S | 71 | LEU |
| 2 | B | 95 | GLN |
| 2 | B | 142 | LEU |
| 3 | C | 77 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 84 | ILE |
| 4 | D | 89 | THR |
| 4 | D | 90 | GLY |
| 4 | D | 102 | ASP |
| 4 | D | 153 | ARG |
| 4 | D | 157 | LEU |
| 5 | E | 39 | GLY |
| 5 | E | 79 | GLU |
| 8 | H | 105 | ARG |
| 9 | I | 56 | LEU |
| 9 | I | 118 | LYS |
| 10 | J | 25 | GLU |
| 10 | J | 72 | VAL |
| 11 | K | 117 | ASN |
| 12 | L | 6 | THR |
| 12 | L | 48 | PRO |
| 12 | L | 115 | LYS |
| 13 | M | 73 | GLU |
| 14 | N | 23 | ARG |
| 15 | O | 34 | LEU |
| 15 | O | 47 | LYS |
| 15 | O | 82 | ILE |
| 16 | P | 10 | GLY |
| 17 | Q | 33 | GLY |
| 17 | Q | 48 | GLU |
| 19 | S | 14 | HIS |
| 19 | S | 16 | LEU |
| 20 | T | 9 | ASN |
| 2 | B | 9 | GLU |
| 2 | B | 26 | PRO |
| 2 | B | 47 | THR |
| 2 | B | 82 | ARG |
| 2 | B | 89 | GLY |
| 2 | B | 131 | PRO |
| 2 | B | 183 | PRO |
| 2 | B | 213 | LEU |
| 3 | C | 60 | ALA |
| 3 | C | 146 | ALA |
| 4 | D | 31 | CYS |
| 4 | D | 45 | GLN |
| 4 | D | 204 | ILE |
| 6 | F | 23 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 93 | PRO |
| 7 | G | 127 | ALA |
| 8 | H | 18 | ARG |
| 8 | H | 30 | ARG |
| 8 | H | 86 | ILE |
| 9 | I | 11 | LYS |
| 10 | J | 30 | SER |
| 15 | O | 12 | ILE |
| 17 | Q | 68 | ARG |
| 20 | T | 38 | LYS |
| 2 | B | 125 | PRO |
| 2 | B | 126 | GLU |
| 3 | C | 42 | LEU |
| 3 | C | 73 | PRO |
| 4 | D | 63 | LYS |
| 4 | D | 200 | GLU |
| 5 | E | 107 | ARG |
| 7 | G | 62 | PHE |
| 15 | O | 72 | ARG |
| 16 | P | 41 | PRO |
| 16 | P | 81 | ARG |
| 20 | T | 73 | HIS |
| 3 | C | 80 | GLY |
| 4 | D | 5 | ILE |
| 5 | E | 115 | VAL |
| 10 | J | 24 | VAL |
| 20 | T | 33 | ILE |
| 3 | C | 51 | GLY |
| 8 | H | 97 | VAL |
| 15 | O | 36 | ILE |
| 20 | T | 97 | ALA |
| 4 | D | 136 | PRO |
| 13 | M | 78 | ILE |
| 4 | D | 133 | VAL |
| 4 | D | 203 | VAL |
| 7 | G | 50 | ILE |
| 7 | G | 87 | VAL |
| 10 | J | 36 | GLY |
| 13 | M | 15 | VAL |
| 17 | Q | 85 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 2 | B | 202/220 (92%) | 183 (91%) | 19 (9%) | 8 | 31 |
| 3 | C | 160/188 (85%) | 142 (89%) | 18 (11%) | 6 | 23 |
| 4 | D | 180/181 (99%) | 164 (91%) | 16 (9%) | 9 | 34 |
| 5 | E | 115/123 (94%) | 102 (89%) | 13 (11%) | 6 | 23 |
| 6 | F | 90/90 (100%) | 84 (93%) | 6 (7%) | 16 | 47 |
| 7 | G | 126/127 (99%) | 120 (95%) | 6 (5%) | 25 | 57 |
| 8 | H | 119/119 (100%) | 109 (92%) | 10 (8%) | 11 | 37 |
| 9 | I | 98/99 (99%) | 88 (90%) | 10 (10%) | 7 | 28 |
| 10 | J | 88/92 (96%) | 81 (92%) | 7 (8%) | 12 | 39 |
| 11 | K | 90/99 (91%) | 85 (94%) | 5 (6%) | 21 | 53 |
| 12 | L | 104/111 (94%) | 96 (92%) | 8 (8%) | 13 | 41 |
| 13 | M | 100/101 (99%) | 84 (84%) | 16 (16%) | 2 | 10 |
| 14 | N | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 | 28 |
| 15 | O | 79/80 (99%) | 72 (91%) | 7 (9%) | 9 | 34 |
| 16 | P | 72/74 (97%) | 68 (94%) | 4 (6%) | 21 | 53 |
| 17 | Q | 96/97 (99%) | 89 (93%) | 7 (7%) | 14 | 43 |
| 18 | R | 64/77 (83%) | 58 (91%) | 6 (9%) | 8 | 31 |
