



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 06:15 PM BST

PDB ID : 3OFO
Title : Crystal structure of the E. coli ribosome bound to erythromycin. This file contains the 30S subunit of the first 70S ribosome.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-15
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

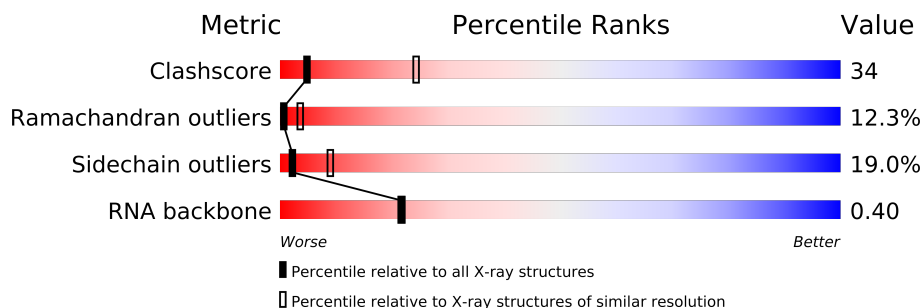
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 79885 | 1078 (3.16-3.04) |
| Ramachandran outliers | 78287 | 1044 (3.16-3.04) |
| Sidechain outliers | 78261 | 1044 (3.16-3.04) |
| RNA backbone | 1838 | 1047 (3.60-2.60) |

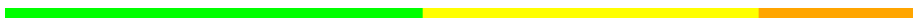
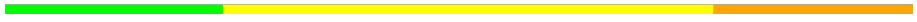




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1533 | |
| 2 | B | 218 | |
| 3 | C | 206 | |
| 4 | D | 205 | |
| 5 | E | 150 | |
| 6 | F | 100 | |
| 7 | G | 151 | |
| 8 | H | 129 | |
| 9 | I | 127 | |
| 10 | J | 98 | |
| 11 | K | 117 | |
| 12 | L | 123 | |
| 13 | M | 114 | |
| 14 | N | 100 | |
| 15 | O | 88 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 16 | P | 82 |  |
| 17 | Q | 80 |  |
| 18 | R | 55 |  |
| 19 | S | 79 |  |
| 20 | T | 85 |  |
| 21 | U | 51 |  |

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51700 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32895 | 14671 | 6036 | 10655 | 1533 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1705 | 1081 | 305 | 312 | 7 | | | |

- 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 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |

- 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 |
| | | | 1106 | 687 | 211 | 202 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 515 | 148 | 149 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | I | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |

- 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 |
| | | | 787 | 493 | 150 | 143 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | K | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | L | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | M | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | N | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |

- 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 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | P | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | Q | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | R | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 288 | 86 | 82 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | S | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | T | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | U | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 426 | 265 | 86 | 74 | 1 | | | |

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22 | A | 41 | Total | Mg | 0 | 0 |
| | | | 41 | 41 | | |
| 22 | N | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 23 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 23 | A | 198 | Total | O | 0 | 0 |
| | | | 198 | 198 | | |
| 23 | L | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 23 | N | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 23 | U | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |

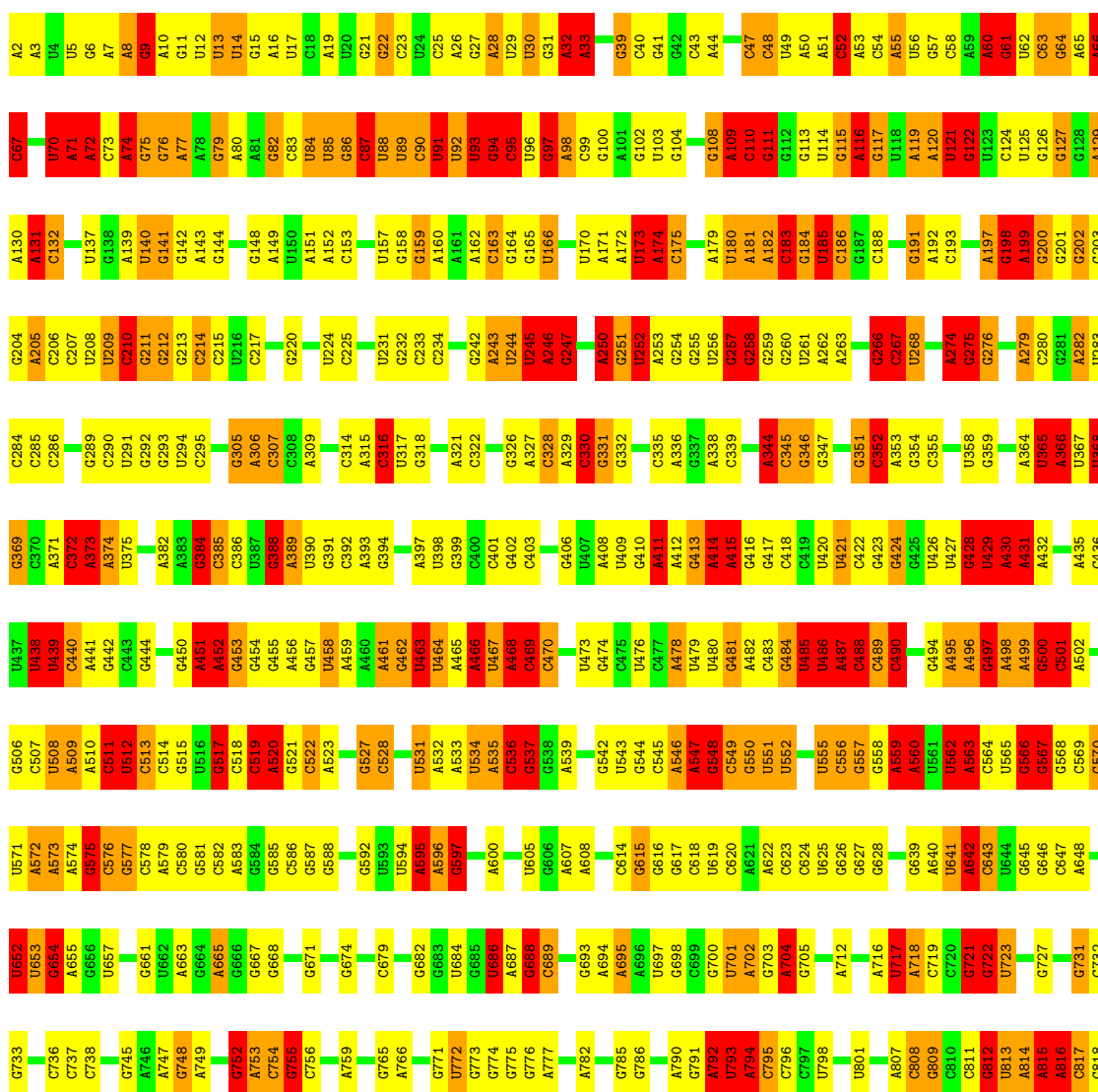
3 Residue-property plots

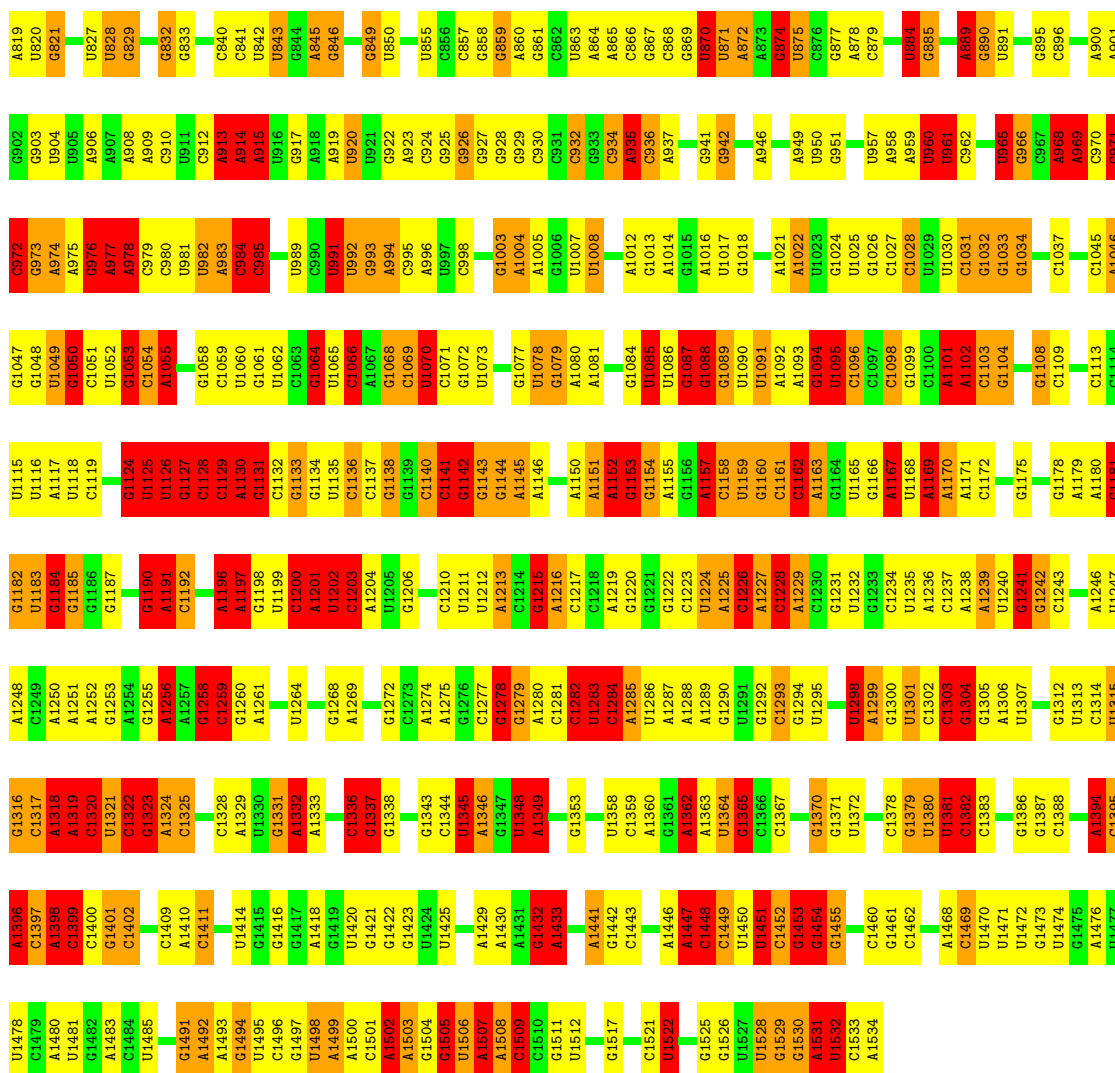
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: 16S rRNA

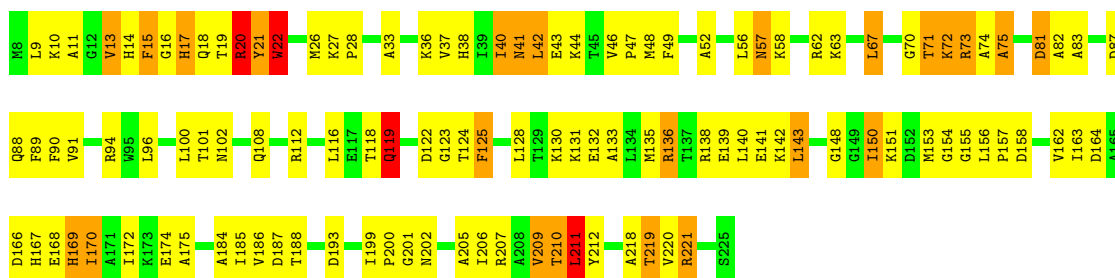
Chain A:





• Molecule 2: 30S ribosomal protein S2

Chain B:



• Molecule 3: 30S ribosomal protein S3

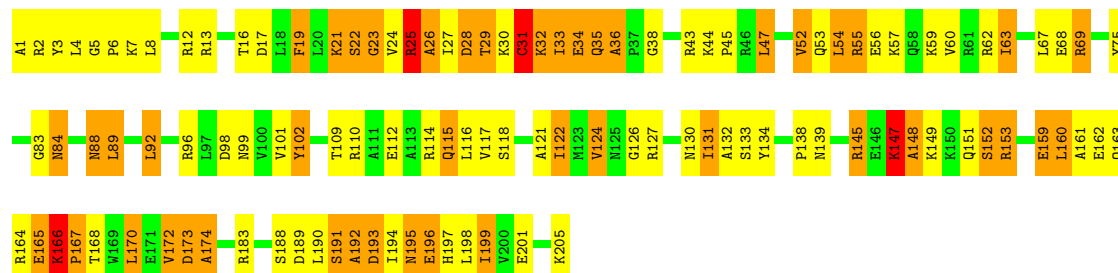
Chain C:





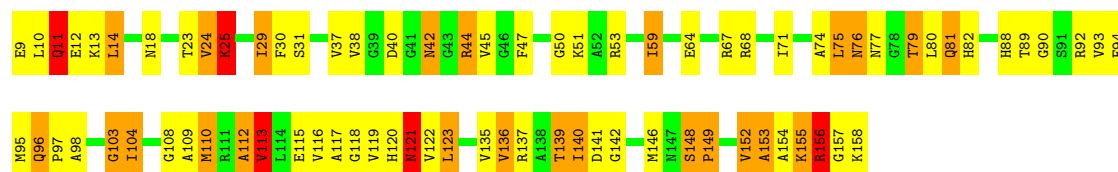
• Molecule 4: 30S ribosomal protein S4

Chain D:



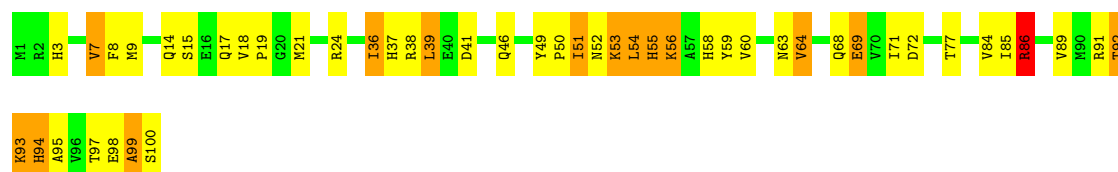
• Molecule 5: 30S ribosomal protein S5

Chain E:



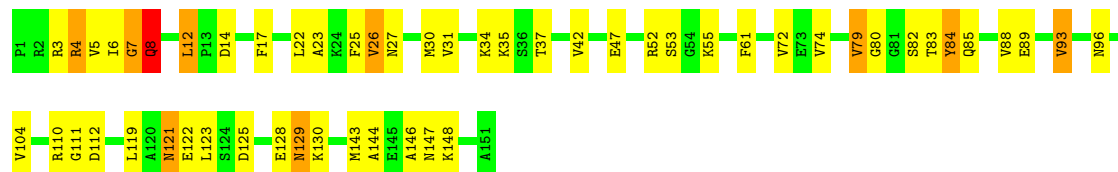
• Molecule 6: 30S ribosomal protein S6

Chain F:



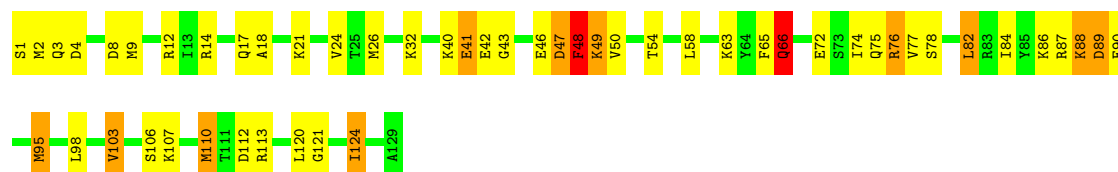
• Molecule 7: 30S ribosomal protein S7

Chain G:



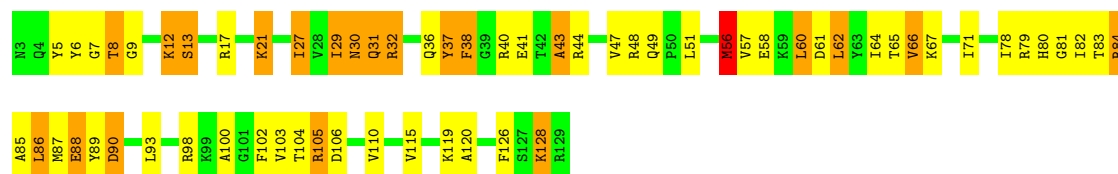
• Molecule 8: 30S ribosomal protein S8

Chain H:



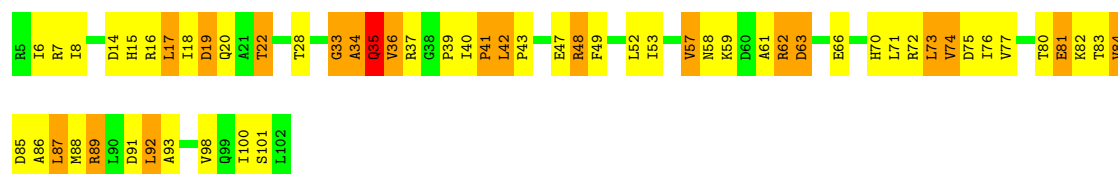
- Molecule 9: 30S ribosomal protein S9

Chain I: 