| 19 | S | 71/80 (89%) | 68 (96%) | 3 (4%) | 30 | 60 |
| 20 | T | 75/82 (92%) | 64 (85%) | 11 (15%) | 3 | 13 |
| 21 | U | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |
| All | All | 1997/2112 (95%) | 1820 (91%) | 177 (9%) | 9 | 34 |

All (177) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 8 | LYS |
| 2 | B | 12 | GLU |
| 2 | B | 17 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 23 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 25 | ASN |
| 2 | B | 26 | PRO |
| 2 | B | 69 | LEU |
| 2 | B | 91 | PRO |
| 2 | B | 96 | ARG |
| 2 | B | 114 | ARG |
| 2 | B | 144 | ARG |
| 2 | B | 147 | LYS |
| 2 | B | 153 | ARG |
| 2 | B | 157 | ARG |
| 2 | B | 170 | GLU |
| 2 | B | 181 | PHE |
| 2 | B | 204 | ASN |
| 2 | B | 231 | GLU |
| 3 | C | 3 | ASN |
| 3 | C | 15 | THR |
| 3 | C | 26 | LYS |
| 3 | C | 29 | TYR |
| 3 | C | 32 | LEU |
| 3 | C | 37 | GLN |
| 3 | C | 82 | GLU |
| 3 | C | 91 | LEU |
| 3 | C | 98 | ASN |
| 3 | C | 99 | VAL |
| 3 | C | 101 | LEU |
| 3 | C | 139 | GLN |
| 3 | C | 162 | GLN |
| 3 | C | 167 | TRP |
| 3 | C | 179 | ARG |
| 3 | C | 188 | LEU |
| 3 | C | 193 | TYR |
| 3 | C | 201 | TYR |
| 4 | D | 9 | CYS |
| 4 | D | 10 | ARG |
| 4 | D | 15 | GLU |
| 4 | D | 25 | ARG |
| 4 | D | 29 | PRO |
| 4 | D | 36 | ARG |
| 4 | D | 53 | ASP |
| 4 | D | 58 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 65 | ARG |
| 4 | D | 92 | VAL |
| 4 | D | 106 | TYR |
| 4 | D | 122 | ARG |
| 4 | D | 138 | TYR |
| 4 | D | 157 | LEU |
| 4 | D | 176 | LEU |
| 4 | D | 199 | ASN |
| 5 | E | 10 | MET |
| 5 | E | 11 | ILE |
| 5 | E | 12 | LEU |
| 5 | E | 15 | ARG |
| 5 | E | 26 | PHE |
| 5 | E | 64 | ARG |
| 5 | E | 68 | GLU |
| 5 | E | 73 | ASN |
| 5 | E | 75 | THR |
| 5 | E | 89 | ILE |
| 5 | E | 120 | THR |
| 5 | E | 147 | ASP |
| 5 | E | 150 | ARG |
| 6 | F | 10 | LEU |
| 6 | F | 24 | GLU |
| 6 | F | 32 | ASN |
| 6 | F | 65 | VAL |
| 6 | F | 69 | GLU |
| 6 | F | 95 | GLU |
| 7 | G | 8 | GLU |
| 7 | G | 12 | LEU |
| 7 | G | 36 | LYS |
| 7 | G | 51 | GLN |
| 7 | G | 113 | GLU |
| 7 | G | 140 | ASP |
| 8 | H | 18 | ARG |
| 8 | H | 25 | ASP |
| 8 | H | 52 | ASP |
| 8 | H | 57 | PRO |
| 8 | H | 63 | LEU |
| 8 | H | 85 | ARG |
| 8 | H | 91 | ARG |
| 8 | H | 92 | ARG |
| 8 | H | 104 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | H | 105 | ARG |
| 9 | I | 2 | GLU |
| 9 | I | 3 | GLN |
| 9 | I | 12 | GLU |
| 9 | I | 23 | ASN |
| 9 | I | 38 | GLN |
| 9 | I | 58 | ARG |
| 9 | I | 91 | ASP |
| 9 | I | 104 | ARG |
| 9 | I | 111 | ARG |
| 9 | I | 121 | ARG |
| 10 | J | 15 | THR |
| 10 | J | 38 | ILE |
| 10 | J | 45 | ARG |
| 10 | J | 71 | LEU |
| 10 | J | 73 | ASP |
| 10 | J | 83 | GLU |
| 10 | J | 95 | GLU |
| 11 | K | 29 | ILE |
| 11 | K | 31 | THR |
| 11 | K | 36 | ASP |
| 11 | K | 51 | LYS |
| 11 | K | 91 | ARG |
| 12 | L | 17 | LYS |
| 12 | L | 53 | ARG |
| 12 | L | 59 | ARG |
| 12 | L | 64 | TYR |
| 12 | L | 81 | SER |
| 12 | L | 98 | TYR |
| 12 | L | 113 | ARG |
| 12 | L | 126 | LYS |
| 13 | M | 9 | ILE |
| 13 | M | 14 | ARG |
| 13 | M | 16 | ASP |
| 13 | M | 40 | ASN |
| 13 | M | 44 | ARG |
| 13 | M | 46 | LYS |
| 13 | M | 63 | THR |
| 13 | M | 70 | LEU |
| 13 | M | 81 | LEU |
| 13 | M | 102 | ARG |
| 13 | M | 105 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | M | 106 | ASN |
| 13 | M | 109 | THR |
| 13 | M | 110 | ARG |
| 13 | M | 124 | PRO |
| 13 | M | 125 | ARG |
| 14 | N | 3 | ARG |
| 14 | N | 17 | LYS |
| 14 | N | 31 | ARG |
| 14 | N | 41 | ARG |
| 14 | N | 44 | LEU |
| 15 | O | 6 | GLU |
| 15 | O | 32 | LEU |
| 15 | O | 39 | LEU |
| 15 | O | 40 | SER |
| 15 | O | 70 | LEU |
| 15 | O | 81 | LEU |
| 15 | O | 83 | GLU |
| 16 | P | 18 | ARG |
| 16 | P | 39 | TYR |
| 16 | P | 55 | ARG |
| 16 | P | 61 | SER |
| 17 | Q | 34 | LYS |
| 17 | Q | 35 | VAL |
| 17 | Q | 38 | ARG |
| 17 | Q | 60 | ILE |
| 17 | Q | 68 | ARG |
| 17 | Q | 98 | LEU |
| 17 | Q | 101 | ARG |
| 18 | R | 28 | GLU |
| 18 | R | 36 | ASN |
| 18 | R | 38 | GLU |
| 18 | R | 55 | ARG |
| 18 | R | 82 | THR |
| 18 | R | 87 | ARG |
| 19 | S | 10 | PHE |
| 19 | S | 15 | LEU |
| 19 | S | 30 | LEU |
| 20 | T | 10 | LEU |
| 20 | T | 13 | LEU |
| 20 | T | 24 | LEU |
| 20 | T | 42 | GLN |
| 20 | T | 57 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | T | 68 | LYS |
| 20 | T | 72 | LEU |
| 20 | T | 73 | HIS |
| 20 | T | 75 | ASN |
| 20 | T | 84 | LEU |
| 20 | T | 86 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 25 | ASN |
| 2 | B | 40 | HIS |
| 2 | B | 94 | ASN |
| 2 | B | 146 | GLN |
| 2 | B | 204 | ASN |
| 2 | B | 212 | GLN |
| 3 | C | 3 | ASN |
| 3 | C | 6 | HIS |
| 3 | C | 63 | ASN |
| 3 | C | 69 | HIS |
| 3 | C | 98 | ASN |
| 3 | C | 110 | ASN |
| 3 | C | 118 | GLN |
| 3 | C | 123 | GLN |
| 3 | C | 139 | GLN |
| 4 | D | 42 | GLN |
| 4 | D | 45 | GLN |
| 4 | D | 62 | GLN |
| 4 | D | 77 | ASN |
| 4 | D | 123 | HIS |
| 4 | D | 160 | GLN |
| 4 | D | 199 | ASN |
| 5 | E | 73 | ASN |
| 6 | F | 13 | ASN |
| 6 | F | 18 | GLN |
| 6 | F | 27 | GLN |
| 6 | F | 32 | ASN |
| 6 | F | 57 | GLN |
| 6 | F | 64 | GLN |
| 6 | F | 94 | GLN |
| 6 | F | 100 | ASN |
| 7 | G | 28 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 37 | ASN |
| 7 | G | 64 | GLN |
| 7 | G | 68 | ASN |
| 7 | G | 86 | GLN |
| 7 | G | 106 | GLN |
| 7 | G | 122 | HIS |
| 8 | H | 82 | HIS |
| 9 | I | 3 | GLN |
| 9 | I | 23 | ASN |
| 9 | I | 31 | GLN |
| 9 | I | 73 | GLN |
| 10 | J | 62 | HIS |
| 10 | J | 76 | ASN |
| 10 | J | 84 | GLN |
| 11 | K | 13 | GLN |
| 11 | K | 93 | GLN |
| 11 | K | 117 | ASN |
| 12 | L | 49 | ASN |
| 12 | L | 75 | HIS |
| 13 | M | 12 | ASN |
| 13 | M | 40 | ASN |
| 13 | M | 62 | ASN |
| 15 | O | 13 | GLN |
| 15 | O | 37 | ASN |
| 16 | P | 16 | HIS |
| 16 | P | 82 | GLN |
| 17 | Q | 16 | GLN |
| 18 | R | 36 | ASN |
| 19 | S | 14 | HIS |
| 19 | S | 23 | ASN |
| 19 | S | 47 | HIS |
| 19 | S | 53 | ASN |
| 19 | S | 56 | GLN |
| 20 | T | 42 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1505/1522 (98%) | 286 (19%) | 164 (10%) |