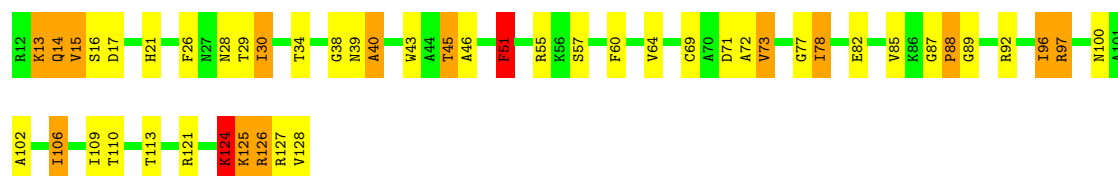
- Molecule 10: 30S ribosomal protein S10

Chain J: 



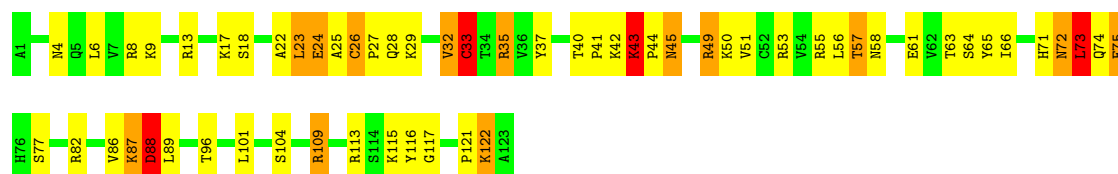
- Molecule 11: 30S ribosomal protein S11

Chain K: 



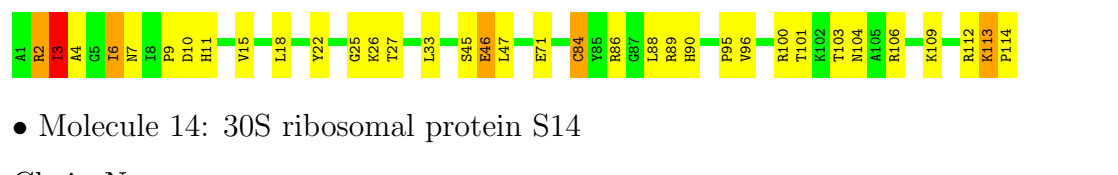
- Molecule 12: 30S ribosomal protein S12

Chain L: 



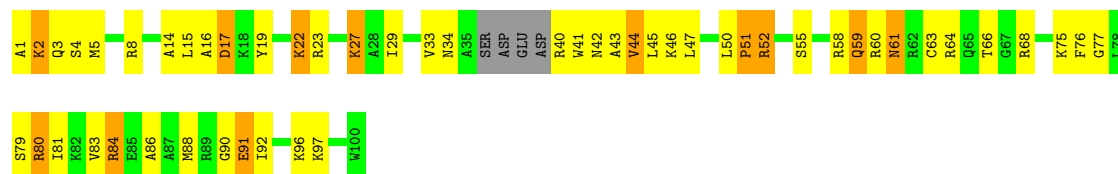
- Molecule 13: 30S ribosomal protein S13

Chain M: 



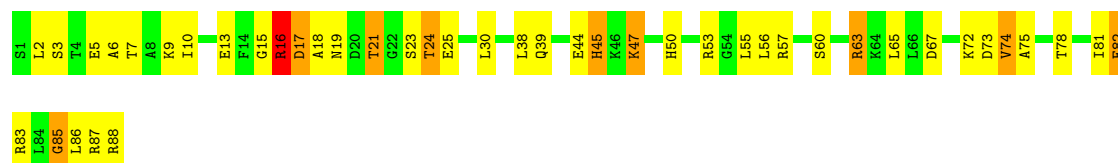
- Molecule 14: 30S ribosomal protein S14

Chain N: 



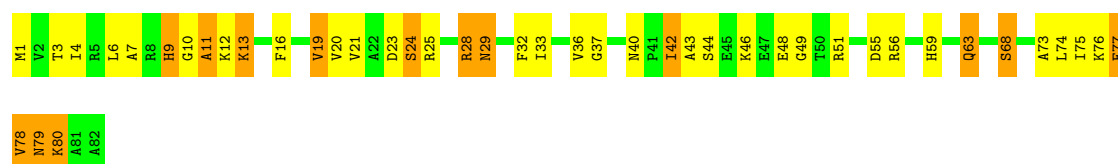
- Molecule 15: 30S ribosomal protein S15

Chain O: 



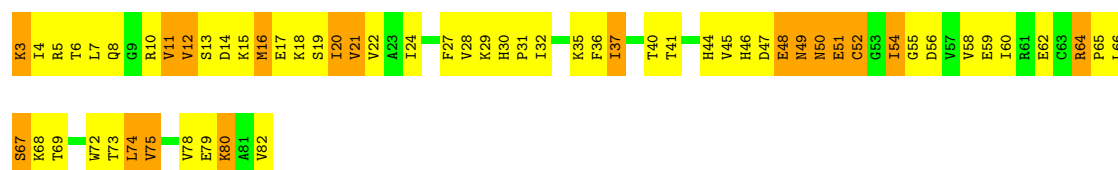
- Molecule 16: 30S ribosomal protein S16

Chain P: 



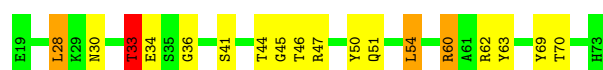
- Molecule 17: 30S ribosomal protein S17

Chain Q: 



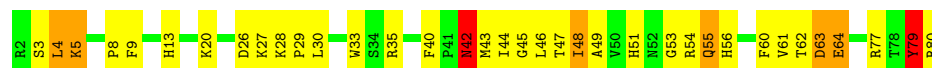
- Molecule 18: 30S ribosomal protein S18

Chain R: 



- Molecule 19: 30S ribosomal protein S19

Chain S: 



- Molecule 20: 30S ribosomal protein S20

Chain T: 



- Molecule 21: 30S ribosomal protein S21

Chain U: 



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.96Å 434.53Å 623.58Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 82.40 – 3.10 | Depositor |
| % Data completeness (in resolution range) | (Not available) (82.40-3.10) | Depositor |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.47 (at 3.13Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.205 , 0.254 | Depositor |
| Wilson B-factor (Å ²) | 54.4 | Xtriage |
| Anisotropy | 0.354 | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 0 of 925668 reflections | Xtriage |
| Total number of atoms | 51700 | wwPDB-VP |
| Average B, all atoms (Å ²) | 95.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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 | 0.53 | 0/36834 | 1.32 | 524/57462 (0.9%) |
| 2 | B | 0.24 | 0/1736 | 0.47 | 0/2338 |
| 3 | C | 0.27 | 0/1652 | 0.50 | 0/2225 |
| 4 | D | 0.30 | 0/1665 | 0.52 | 0/2227 |
| 5 | E | 0.34 | 0/1119 | 0.61 | 0/1504 |
| 6 | F | 0.29 | 0/836 | 0.47 | 0/1128 |
| 7 | G | 0.22 | 0/1196 | 0.44 | 0/1602 |
| 8 | H | 0.32 | 0/989 | 0.56 | 0/1326 |
| 9 | I | 0.23 | 0/1034 | 0.45 | 0/1375 |
| 10 | J | 0.24 | 0/797 | 0.47 | 0/1077 |
| 11 | K | 0.27 | 0/893 | 0.53 | 0/1205 |
| 12 | L | 0.38 | 0/969 | 0.69 | 0/1300 |
| 13 | M | 0.23 | 0/893 | 0.49 | 0/1193 |
| 14 | N | 0.25 | 0/785 | 0.48 | 0/1043 |
| 15 | O | 0.30 | 0/722 | 0.49 | 0/964 |
| 16 | P | 0.31 | 0/659 | 0.51 | 0/884 |
| 17 | Q | 0.37 | 0/658 | 0.59 | 0/881 |
| 18 | R | 0.29 | 0/463 | 0.49 | 0/621 |
| 19 | S | 0.23 | 0/653 | 0.46 | 0/877 |
| 20 | T | 0.34 | 0/671 | 0.57 | 0/888 |
| 21 | U | 0.25 | 0/431 | 0.46 | 0/570 |
| All | All | 0.46 | 0/55655 | 1.14 | 524/82690 (0.6%) |

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 |
|-----|-------|---------------------|---------------------|
| 12 | L | 0 | 1 |
| 20 | T | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All | 0 | 2 |

There are no bond length outliers.