All (286) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 7 | G |
| 1 | A | 8 | G |
| 1 | A | 9 | A |
| 1 | A | 10 | G |
| 1 | A | 14 | U |
| 1 | A | 15 | U |
| 1 | A | 32 | G |
| 1 | A | 33 | A |
| 1 | A | 40 | G |
| 1 | A | 48 | C |
| 1 | A | 49 | C |
| 1 | A | 50 | U |
| 1 | A | 51 | A |
| 1 | A | 52 | A |
| 1 | A | 53 | G |
| 1 | A | 62 | G |
| 1 | A | 65 | G |
| 1 | A | 66 | U |
| 1 | A | 67 | G |
| 1 | A | 80 | U |
| 1 | A | 103 | A |
| 1 | A | 104 | C |
| 1 | A | 110 | A |
| 1 | A | 114 | A |
| 1 | A | 115 | C |
| 1 | A | 116 | G |
| 1 | A | 124 | G |
| 1 | A | 125 | A |
| 1 | A | 177 | U |
| 1 | A | 190 | U |
| 1 | A | 191 | G |
| 1 | A | 192 | G |
| 1 | A | 202 | A |
| 1 | A | 204 | A |
| 1 | A | 205 | G |
| 1 | A | 210 | U |
| 1 | A | 211 | U |
| 1 | A | 212 | G |
| 1 | A | 240 | U |
| 1 | A | 241 | C |
| 1 | A | 243 | G |
| 1 | A | 247 | G |
| 1 | A | 248 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 262 | G |
| 1 | A | 263 | C |
| 1 | A | 271 | G |
| 1 | A | 275 | A |
| 1 | A | 276 | C |
| 1 | A | 277 | G |
| 1 | A | 278 | A |
| 1 | A | 285 | G |
| 1 | A | 301 | G |
| 1 | A | 302 | G |
| 1 | A | 312 | G |
| 1 | A | 324 | C |
| 1 | A | 325 | A |
| 1 | A | 326 | C |
| 1 | A | 328 | G |
| 1 | A | 340 | A |
| 1 | A | 341 | C |
| 1 | A | 342 | G |
| 1 | A | 348 | C |
| 1 | A | 349 | A |
| 1 | A | 350 | G |
| 1 | A | 363 | U |
| 1 | A | 364 | U |
| 1 | A | 369 | A |
| 1 | A | 385 | A |
| 1 | A | 393 | A |
| 1 | A | 394 | C |
| 1 | A | 402 | G |
| 1 | A | 408 | A |
| 1 | A | 409 | G |
| 1 | A | 417 | U |
| 1 | A | 418 | C |
| 1 | A | 419 | G |
| 1 | A | 424 | G |
| 1 | A | 425 | U |
| 1 | A | 426 | A |
| 1 | A | 435 | A |
| 1 | A | 446 | A |
| 1 | A | 447 | A |
| 1 | A | 455 | A |
| 1 | A | 456 | C |
| 1 | A | 457 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 466 | G |
| 1 | A | 469 | G |
| 1 | A | 470 | G |
| 1 | A | 471 | U |
| 1 | A | 480 | A |
| 1 | A | 481 | A |
| 1 | A | 482 | U |
| 1 | A | 484 | G |
| 1 | A | 492 | C |
| 1 | A | 493 | A |
| 1 | A | 494 | A |
| 1 | A | 495 | C |
| 1 | A | 502 | C |
| 1 | A | 503 | C |
| 1 | A | 511 | G |
| 1 | A | 516 | A |
| 1 | A | 517 | A |
| 1 | A | 518 | U |
| 1 | A | 520 | C |
| 1 | A | 532 | G |
| 1 | A | 543 | A |
| 1 | A | 544 | U |
| 1 | A | 545 | U |
| 1 | A | 546 | C |
| 1 | A | 547 | A |
| 1 | A | 550 | G |
| 1 | A | 551 | G |
| 1 | A | 556 | A |
| 1 | A | 557 | A |
| 1 | A | 559 | G |
| 1 | A | 560 | G |
| 1 | A | 561 | G |
| 1 | A | 580 | C |
| 1 | A | 626 | A |
| 1 | A | 636 | U |
| 1 | A | 637 | A |
| 1 | A | 649 | A |
| 1 | A | 670 | U |
| 1 | A | 672 | G |
| 1 | A | 679 | A |
| 1 | A | 685 | C |
| 1 | A | 686 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 687 | G |
| 1 | A | 688 | A |
| 1 | A | 701 | C |
| 1 | A | 702 | G |
| 1 | A | 705 | G |
| 1 | A | 706 | A |
| 1 | A | 707 | U |
| 1 | A | 715 | G |
| 1 | A | 733 | C |
| 1 | A | 737 | A |
| 1 | A | 738 | C |
| 1 | A | 739 | G |
| 1 | A | 761 | A |
| 1 | A | 765 | A |
| 1 | A | 776 | A |