All (524) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | A | 111 | G | P-O3'-C3' | -15.18 | 101.49 | 119.70 |
| 1 | A | 1202 | U | N1-C1'-C2' | -14.12 | 95.64 | 114.00 |
| 1 | A | 352 | C | N1-C1'-C2' | -13.67 | 96.23 | 114.00 |
| 1 | A | 52 | C | N1-C1'-C2' | -13.24 | 96.79 | 114.00 |
| 1 | A | 267 | C | N1-C1'-C2' | -12.43 | 97.84 | 114.00 |
| 1 | A | 1202 | U | O4'-C1'-N1 | 12.41 | 118.13 | 108.20 |
| 1 | A | 960 | U | P-O3'-C3' | 12.27 | 134.42 | 119.70 |
| 1 | A | 32 | A | P-O3'-C3' | -11.79 | 105.56 | 119.70 |
| 1 | A | 870 | U | P-O3'-C3' | 11.67 | 133.70 | 119.70 |
| 1 | A | 1282 | C | N1-C1'-C2' | -11.57 | 98.96 | 114.00 |
| 1 | A | 597 | G | P-O3'-C3' | -11.49 | 105.91 | 119.70 |
| 1 | A | 1284 | C | N1-C1'-C2' | -11.42 | 99.16 | 114.00 |
| 1 | A | 122 | G | P-O3'-C3' | -11.23 | 106.23 | 119.70 |
| 1 | A | 972 | C | N1-C1'-C2' | -11.08 | 99.59 | 114.00 |
| 1 | A | 488 | C | N1-C1'-C2' | -11.00 | 99.70 | 114.00 |
| 1 | A | 512 | U | N1-C1'-C2' | -10.90 | 99.83 | 114.00 |
| 1 | A | 1345 | U | O4'-C1'-N1 | 10.74 | 116.79 | 108.20 |
| 1 | A | 275 | G | P-O3'-C3' | -10.71 | 106.85 | 119.70 |
| 1 | A | 812 | G | P-O3'-C3' | 10.70 | 132.54 | 119.70 |
| 1 | A | 1532 | U | N1-C1'-C2' | -10.70 | 100.09 | 114.00 |
| 1 | A | 330 | C | N1-C1'-C2' | -10.64 | 100.17 | 114.00 |
| 1 | A | 1507 | A | P-O3'-C3' | -10.59 | 106.99 | 119.70 |
| 1 | A | 915 | A | P-O3'-C3' | -10.54 | 107.05 | 119.70 |
| 1 | A | 1528 | U | P-O3'-C3' | 10.45 | 132.24 | 119.70 |
| 1 | A | 985 | C | N1-C1'-C2' | -10.42 | 100.45 | 114.00 |
| 1 | A | 874 | G | P-O3'-C3' | -10.42 | 107.19 | 119.70 |
| 1 | A | 66 | A | P-O3'-C3' | -10.41 | 107.20 | 119.70 |
| 1 | A | 1448 | C | N1-C1'-C2' | -10.35 | 100.54 | 114.00 |
| 1 | A | 1162 | C | N1-C1'-C2' | -10.29 | 100.63 | 114.00 |
| 1 | A | 1224 | U | P-O3'-C3' | 10.24 | 131.99 | 119.70 |
| 1 | A | 13 | U | P-O3'-C3' | 10.13 | 131.85 | 119.70 |
| 1 | A | 490 | C | N1-C1'-C2' | -10.10 | 100.87 | 114.00 |
| 1 | A | 889 | A | P-O3'-C3' | 10.05 | 131.77 | 119.70 |
| 1 | A | 119 | A | P-O3'-C3' | 10.02 | 131.72 | 119.70 |
| 1 | A | 1203 | C | N1-C1'-C2' | -10.01 | 100.99 | 114.00 |
| 1 | A | 891 | U | N1-C1'-C2' | -10.01 | 100.99 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 511 | C | P-O3'-C3' | 9.91 | 131.59 | 119.70 |
| 1 | A | 534 | U | N1-C1'-C2' | -9.90 | 101.11 | 112.00 |
| 1 | A | 33 | A | P-O3'-C3' | -9.87 | 107.86 | 119.70 |
| 1 | A | 1181 | G | P-O3'-C3' | 9.83 | 131.50 | 119.70 |
| 1 | A | 1088 | G | P-O3'-C3' | -9.81 | 107.93 | 119.70 |
| 1 | A | 1128 | C | N1-C1'-C2' | -9.73 | 101.29 | 112.00 |
| 1 | A | 934 | C | O4'-C1'-N1 | 9.64 | 115.91 | 108.20 |
| 1 | A | 93 | U | N1-C1'-C2' | -9.55 | 101.50 | 112.00 |
| 1 | A | 969 | A | P-O3'-C3' | -9.52 | 108.28 | 119.70 |
| 1 | A | 1095 | U | N1-C1'-C2' | -9.51 | 101.54 | 112.00 |
| 1 | A | 279 | A | P-O3'-C3' | 9.50 | 131.10 | 119.70 |
| 1 | A | 1298 | U | P-O3'-C3' | 9.45 | 131.04 | 119.70 |
| 1 | A | 173 | U | O4'-C1'-N1 | 9.45 | 115.76 | 108.20 |
| 1 | A | 1381 | U | N1-C1'-C2' | -9.44 | 101.62 | 112.00 |
| 1 | A | 1451 | U | P-O3'-C3' | 9.36 | 130.94 | 119.70 |
| 1 | A | 305 | G | P-O3'-C3' | 9.33 | 130.90 | 119.70 |
| 1 | A | 984 | C | N1-C1'-C2' | -9.29 | 101.78 | 112.00 |
| 1 | A | 1259 | C | N1-C1'-C2' | -9.28 | 101.79 | 112.00 |
| 1 | A | 961 | U | N1-C1'-C2' | -9.27 | 101.81 | 112.00 |
| 1 | A | 595 | A | P-O3'-C3' | 9.26 | 130.81 | 119.70 |
| 1 | A | 547 | A | P-O3'-C3' | 9.23 | 130.77 | 119.70 |
| 1 | A | 1283 | U | N1-C1'-C2' | -9.22 | 101.85 | 112.00 |
| 1 | A | 173 | U | P-O3'-C3' | 9.19 | 130.72 | 119.70 |
| 1 | A | 793 | U | P-O3'-C3' | -9.18 | 108.69 | 119.70 |
| 1 | A | 1349 | A | P-O3'-C3' | -9.16 | 108.71 | 119.70 |
| 1 | A | 575 | G | P-O3'-C3' | 9.14 | 130.67 | 119.70 |
| 1 | A | 972 | C | O4'-C1'-N1 | 9.14 | 115.52 | 108.20 |
| 1 | A | 1228 | C | N1-C1'-C2' | -9.11 | 101.98 | 112.00 |
| 1 | A | 1399 | C | P-O3'-C3' | 9.10 | 130.61 | 119.70 |
| 1 | A | 307 | C | P-O3'-C3' | -9.06 | 108.83 | 119.70 |
| 1 | A | 110 | C | N1-C1'-C2' | -9.06 | 102.04 | 112.00 |
| 1 | A | 1068 | G | P-O3'-C3' | -8.98 | 108.93 | 119.70 |
| 1 | A | 1380 | U | P-O3'-C3' | 8.96 | 130.45 | 119.70 |
| 1 | A | 1125 | U | P-O3'-C3' | 8.96 | 130.45 | 119.70 |
| 1 | A | 821 | G | P-O3'-C3' | -8.96 | 108.95 | 119.70 |
| 1 | A | 577 | G | P-O3'-C3' | -8.86 | 109.06 | 119.70 |
| 1 | A | 1502 | A | P-O3'-C3' | 8.86 | 130.33 | 119.70 |
| 1 | A | 1348 | U | N1-C1'-C2' | -8.85 | 102.26 | 112.00 |
| 1 | A | 815 | A | P-O3'-C3' | 8.80 | 130.27 | 119.70 |
| 1 | A | 1398 | A | P-O3'-C3' | -8.77 | 109.18 | 119.70 |
| 1 | A | 792 | A | O4'-C1'-N9 | 8.72 | 115.18 | 108.20 |
| 1 | A | 9 | G | P-O3'-C3' | -8.71 | 109.25 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 141 | G | P-O3'-C3' | -8.61 | 109.37 | 119.70 |
| 1 | A | 438 | U | P-O3'-C3' | 8.57 | 129.99 | 119.70 |
| 1 | A | 519 | C | P-O3'-C3' | -8.55 | 109.44 | 119.70 |
| 1 | A | 752 | G | P-O3'-C3' | 8.53 | 129.94 | 119.70 |
| 1 | A | 501 | C | N1-C1'-C2' | -8.52 | 102.63 | 112.00 |
| 1 | A | 469 | C | N1-C1'-C2' | -8.50 | 102.65 | 112.00 |
| 1 | A | 1157 | A | P-O3'-C3' | 8.47 | 129.86 | 119.70 |
| 1 | A | 306 | A | P-O3'-C3' | -8.46 | 109.55 | 119.70 |
| 1 | A | 889 | A | O4'-C1'-N9 | 8.44 | 114.95 | 108.20 |
| 1 | A | 1200 | C | P-O3'-C3' | 8.43 | 129.81 | 119.70 |
| 1 | A | 813 | U | P-O3'-C3' | -8.31 | 109.73 | 119.70 |
| 1 | A | 1433 | A | P-O3'-C3' | -8.28 | 109.77 | 119.70 |
| 1 | A | 252 | U | N1-C1'-C2' | -8.26 | 102.91 | 112.00 |
| 1 | A | 1203 | C | P-O3'-C3' | -8.23 | 109.82 | 119.70 |
| 1 | A | 1284 | C | P-O3'-C3' | -8.21 | 109.85 | 119.70 |
| 1 | A | 1303 | C | N1-C1'-C2' | -8.12 | 103.07 | 112.00 |
| 1 | A | 985 | C | P-O3'-C3' | -8.11 | 109.97 | 119.70 |
| 1 | A | 316 | C | P-O3'-C3' | -8.11 | 109.97 | 119.70 |
| 1 | A | 431 | A | P-O3'-C3' | -8.08 | 110.01 | 119.70 |
| 1 | A | 1365 | G | P-O3'-C3' | -8.06 | 110.02 | 119.70 |
| 1 | A | 1380 | U | O4'-C1'-N1 | 8.06 | 114.65 | 108.20 |
| 1 | A | 654 | G | P-O3'-C3' | -8.02 | 110.08 | 119.70 |
| 1 | A | 1332 | A | P-O3'-C3' | -8.02 | 110.08 | 119.70 |
| 1 | A | 1256 | A | P-O3'-C3' | 8.01 | 129.31 | 119.70 |
| 1 | A | 816 | A | P-O3'-C3' | -8.01 | 110.09 | 119.70 |
| 1 | A | 934 | C | P-O3'-C3' | 7.96 | 129.25 | 119.70 |
| 1 | A | 115 | G | P-O3'-C3' | 7.93 | 129.21 | 119.70 |
| 1 | A | 486 | U | N1-C1'-C2' | -7.92 | 103.29 | 112.00 |