| 1 | A | 777 | U |
| 1 | A | 796 | C |
| 1 | A | 797 | U |
| 1 | A | 799 | A |
| 1 | A | 800 | A |
| 1 | A | 801 | C |
| 1 | A | 802 | G |
| 1 | A | 803 | A |
| 1 | A | 804 | U |
| 1 | A | 805 | G |
| 1 | A | 812 | A |
| 1 | A | 823 | U |
| 1 | A | 824 | C |
| 1 | A | 825 | U |
| 1 | A | 849 | U |
| 1 | A | 850 | A |
| 1 | A | 851 | A |
| 1 | A | 852 | G |
| 1 | A | 862 | U |
| 1 | A | 863 | G |
| 1 | A | 867 | A |
| 1 | A | 868 | G |
| 1 | A | 869 | U |
| 1 | A | 880 | G |
| 1 | A | 892 | A |
| 1 | A | 904 | G |
| 1 | A | 905 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 912 | C |
| 1 | A | 913 | A |
| 1 | A | 923 | G |
| 1 | A | 938 | U |
| 1 | A | 939 | U |
| 1 | A | 944 | G |
| 1 | A | 946 | A |
| 1 | A | 947 | A |
| 1 | A | 949 | G |
| 1 | A | 950 | C |
| 1 | A | 952 | A |
| 1 | A | 953 | A |
| 1 | A | 954 | G |
| 1 | A | 955 | A |
| 1 | A | 960 | U |
| 1 | A | 961 | A |
| 1 | A | 969 | U |
| 1 | A | 970 | U |
| 1 | A | 971 | G |
| 1 | A | 972 | A |
| 1 | A | 983 | A |
| 1 | A | 984 | A |
| 1 | A | 1002 | G |
| 1 | A | 1003 | G |
| 1 | A | 1005 | G |
| 1 | A | 1007 | C |
| 1 | A | 1033 | G |
| 1 | A | 1037 | C |
| 1 | A | 1047 | G |
| 1 | A | 1048 | U |
| 1 | A | 1049 | C |
| 1 | A | 1051 | G |
| 1 | A | 1068 | U |
| 1 | A | 1069 | U |
| 1 | A | 1077 | G |
| 1 | A | 1084 | A |
| 1 | A | 1085 | A |
| 1 | A | 1100 | G |
| 1 | A | 1107 | G |
| 1 | A | 1108 | U |
| 1 | A | 1109 | U |
| 1 | A | 1112 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1113 | A |
| 1 | A | 1114 | G |
| 1 | A | 1120 | C |
| 1 | A | 1121 | G |
| 1 | A | 1122 | G |
| 1 | A | 1128 | C |
| 1 | A | 1129 | A |
| 1 | A | 1141 | C |
| 1 | A | 1142 | U |
| 1 | A | 1143 | G |
| 1 | A | 1165 | A |
| 1 | A | 1166 | G |
| 1 | A | 1173 | A |
| 1 | A | 1174 | C |
| 1 | A | 1178 | U |
| 1 | A | 1179 | G |
| 1 | A | 1183 | A |
| 1 | A | 1184 | G |
| 1 | A | 1194 | U |
| 1 | A | 1197 | G |
| 1 | A | 1207 | A |
| 1 | A | 1208 | C |
| 1 | A | 1209 | A |
| 1 | A | 1220 | A |
| 1 | A | 1221 | A |
| 1 | A | 1222 | U |
| 1 | A | 1223 | G |
| 1 | A | 1239 | U |
| 1 | A | 1240 | G |
| 1 | A | 1261 | A |
| 1 | A | 1264 | C |
| 1 | A | 1267 | A |
| 1 | A | 1268 | A |
| 1 | A | 1269 | A |
| 1 | A | 1281 | A |
| 1 | A | 1282 | G |
| 1 | A | 1283 | U |
| 1 | A | 1285 | C |
| 1 | A | 1287 | G |
| 1 | A | 1302 | C |
| 1 | A | 1304 | C |
| 1 | A | 1314 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1319 | G |
| 1 | A | 1327 | U |
| 1 | A | 1328 | A |
| 1 | A | 1329 | G |
| 1 | A | 1330 | U |
| 1 | A | 1346 | A |
| 1 | A | 1347 | U |
| 1 | A | 1348 | G |
| 1 | A | 1353 | G |
| 1 | A | 1364 | U |
| 1 | A | 1378 | C |
| 1 | A | 1379 | A |
| 1 | A | 1380 | C |
| 1 | A | 1381 | A |
| 1 | A | 1383 | C |
| 1 | A | 1384 | G |
| 1 | A | 1425 | G |
| 1 | A | 1427 | A |
| 1 | A | 1428 | G |
| 1 | A | 1433 | C |
| 1 | A | 1434 | G |
| 1 | A | 1468 | C |
| 1 | A | 1477 | A |
| 1 | A | 1480 | A |
| 1 | A | 1481 | A |
| 1 | A | 1482 | G |