| 1 | A | 48 | C | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 1 | A | 479 | U | O4'-C1'-N1 | 7.86 | 114.48 | 108.20 |
| 1 | A | 718 | A | P-O3'-C3' | -7.84 | 110.30 | 119.70 |
| 1 | A | 1447 | A | P-O3'-C3' | 7.83 | 129.10 | 119.70 |
| 1 | A | 511 | C | N1-C1'-C2' | 7.82 | 124.17 | 114.00 |
| 1 | A | 1196 | A | P-O3'-C3' | 7.82 | 129.09 | 119.70 |
| 1 | A | 389 | A | P-O3'-C3' | -7.82 | 110.32 | 119.70 |
| 1 | A | 490 | C | P-O3'-C3' | -7.79 | 110.35 | 119.70 |
| 1 | A | 373 | A | P-O3'-C3' | -7.78 | 110.36 | 119.70 |
| 1 | A | 1055 | A | P-O3'-C3' | -7.77 | 110.38 | 119.70 |
| 1 | A | 365 | U | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 1 | A | 688 | G | P-O3'-C3' | -7.75 | 110.40 | 119.70 |
| 1 | A | 1066 | C | O4'-C1'-N1 | -7.75 | 102.00 | 108.20 |
| 1 | A | 439 | U | N1-C1'-C2' | -7.74 | 103.49 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 129 | A | P-O3'-C3' | 7.72 | 128.96 | 119.70 |
| 1 | A | 109 | A | P-O3'-C3' | 7.71 | 128.96 | 119.70 |
| 1 | A | 794 | A | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 1 | A | 1128 | C | P-O3'-C3' | -7.70 | 110.46 | 119.70 |
| 1 | A | 717 | U | P-O3'-C3' | 7.68 | 128.91 | 119.70 |
| 1 | A | 1201 | A | P-O3'-C3' | 7.66 | 128.89 | 119.70 |
| 1 | A | 198 | G | P-O3'-C3' | -7.62 | 110.55 | 119.70 |
| 1 | A | 72 | A | P-O3'-C3' | -7.61 | 110.57 | 119.70 |
| 1 | A | 1200 | C | N1-C1'-C2' | 7.61 | 123.89 | 114.00 |
| 1 | A | 336 | A | P-O3'-C3' | -7.57 | 110.62 | 119.70 |
| 1 | A | 512 | U | P-O3'-C3' | -7.55 | 110.64 | 119.70 |
| 1 | A | 1394 | A | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 1 | A | 1395 | C | P-O5'-C5' | -7.53 | 108.85 | 120.90 |
| 1 | A | 974 | A | P-O3'-C3' | 7.52 | 128.72 | 119.70 |
| 1 | A | 1382 | C | N1-C1'-C2' | -7.51 | 103.74 | 112.00 |
| 1 | A | 1259 | C | P-O3'-C3' | -7.50 | 110.70 | 119.70 |
| 1 | A | 415 | A | P-O3'-C3' | -7.50 | 110.70 | 119.70 |
| 1 | A | 95 | C | N1-C1'-C2' | -7.50 | 103.76 | 112.00 |
| 1 | A | 642 | A | P-O3'-C3' | -7.47 | 110.74 | 119.70 |
| 1 | A | 536 | C | P-O3'-C3' | -7.43 | 110.78 | 119.70 |
| 1 | A | 641 | U | P-O3'-C3' | 7.42 | 128.61 | 119.70 |
| 1 | A | 517 | G | P-O3'-C3' | 7.35 | 128.52 | 119.70 |
| 1 | A | 960 | U | N1-C1'-C2' | 7.33 | 123.53 | 114.00 |
| 1 | A | 245 | U | N1-C1'-C2' | -7.32 | 103.94 | 112.00 |
| 1 | A | 704 | A | P-O3'-C3' | -7.31 | 110.93 | 119.70 |
| 1 | A | 885 | G | P-O3'-C3' | -7.29 | 110.95 | 119.70 |
| 1 | A | 935 | A | P-O3'-C3' | -7.29 | 110.96 | 119.70 |
| 1 | A | 520 | A | P-O3'-C3' | -7.28 | 110.97 | 119.70 |
| 1 | A | 913 | A | P-O3'-C3' | 7.27 | 128.42 | 119.70 |
| 1 | A | 1320 | C | P-O3'-C3' | -7.27 | 110.98 | 119.70 |
| 1 | A | 1345 | U | P-O3'-C3' | 7.27 | 128.42 | 119.70 |
| 1 | A | 1141 | C | N1-C1'-C2' | -7.24 | 104.04 | 112.00 |
| 1 | A | 961 | U | P-O3'-C3' | -7.23 | 111.03 | 119.70 |
| 1 | A | 388 | G | P-O3'-C3' | 7.22 | 128.37 | 119.70 |
| 1 | A | 346 | G | P-O5'-C5' | -7.22 | 109.34 | 120.90 |
| 1 | A | 531 | U | P-O3'-C3' | 7.19 | 128.32 | 119.70 |
| 1 | A | 1101 | A | P-O3'-C3' | 7.19 | 128.33 | 119.70 |
| 1 | A | 1053 | G | P-O3'-C3' | 7.17 | 128.30 | 119.70 |
| 1 | A | 519 | C | N1-C1'-C2' | -7.16 | 104.12 | 112.00 |
| 1 | A | 1320 | C | N1-C1'-C2' | -7.14 | 104.15 | 112.00 |
| 1 | A | 282 | A | P-O3'-C3' | -7.14 | 111.14 | 119.70 |
| 1 | A | 485 | U | P-O3'-C3' | 7.13 | 128.26 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 652 | U | P-O3'-C3' | 7.13 | 128.25 | 119.70 |
| 1 | A | 14 | U | P-O5'-C5' | -7.12 | 109.51 | 120.90 |
| 1 | A | 1131 | G | P-O3'-C3' | -7.11 | 111.17 | 119.70 |
| 1 | A | 344 | A | P-O3'-C3' | 7.10 | 128.22 | 119.70 |
| 1 | A | 452 | A | P-O3'-C3' | -7.08 | 111.21 | 119.70 |
| 1 | A | 1453 | G | P-O3'-C3' | -7.05 | 111.23 | 119.70 |
| 1 | A | 411 | A | P-O3'-C3' | 7.03 | 128.13 | 119.70 |
| 1 | A | 316 | C | N1-C1'-C2' | -7.01 | 104.28 | 112.00 |
| 1 | A | 372 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 1 | A | 1362 | A | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 1 | A | 1283 | U | P-O3'-C3' | -6.98 | 111.32 | 119.70 |
| 1 | A | 1190 | G | P-O3'-C3' | 6.97 | 128.06 | 119.70 |
| 1 | A | 1401 | G | P-O3'-C3' | -6.97 | 111.34 | 119.70 |
| 1 | A | 1167 | A | P-O3'-C3' | 6.96 | 128.05 | 119.70 |
| 1 | A | 1068 | G | N9-C1'-C2' | -6.93 | 104.38 | 112.00 |
| 1 | A | 972 | C | P-O3'-C3' | -6.92 | 111.40 | 119.70 |
| 1 | A | 438 | U | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 1 | A | 60 | A | P-O3'-C3' | 6.89 | 127.97 | 119.70 |
| 1 | A | 1094 | G | O4'-C1'-N9 | 6.89 | 113.72 | 108.20 |
| 1 | A | 52 | C | P-O3'-C3' | -6.88 | 111.44 | 119.70 |
| 1 | A | 919 | A | P-O3'-C3' | 6.88 | 127.96 | 119.70 |
| 1 | A | 258 | G | N9-C1'-C2' | -6.87 | 104.45 | 112.00 |
| 1 | A | 965 | U | P-O3'-C3' | 6.87 | 127.94 | 119.70 |
| 1 | A | 463 | U | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 1 | A | 1197 | A | P-O3'-C3' | -6.85 | 111.48 | 119.70 |
| 1 | A | 1085 | U | N1-C1'-C2' | 6.84 | 122.89 | 114.00 |
| 1 | A | 1381 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 1 | A | 9 | G | N9-C1'-C2' | -6.79 | 104.53 | 112.00 |
| 1 | A | 1318 | A | P-O3'-C3' | 6.79 | 127.85 | 119.70 |
| 1 | A | 566 | G | P-O3'-C3' | 6.77 | 127.83 | 119.70 |
| 1 | A | 1152 | A | P-O3'-C3' | -6.77 | 111.58 | 119.70 |
| 1 | A | 1531 | A | P-O3'-C3' | -6.76 | 111.58 | 119.70 |
| 1 | A | 1382 | C | P-O3'-C3' | -6.75 | 111.60 | 119.70 |
| 1 | A | 366 | A | P-O3'-C3' | 6.75 | 127.80 | 119.70 |
| 1 | A | 1228 | C | P-O3'-C3' | -6.71 | 111.64 | 119.70 |
| 1 | A | 372 | C | P-O3'-C3' | 6.71 | 127.75 | 119.70 |
| 1 | A | 469 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 1 | A | 314 | C | P-O3'-C3' | 6.68 | 127.72 | 119.70 |
| 1 | A | 266 | G | P-O3'-C3' | 6.66 | 127.69 | 119.70 |
| 1 | A | 497 | G | P-O3'-C3' | -6.65 | 111.72 | 119.70 |
| 1 | A | 1336 | C | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 1 | A | 451 | A | P-O3'-C3' | 6.62 | 127.65 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 14 | U | N1-C1'-C2' | -6.61 | 104.73 | 112.00 |
| 1 | A | 121 | U | N1-C1'-C2' | -6.61 | 104.73 | 112.00 |
| 1 | A | 686 | U | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 1 | A | 688 | G | N9-C1'-C2' | -6.61 | 104.73 | 112.00 |
| 1 | A | 428 | G | P-O3'-C3' | 6.58 | 127.60 | 119.70 |
| 1 | A | 984 | C | P-O3'-C3' | -6.55 | 111.83 | 119.70 |
| 1 | A | 1278 | G | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 1 | A | 486 | U | P-O3'-C3' | -6.53 | 111.86 | 119.70 |
| 1 | A | 872 | A | O4'-C1'-N9 | 6.53 | 113.42 | 108.20 |
| 1 | A | 1126 | U | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 1 | A | 424 | G | P-O3'-C3' | -6.49 | 111.92 | 119.70 |
| 1 | A | 722 | G | P-O3'-C3' | -6.48 | 111.92 | 119.70 |
| 1 | A | 344 | A | O4'-C1'-N9 | 6.48 | 113.39 | 108.20 |
| 1 | A | 14 | U | P-O3'-C3' | -6.48 | 111.93 | 119.70 |
| 1 | A | 792 | A | P-O3'-C3' | 6.48 | 127.47 | 119.70 |
| 1 | A | 1283 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 1 | A | 184 | G | P-O3'-C3' | -6.45 | 111.96 | 119.70 |
| 1 | A | 857 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 1 | A | 365 | U | C5-C6-N1 | -6.43 | 119.48 | 122.70 |
| 1 | A | 108 | G | P-O3'-C3' | -6.42 | 112.00 | 119.70 |
| 1 | A | 258 | G | P-O5'-C5' | -6.41 | 110.64 | 120.90 |
| 1 | A | 469 | C | P-O3'-C3' | -6.39 | 112.03 | 119.70 |
| 1 | A | 1320 | C | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 1 | A | 985 | C | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 1 | A | 318 | G | N3-C4-N9 | -6.35 | 122.19 | 126.00 |
| 1 | A | 67 | C | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 1 | A | 245 | U | O4'-C1'-N1 | 6.34 | 113.28 | 108.20 |
| 1 | A | 267 | C | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 1 | A | 110 | C | P-O3'-C3' | -6.33 | 112.10 | 119.70 |
| 1 | A | 1224 | U | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 1 | A | 124 | C | O4'-C1'-N1 | -6.32 | 103.15 | 108.20 |
| 1 | A | 1396 | A | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 1 | A | 733 | G | O4'-C1'-N9 | 6.31 | 113.25 | 108.20 |
| 1 | A | 1478 | U | P-O5'-C5' | -6.29 | 110.83 | 120.90 |
| 1 | A | 1087 | G | P-O3'-C3' | -6.29 | 112.15 | 119.70 |
| 1 | A | 85 | U | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 1 | A | 1282 | C | P-O3'-C3' | -6.28 | 112.17 | 119.70 |
| 1 | A | 1064 | G | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 1 | A | 257 | G | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 1 | A | 1066 | C | P-O3'-C3' | -6.25 | 112.21 | 119.70 |
| 1 | A | 811 | C | P-O3'-C3' | 6.24 | 127.19 | 119.70 |
| 1 | A | 368 | U | P-O3'-C3' | -6.23 | 112.22 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 884 | U | N1-C1'-C2' | 6.23 | 122.10 | 114.00 |
| 1 | A | 414 | A | C3'-C2'-C1' | 6.22 | 106.48 | 101.50 |
| 1 | A | 1348 | U | P-O3'-C3' | -6.21 | 112.25 | 119.70 |
| 1 | A | 1398 | A | N9-C1'-C2' | -6.21 | 105.17 | 112.00 |
| 1 | A | 141 | G | N9-C1'-C2' | -6.20 | 105.18 | 112.00 |
| 1 | A | 562 | U | O4'-C1'-N1 | -6.20 | 103.24 | 108.20 |
| 1 | A | 534 | U | P-O3'-C3' | -6.20 | 112.26 | 119.70 |
| 1 | A | 247 | G | N9-C1'-C2' | -6.19 | 105.19 | 112.00 |
| 1 | A | 567 | G | C3'-C2'-C1' | 6.19 | 106.45 | 101.50 |
| 1 | A | 884 | U | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 1 | A | 594 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 1 | A | 575 | G | P-O5'-C5' | -6.15 | 111.06 | 120.90 |
| 1 | A | 935 | A | C3'-C2'-C1' | 6.15 | 106.42 | 101.50 |
| 1 | A | 1066 | C | N1-C1'-C2' | -6.14 | 105.24 | 112.00 |
| 1 | A | 971 | G | O4'-C1'-N9 | 6.13 | 113.10 | 108.20 |
| 1 | A | 1451 | U | N1-C1'-C2' | 6.13 | 121.96 | 114.00 |
| 1 | A | 559 | A | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 1 | A | 547 | A | O4'-C1'-N9 | 6.11 | 113.09 | 108.20 |
| 1 | A | 1203 | C | O4'-C1'-N1 | 6.11 | 113.08 | 108.20 |
| 1 | A | 1302 | C | N1-C1'-C2' | -6.11 | 105.28 | 112.00 |
| 1 | A | 183 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 1 | A | 452 | A | N9-C1'-C2' | -6.09 | 105.30 | 112.00 |
| 1 | A | 1509 | C | C6-N1-C2 | 6.09 | 122.73 | 120.30 |
| 1 | A | 97 | G | C3'-C2'-C1' | 6.08 | 106.36 | 101.50 |
| 1 | A | 1258 | G | P-O3'-C3' | -6.08 | 112.41 | 119.70 |
| 1 | A | 247 | G | P-O3'-C3' | -6.07 | 112.42 | 119.70 |
| 1 | A | 991 | U | P-O3'-C3' | 6.06 | 126.97 | 119.70 |
| 1 | A | 345 | C | O4'-C1'-N1 | -6.06 | 103.35 | 108.20 |
| 1 | A | 914 | A | C3'-C2'-C1' | 6.05 | 106.34 | 101.50 |
| 1 | A | 316 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 1 | A | 1162 | C | C3'-C2'-C1' | 6.05 | 106.34 | 101.50 |
| 1 | A | 1478 | U | O4'-C1'-N1 | -6.04 | 103.36 | 108.20 |
| 1 | A | 185 | U | N1-C1'-C2' | -6.04 | 105.35 | 112.00 |
| 1 | A | 1187 | G | P-O3'-C3' | -6.04 | 112.45 | 119.70 |
| 1 | A | 1153 | G | P-O3'-C3' | -6.03 | 112.46 | 119.70 |
| 1 | A | 497 | G | C3'-C2'-C1' | 6.03 | 106.32 | 101.50 |
| 1 | A | 30 | U | N1-C1'-C2' | 6.03 | 121.84 | 114.00 |
| 1 | A | 198 | G | C3'-C2'-C1' | 6.02 | 106.31 | 101.50 |
| 1 | A | 723 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 1 | A | 1095 | U | C3'-C2'-C1' | 6.01 | 106.31 | 101.50 |
| 1 | A | 330 | C | P-O3'-C3' | -6.00 | 112.50 | 119.70 |
| 1 | A | 501 | C | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 551 | U | O4'-C1'-N1 | -6.00 | 103.40 | 108.20 |
| 1 | A | 1448 | C | P-O3'-C3' | -6.00 | 112.50 | 119.70 |
| 1 | A | 1241 | G | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 1 | A | 267 | C | C3'-C2'-C1' | 5.98 | 106.28 | 101.50 |
| 1 | A | 537 | G | P-O3'-C3' | -5.97 | 112.53 | 119.70 |
| 1 | A | 47 | C | N1-C1'-C2' | 5.97 | 121.76 | 114.00 |
| 1 | A | 840 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 1 | A | 199 | A | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 1 | A | 1505 | G | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 1 | A | 93 | U | P-O3'-C3' | -5.95 | 112.56 | 119.70 |
| 1 | A | 386 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 1 | A | 174 | A | P-O3'-C3' | -5.94 | 112.57 | 119.70 |
| 1 | A | 559 | A | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 1 | A | 252 | U | P-O3'-C3' | -5.94 | 112.57 | 119.70 |
| 1 | A | 1365 | G | N9-C1'-C2' | -5.93 | 105.48 | 112.00 |
| 1 | A | 912 | C | O4'-C1'-N1 | -5.92 | 103.46 | 108.20 |
| 1 | A | 1142 | G | C3'-C2'-C1' | 5.91 | 106.22 | 101.50 |
| 1 | A | 244 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 1 | A | 1213 | A | P-O3'-C3' | 5.89 | 126.77 | 119.70 |
| 1 | A | 111 | G | N9-C1'-C2' | -5.88 | 105.53 | 112.00 |
| 1 | A | 244 | U | N3-C2-O2 | -5.88 | 118.09 | 122.20 |
| 1 | A | 185 | U | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 1 | A | 1202 | U | C3'-C2'-C1' | 5.87 | 106.20 | 101.50 |
| 1 | A | 488 | C | C3'-C2'-C1' | 5.87 | 106.19 | 101.50 |
| 1 | A | 509 | A | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 1 | A | 1162 | C | P-O3'-C3' | -5.86 | 112.66 | 119.70 |