| 1 | A | 1483 | G |
| 1 | A | 1484 | U |
| 1 | A | 1485 | A |
| 1 | A | 1495 | G |
| 1 | A | 1498 | G |
| 1 | A | 1507 | G |
| 1 | A | 1508 | G |

All (164) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | U |
| 1 | A | 8 | G |
| 1 | A | 9 | A |
| 1 | A | 14 | U |
| 1 | A | 31 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 32 | G |
| 1 | A | 48 | C |
| 1 | A | 49 | C |
| 1 | A | 50 | U |
| 1 | A | 51 | A |
| 1 | A | 52 | A |
| 1 | A | 61 | A |
| 1 | A | 65 | G |
| 1 | A | 103 | A |
| 1 | A | 109 | G |
| 1 | A | 113 | A |
| 1 | A | 115 | C |
| 1 | A | 124 | G |
| 1 | A | 168 | U |
| 1 | A | 176 | G |
| 1 | A | 190 | U |
| 1 | A | 191 | G |
| 1 | A | 204 | A |
| 1 | A | 209 | U |
| 1 | A | 211 | U |
| 1 | A | 239 | A |
| 1 | A | 240 | U |
| 1 | A | 242 | A |
| 1 | A | 246 | A |
| 1 | A | 247 | G |
| 1 | A | 262 | G |
| 1 | A | 270 | A |
| 1 | A | 275 | A |
| 1 | A | 276 | C |
| 1 | A | 277 | G |
| 1 | A | 301 | G |
| 1 | A | 323 | A |
| 1 | A | 324 | C |
| 1 | A | 325 | A |
| 1 | A | 340 | A |
| 1 | A | 341 | C |
| 1 | A | 347 | G |
| 1 | A | 362 | C |
| 1 | A | 363 | U |
| 1 | A | 368 | C |
| 1 | A | 384 | G |
| 1 | A | 417 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 424 | G |
| 1 | A | 425 | U |
| 1 | A | 434 | G |
| 1 | A | 446 | A |
| 1 | A | 469 | G |
| 1 | A | 470 | G |
| 1 | A | 480 | A |
| 1 | A | 481 | A |
| 1 | A | 483 | A |
| 1 | A | 492 | C |
| 1 | A | 493 | A |
| 1 | A | 495 | C |
| 1 | A | 502 | C |
| 1 | A | 515 | U |
| 1 | A | 517 | A |
| 1 | A | 519 | A |
| 1 | A | 531 | A |
| 1 | A | 543 | A |
| 1 | A | 544 | U |
| 1 | A | 545 | U |
| 1 | A | 546 | C |
| 1 | A | 550 | G |
| 1 | A | 559 | G |
| 1 | A | 560 | G |
| 1 | A | 579 | G |
| 1 | A | 625 | U |
| 1 | A | 636 | U |
| 1 | A | 637 | A |
| 1 | A | 671 | A |
| 1 | A | 685 | C |
| 1 | A | 687 | G |
| 1 | A | 701 | C |
| 1 | A | 705 | G |
| 1 | A | 732 | C |
| 1 | A | 736 | G |
| 1 | A | 737 | A |
| 1 | A | 776 | A |
| 1 | A | 796 | C |
| 1 | A | 799 | A |
| 1 | A | 801 | C |
| 1 | A | 802 | G |
| 1 | A | 803 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 804 | U |
| 1 | A | 824 | C |
| 1 | A | 848 | U |
| 1 | A | 849 | U |
| 1 | A | 850 | A |
| 1 | A | 851 | A |
| 1 | A | 862 | U |
| 1 | A | 867 | A |
| 1 | A | 868 | G |
| 1 | A | 891 | A |
| 1 | A | 912 | C |
| 1 | A | 938 | U |
| 1 | A | 943 | A |
| 1 | A | 946 | A |
| 1 | A | 949 | G |
| 1 | A | 952 | A |
| 1 | A | 953 | A |
| 1 | A | 954 | G |
| 1 | A | 960 | U |
| 1 | A | 970 | U |
| 1 | A | 971 | G |
| 1 | A | 1032 | U |
| 1 | A | 1047 | G |
| 1 | A | 1048 | U |
| 1 | A | 1050 | A |
| 1 | A | 1068 | U |
| 1 | A | 1077 | G |
| 1 | A | 1084 | A |
| 1 | A | 1112 | C |
| 1 | A | 1128 | C |
| 1 | A | 1134 | A |
| 1 | A | 1140 | A |
| 1 | A | 1142 | U |
| 1 | A | 1164 | G |
| 1 | A | 1165 | A |
| 1 | A | 1172 | G |
| 1 | A | 1178 | U |
| 1 | A | 1183 | A |
| 1 | A | 1196 | C |
| 1 | A | 1206 | G |
| 1 | A | 1208 | C |
| 1 | A | 1221 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1222 | U |
| 1 | A | 1238 | A |
| 1 | A | 1239 | U |
| 1 | A | 1260 | U |
| 1 | A | 1262 | A |
| 1 | A | 1263 | U |
| 1 | A | 1267 | A |
| 1 | A | 1282 | G |
| 1 | A | 1284 | U |
| 1 | A | 1301 | A |
| 1 | A | 1304 | C |
| 1 | A | 1313 | G |
| 1 | A | 1327 | U |
| 1 | A | 1328 | A |
| 1 | A | 1329 | G |
| 1 | A | 1346 | A |
| 1 | A | 1347 | U |
| 1 | A | 1363 | U |
| 1 | A | 1377 | A |
| 1 | A | 1379 | A |
| 1 | A | 1380 | C |
| 1 | A | 1382 | C |
| 1 | A | 1383 | C |
| 1 | A | 1432 | A |
| 1 | A | 1433 | C |
| 1 | A | 1476 | U |
| 1 | A | 1480 | A |
| 1 | A | 1481 | A |
| 1 | A | 1482 | G |
| 1 | A | 1483 | G |
| 1 | A | 1484 | U |
| 1 | A | 1506 | U |
| 1 | A | 1507 | G |

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | KSG | A | 1524 | - | 24,27,27 | 1.47 | 1 (4%) | 29,40,40 | 1.24 | 2 (6%) |
| 22 | KSG | A | 1523 | - | 24,27,27 | 1.46 | 1 (4%) | 29,40,40 | 1.23 | 2 (6%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 22 | KSG | A | 1524 | - | - | 1/8/52/52 | 0/2/2/2 |
| 22 | KSG | A | 1523 | - | - | 3/8/52/52 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | A | 1524 | KSG | C14-C13 | -6.81 | 1.49 | 1.53 |
| 22 | A | 1523 | KSG | C14-C13 | -6.78 | 1.49 | 1.53 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | A | 1524 | KSG | C1-O1-C2 | -4.51 | 106.80 | 117.96 |
| 22 | A | 1523 | KSG | C1-O1-C2 | -4.50 | 106.83 | 117.96 |
| 22 | A | 1524 | KSG | C1-O7-C8 | -3.56 | 107.55 | 113.67 |
| 22 | A | 1523 | KSG | C1-O7-C8 | -3.54 | 107.58 | 113.67 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

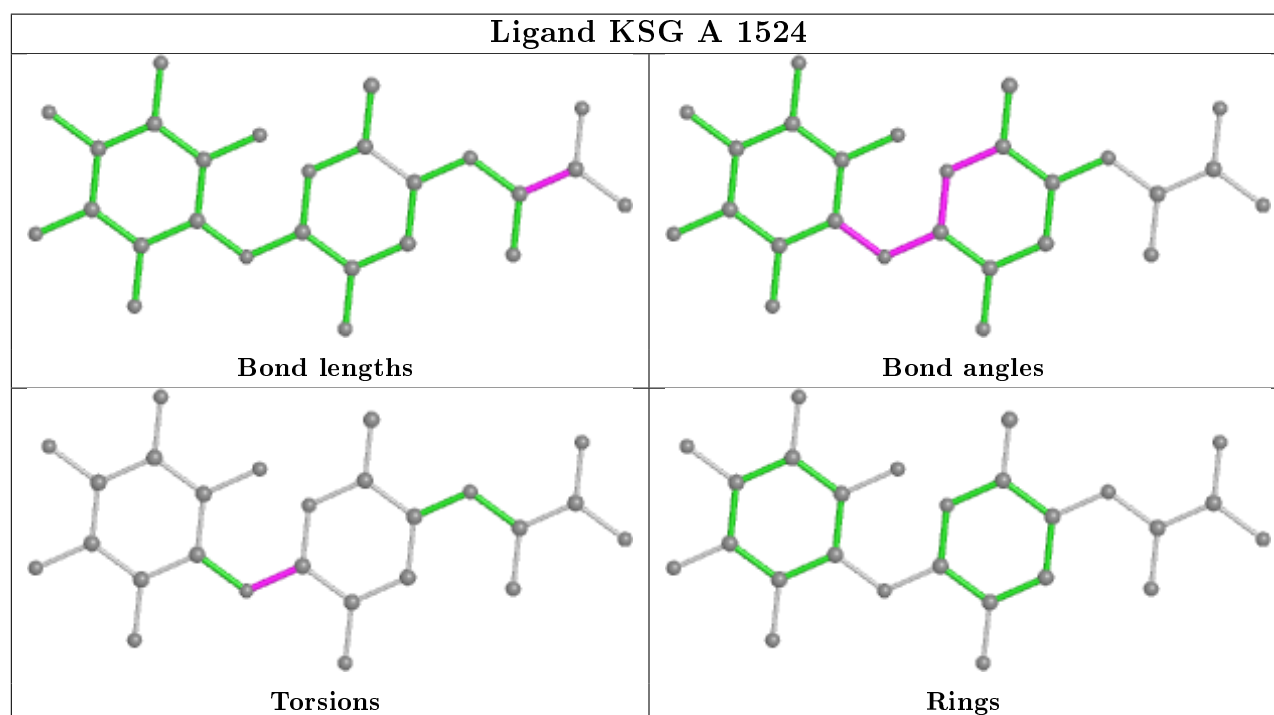
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 22 | A | 1523 | KSG | C14-C13-N2-C10 |
| 22 | A | 1523 | KSG | N3-C13-N2-C10 |
| 22 | A | 1524 | KSG | O7-C1-O1-C2 |
| 22 | A | 1523 | KSG | O7-C1-O1-C2 |

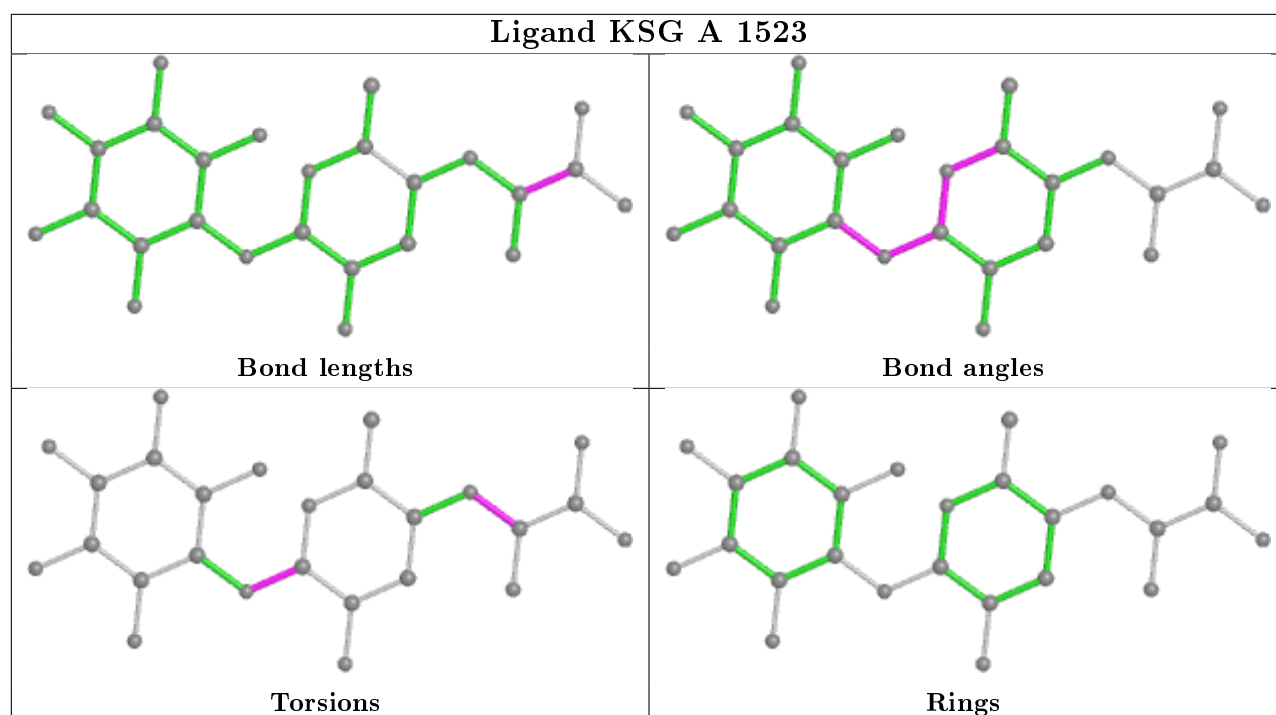
There are no ring outliers.

2 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22 | A | 1524 | KSG | 7 | 0 |
| 22 | A | 1523 | KSG | 5 | 0 |

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





5.7 Other polymers [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 1503/1522 (98%) | -0.55 | 12 (0%) 86 89 | 1, 29, 110, 161 | 0 |
| 2 | B | 234/256 (91%) | -0.25 | 12 (5%) 28 30 | 4, 41, 109, 134 | 0 |
| 3 | C | 206/239 (86%) | -0.60 | 0 100 100 | 7, 46, 83, 93 | 0 |
| 4 | D | 208/209 (99%) | -0.57 | 3 (1%) 75 78 | 1, 27, 57, 70 | 0 |
| 5 | E | 150/162 (92%) | -0.78 | 0 100 100 | 1, 10, 35, 60 | 0 |
| 6 | F | 101/101 (100%) | -0.57 | 0 100 100 | 25, 52, 71, 80 | 0 |
| 7 | G | 155/156 (99%) | -0.44 | 4 (2%) 56 58 | 27, 54, 85, 102 | 0 |
| 8 | H | 138/138 (100%) | -0.84 | 0 100 100 | 1, 6, 34, 41 | 0 |
| 9 | I | 127/128 (99%) | -0.36 | 1 (0%) 86 89 | 9, 59, 87, 96 | 0 |
| 10 | J | 98/105 (93%) | -0.09 | 4 (4%) 37 39 | 15, 78, 118, 124 | 0 |
| 11 | K | 119/129 (92%) | -0.42 | 2 (1%) 70 73 | 18, 39, 66, 110 | 0 |
| 12 | L | 124/135 (91%) | -0.59 | 0 100 100 | 1, 32, 55, 98 | 0 |