| 1 | A | 279 | A | O4'-C1'-N9 | -5.85 | 103.52 | 108.20 |
| 1 | A | 250 | A | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 1 | A | 874 | G | N9-C1'-C2' | -5.85 | 105.57 | 112.00 |
| 1 | A | 1184 | G | P-O3'-C3' | -5.84 | 112.69 | 119.70 |
| 1 | A | 686 | U | N1-C1'-C2' | 5.83 | 121.58 | 114.00 |
| 1 | A | 816 | A | C3'-C2'-C1' | 5.83 | 106.17 | 101.50 |
| 1 | A | 560 | A | O4'-C1'-N9 | -5.83 | 103.54 | 108.20 |
| 1 | A | 605 | U | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 1 | A | 429 | U | P-O3'-C3' | 5.82 | 126.68 | 119.70 |
| 1 | A | 439 | U | C3'-C2'-C1' | 5.81 | 106.15 | 101.50 |
| 1 | A | 772 | U | P-O3'-C3' | -5.81 | 112.73 | 119.70 |
| 1 | A | 801 | U | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 1 | A | 974 | A | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 1 | A | 817 | C | N1-C1'-C2' | 5.80 | 121.54 | 114.00 |
| 1 | A | 87 | C | N1-C1'-C2' | -5.80 | 105.62 | 112.00 |
| 1 | A | 512 | U | C3'-C2'-C1' | 5.78 | 106.13 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1226 | C | O4'-C1'-N1 | -5.77 | 103.58 | 108.20 |
| 1 | A | 1323 | G | P-O3'-C3' | -5.77 | 112.78 | 119.70 |
| 1 | A | 1365 | G | C3'-C2'-C1' | 5.77 | 106.11 | 101.50 |
| 1 | A | 1228 | C | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 1 | A | 686 | U | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 1 | A | 368 | U | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 1 | A | 1268 | G | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 1 | A | 469 | C | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 1 | A | 463 | U | N1-C1'-C2' | -5.75 | 105.68 | 112.00 |
| 1 | A | 1191 | A | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 1 | A | 935 | A | N9-C1'-C2' | -5.73 | 105.70 | 112.00 |
| 1 | A | 508 | U | P-O3'-C3' | 5.73 | 126.57 | 119.70 |
| 1 | A | 1095 | U | P-O3'-C3' | -5.72 | 112.84 | 119.70 |
| 1 | A | 704 | A | C3'-C2'-C1' | 5.72 | 106.07 | 101.50 |
| 1 | A | 1085 | U | P-O3'-C3' | 5.71 | 126.55 | 119.70 |
| 1 | A | 1532 | U | P-O3'-C3' | -5.69 | 112.87 | 119.70 |
| 1 | A | 1088 | G | C3'-C2'-C1' | 5.68 | 106.05 | 101.50 |
| 1 | A | 295 | C | P-O3'-C3' | -5.68 | 112.89 | 119.70 |
| 1 | A | 231 | U | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 1 | A | 1302 | C | O4'-C1'-N1 | -5.67 | 103.66 | 108.20 |
| 1 | A | 1447 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 1 | A | 1395 | C | O4'-C1'-N1 | -5.67 | 103.66 | 108.20 |
| 1 | A | 74 | A | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 1 | A | 1395 | C | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 1 | A | 430 | A | P-O3'-C3' | -5.67 | 112.90 | 119.70 |
| 1 | A | 415 | A | C3'-C2'-C1' | 5.66 | 106.03 | 101.50 |
| 1 | A | 131 | A | C3'-C2'-C1' | 5.66 | 106.03 | 101.50 |
| 1 | A | 808 | C | O4'-C1'-N1 | 5.66 | 112.72 | 108.20 |
| 1 | A | 173 | U | N1-C1'-C2' | 5.65 | 121.35 | 114.00 |
| 1 | A | 555 | U | O4'-C1'-N1 | -5.65 | 103.68 | 108.20 |
| 1 | A | 1124 | G | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 1 | A | 976 | G | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 1 | A | 1499 | A | P-O5'-C5' | -5.65 | 111.86 | 120.90 |
| 1 | A | 116 | A | N9-C1'-C2' | -5.64 | 105.79 | 112.00 |
| 1 | A | 486 | U | P-O5'-C5' | -5.64 | 111.88 | 120.90 |
| 1 | A | 972 | C | C3'-C2'-C1' | 5.64 | 106.01 | 101.50 |
| 1 | A | 1448 | C | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 1 | A | 64 | G | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 1 | A | 968 | A | P-O3'-C3' | 5.59 | 126.42 | 119.70 |
| 1 | A | 817 | C | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 1 | A | 654 | G | C3'-C2'-C1' | 5.59 | 105.97 | 101.50 |
| 1 | A | 1130 | A | P-O3'-C3' | -5.58 | 113.00 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 61 | G | P-O3'-C3' | -5.58 | 113.00 | 119.70 |
| 1 | A | 93 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 1 | A | 318 | G | N3-C4-C5 | 5.58 | 131.39 | 128.60 |
| 1 | A | 500 | G | P-O3'-C3' | -5.57 | 113.01 | 119.70 |
| 1 | A | 1203 | C | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 1 | A | 352 | C | C3'-C2'-C1' | 5.56 | 105.94 | 101.50 |
| 1 | A | 994 | A | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 1 | A | 528 | C | O4'-C1'-N1 | -5.54 | 103.77 | 108.20 |
| 1 | A | 548 | G | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 1 | A | 1337 | G | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 1 | A | 373 | A | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 1 | A | 14 | U | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 1 | A | 998 | C | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 1 | A | 1127 | G | P-O3'-C3' | -5.52 | 113.07 | 119.70 |
| 1 | A | 267 | C | P-O5'-C5' | -5.52 | 112.07 | 120.90 |
| 1 | A | 47 | C | P-O3'-C3' | 5.51 | 126.32 | 119.70 |
| 1 | A | 1259 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 1 | A | 1191 | A | P-O3'-C3' | -5.51 | 113.09 | 119.70 |
| 1 | A | 1322 | C | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 1 | A | 345 | C | P-O5'-C5' | -5.51 | 112.08 | 120.90 |
| 1 | A | 1152 | A | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |
| 1 | A | 1349 | A | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |
| 1 | A | 1496 | C | P-O3'-C3' | -5.51 | 113.09 | 119.70 |
| 1 | A | 430 | A | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 1 | A | 1126 | U | N1-C1'-C2' | 5.50 | 121.16 | 114.00 |
| 1 | A | 71 | A | P-O3'-C3' | -5.50 | 113.09 | 119.70 |
| 1 | A | 163 | C | O4'-C1'-N1 | -5.50 | 103.80 | 108.20 |
| 1 | A | 91 | U | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 1 | A | 115 | G | C4'-C3'-C2' | 5.50 | 108.10 | 102.60 |
| 1 | A | 1129 | C | N1-C1'-C2' | 5.50 | 121.15 | 114.00 |
| 1 | A | 1183 | U | N1-C1'-C2' | -5.50 | 105.95 | 112.00 |
| 1 | A | 1381 | U | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 1 | A | 509 | A | P-O3'-C3' | -5.50 | 113.11 | 119.70 |
| 1 | A | 94 | G | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 1 | A | 994 | A | P-O3'-C3' | -5.49 | 113.11 | 119.70 |
| 1 | A | 174 | A | C3'-C2'-C1' | 5.49 | 105.89 | 101.50 |
| 1 | A | 1323 | G | C3'-C2'-C1' | 5.48 | 105.89 | 101.50 |
| 1 | A | 537 | G | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 1 | A | 191 | G | O4'-C1'-N9 | -5.48 | 103.82 | 108.20 |
| 1 | A | 331 | G | N9-C1'-C2' | -5.47 | 105.98 | 112.00 |