| 13 | M | 125/126 (99%) | -0.05 | 7 (5%) 24 26 | 32, 53, 94, 133 | 0 |
| 14 | N | 60/61 (98%) | -0.44 | 0 100 100 | 15, 37, 78, 93 | 0 |
| 15 | O | 88/89 (98%) | -0.78 | 0 100 100 | 2, 30, 61, 95 | 0 |
| 16 | P | 83/88 (94%) | -0.76 | 0 100 100 | 3, 22, 42, 75 | 0 |
| 17 | Q | 104/105 (99%) | -0.55 | 4 (3%) 40 42 | 1, 22, 93, 153 | 0 |
| 18 | R | 73/88 (82%) | -0.43 | 2 (2%) 54 57 | 10, 33, 95, 136 | 0 |
| 19 | S | 80/93 (86%) | -0.10 | 2 (2%) 57 59 | 47, 64, 106, 120 | 0 |
| 20 | T | 99/106 (93%) | -0.51 | 1 (1%) 82 86 | 22, 37, 80, 87 | 0 |
| 21 | U | 24/27 (88%) | -0.19 | 0 100 100 | 27, 38, 62, 78 | 0 |
| All | All | 3899/4063 (95%) | -0.51 | 54 (1%) 75 78 | 1, 35, 95, 161 | 0 |

All (54) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | M | 123 | ALA | 10.6 |
| 11 | K | 129 | SER | 8.9 |
| 2 | B | 234 | PRO | 8.7 |
| 13 | M | 124 | PRO | 8.2 |
| 13 | M | 121 | LYS | 7.3 |
| 17 | Q | 102 | GLY | 6.3 |
| 2 | B | 235 | SER | 6.1 |
| 2 | B | 233 | SER | 6.1 |
| 17 | Q | 104 | LYS | 5.8 |
| 17 | Q | 103 | GLY | 5.4 |
| 13 | M | 122 | LYS | 5.4 |
| 18 | R | 16 | PRO | 5.3 |
| 17 | Q | 105 | ALA | 5.2 |
| 2 | B | 231 | GLU | 5.2 |
| 2 | B | 236 | TYR | 5.0 |
| 18 | R | 17 | SER | 4.9 |
| 1 | A | 1013 | A | 4.9 |
| 19 | S | 2 | PRO | 4.5 |
| 7 | G | 156 | TRP | 4.5 |
| 1 | A | 1011 | C | 4.5 |
| 11 | K | 128 | ALA | 4.4 |
| 19 | S | 3 | ARG | 4.4 |
| 2 | B | 232 | PRO | 4.2 |
| 2 | B | 230 | VAL | 4.1 |
| 13 | M | 120 | LYS | 4.1 |
| 1 | A | 1112 | C | 4.0 |
| 2 | B | 239 | VAL | 3.9 |
| 10 | J | 73 | ASP | 3.2 |
| 2 | B | 229 | VAL | 3.2 |
| 2 | B | 237 | ALA | 3.1 |
| 1 | A | 982 | G | 3.1 |
| 1 | A | 456 | C | 3.0 |
| 1 | A | 1014 | G | 2.9 |
| 7 | G | 5 | ARG | 2.9 |
| 2 | B | 238 | LEU | 2.9 |
| 9 | I | 128 | ARG | 2.9 |
| 1 | A | 1006 | C | 2.9 |
| 1 | A | 1402 | G | 2.8 |
| 10 | J | 72 | VAL | 2.7 |
| 4 | D | 26 | CYS | 2.6 |
| 20 | T | 103 | GLY | 2.6 |
| 7 | G | 155 | ARG | 2.6 |
| 1 | A | 81 | U | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | D | 31 | CYS | 2.5 |
| 13 | M | 126 | LYS | 2.3 |
| 2 | B | 240 | GLN | 2.3 |
| 10 | J | 71 | LEU | 2.3 |
| 10 | J | 33 | GLN | 2.3 |
| 1 | A | 1010 | G | 2.3 |
| 13 | M | 125 | ARG | 2.2 |
| 7 | G | 81 | GLY | 2.2 |
| 4 | D | 9 | CYS | 2.1 |
| 1 | A | 1399 | G | 2.1 |
| 1 | A | 1009 | C | 2.1 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

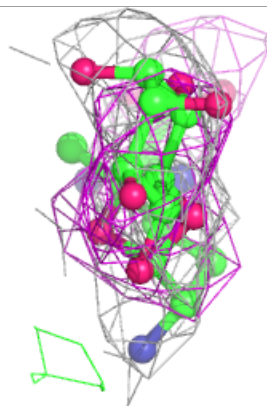
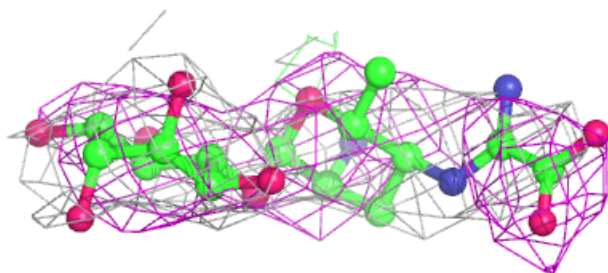
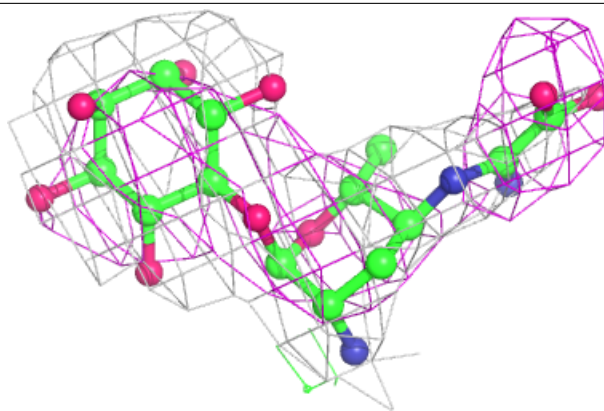
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | KSG | A | 1524 | 26/26 | 0.80 | 0.62 | 28,32,34,36 | 0 |
| 22 | KSG | A | 1523 | 26/26 | 0.88 | 0.40 | 27,31,32,33 | 0 |

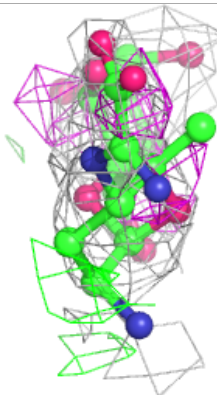
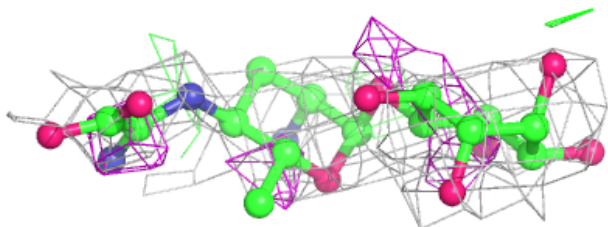
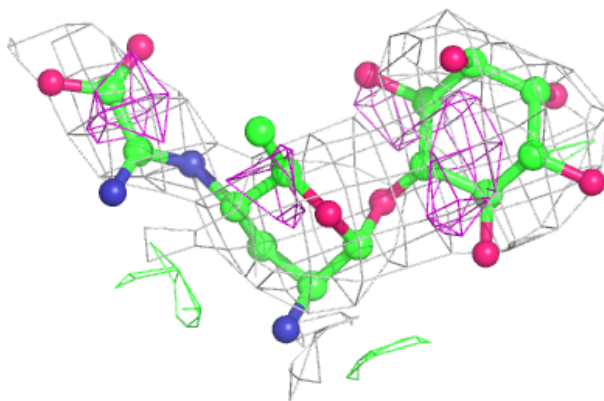
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KSG A 1524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around KSG A 1523:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.