| 1 | A | 874 | G | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 1 | A | 1381 | U | P-O3'-C3' | -5.47 | 113.13 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 794 | A | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 1 | A | 1322 | C | N1-C1'-C2' | 5.46 | 121.10 | 114.00 |
| 1 | A | 1498 | U | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 1 | A | 1046 | A | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 1 | A | 84 | U | O4'-C1'-N1 | 5.43 | 112.55 | 108.20 |
| 1 | A | 1348 | U | C3'-C2'-C1' | 5.43 | 105.85 | 101.50 |
| 1 | A | 1128 | C | P-O5'-C5' | -5.43 | 112.21 | 120.90 |
| 1 | A | 352 | C | O4'-C1'-N1 | -5.42 | 103.86 | 108.20 |
| 1 | A | 721 | G | P-O3'-C3' | 5.42 | 126.21 | 119.70 |
| 1 | A | 978 | A | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 1 | A | 487 | A | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 1 | A | 1215 | G | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 1 | A | 1153 | G | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 1 | A | 64 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 1 | A | 1131 | G | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 1 | A | 1259 | C | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 1 | A | 576 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 1 | A | 1087 | G | C3'-C2'-C1' | 5.38 | 105.81 | 101.50 |
| 1 | A | 61 | G | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 1 | A | 1131 | G | N9-C1'-C2' | -5.38 | 106.08 | 112.00 |
| 1 | A | 536 | C | N1-C1'-C2' | -5.38 | 106.08 | 112.00 |
| 1 | A | 754 | C | N1-C1'-C2' | -5.38 | 106.08 | 112.00 |
| 1 | A | 1304 | G | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 1 | A | 1454 | G | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 1 | A | 252 | U | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 1 | A | 642 | A | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 1 | A | 384 | G | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 1 | A | 352 | C | P-O3'-C3' | -5.37 | 113.26 | 119.70 |
| 1 | A | 1184 | G | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 1 | A | 1304 | G | P-O3'-C3' | -5.36 | 113.27 | 119.70 |
| 1 | A | 966 | G | P-O3'-C3' | -5.35 | 113.28 | 119.70 |
| 1 | A | 286 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 1 | A | 1522 | U | P-O5'-C5' | -5.35 | 112.34 | 120.90 |
| 1 | A | 722 | G | C3'-C2'-C1' | 5.34 | 105.77 | 101.50 |
| 1 | A | 718 | A | C3'-C2'-C1' | 5.32 | 105.76 | 101.50 |
| 1 | A | 339 | C | C5-C6-N1 | -5.32 | 118.34 | 121.00 |
| 1 | A | 368 | U | N1-C1'-C2' | -5.32 | 106.15 | 112.00 |
| 1 | A | 1108 | G | P-O3'-C3' | -5.31 | 113.32 | 119.70 |
| 1 | A | 1401 | G | P-O5'-C5' | -5.31 | 112.40 | 120.90 |
| 1 | A | 52 | C | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 1 | A | 85 | U | N1-C1'-C2' | 5.31 | 120.90 | 114.00 |
| 1 | A | 439 | U | P-O3'-C3' | -5.31 | 113.33 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 246 | A | P-O3'-C3' | 5.31 | 126.07 | 119.70 |
| 1 | A | 71 | A | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 1 | A | 1382 | C | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 1 | A | 1130 | A | O4'-C1'-N9 | -5.30 | 103.96 | 108.20 |
| 1 | A | 23 | C | P-O3'-C3' | -5.29 | 113.35 | 119.70 |
| 1 | A | 1129 | C | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 1 | A | 534 | U | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 1 | A | 1402 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 1 | A | 110 | C | C3'-C2'-C1' | 5.27 | 105.72 | 101.50 |
| 1 | A | 275 | G | C8-N9-C4 | -5.26 | 104.30 | 106.40 |
| 1 | A | 468 | A | P-O3'-C3' | -5.25 | 113.40 | 119.70 |
| 1 | A | 1420 | U | N3-C2-O2 | 5.25 | 125.88 | 122.20 |
| 1 | A | 885 | G | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 1 | A | 331 | G | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 1 | A | 468 | A | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 1 | A | 72 | A | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 1 | A | 733 | G | P-O3'-C3' | 5.23 | 125.97 | 119.70 |
| 1 | A | 346 | G | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 1 | A | 1432 | G | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 1 | A | 977 | A | P-O3'-C3' | -5.22 | 113.44 | 119.70 |
| 1 | A | 490 | C | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 1 | A | 891 | U | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 1 | A | 1169 | A | P-O3'-C3' | -5.21 | 113.45 | 119.70 |
| 1 | A | 961 | U | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 1 | A | 519 | C | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 1 | A | 1070 | U | O4'-C1'-N1 | -5.20 | 104.04 | 108.20 |
| 1 | A | 812 | G | O3'-P-O5' | -5.19 | 94.13 | 104.00 |
| 1 | A | 1050 | G | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 1 | A | 436 | C | O4'-C1'-N1 | 5.18 | 112.34 | 108.20 |
| 1 | A | 466 | A | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 1 | A | 166 | U | P-O3'-C3' | -5.17 | 113.49 | 119.70 |
| 1 | A | 1088 | G | N9-C1'-C2' | -5.17 | 106.31 | 112.00 |
| 1 | A | 1258 | G | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 1 | A | 486 | U | O4'-C1'-N1 | -5.17 | 104.06 | 108.20 |
| 1 | A | 93 | U | C3'-C2'-C1' | 5.16 | 105.63 | 101.50 |
| 1 | A | 28 | A | P-O5'-C5' | -5.15 | 112.67 | 120.90 |
| 1 | A | 346 | G | P-O3'-C3' | -5.15 | 113.52 | 119.70 |
| 1 | A | 274 | A | O4'-C1'-N9 | 5.14 | 112.32 | 108.20 |
| 1 | A | 500 | G | N9-C1'-C2' | -5.14 | 106.35 | 112.00 |
| 1 | A | 1098 | C | O4'-C1'-N1 | -5.13 | 104.10 | 108.20 |
| 1 | A | 210 | C | P-O3'-C3' | 5.12 | 125.85 | 119.70 |
| 1 | A | 563 | A | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 969 | A | C3'-C2'-C1' | 5.12 | 105.59 | 101.50 |
| 1 | A | 786 | G | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | A | 95 | C | O4'-C1'-N1 | -5.11 | 104.11 | 108.20 |
| 1 | A | 1284 | C | C3'-C2'-C1' | 5.10 | 105.58 | 101.50 |
| 1 | A | 316 | C | C3'-C2'-C1' | 5.09 | 105.58 | 101.50 |
| 1 | A | 755 | G | C3'-C2'-C1' | 5.09 | 105.58 | 101.50 |
| 1 | A | 41 | G | P-O3'-C3' | -5.09 | 113.59 | 119.70 |
| 1 | A | 245 | U | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 1 | A | 1066 | C | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |
| 1 | A | 258 | G | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 1 | A | 756 | C | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 1 | A | 984 | C | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 1 | A | 116 | A | O5'-P-OP2 | -5.05 | 101.16 | 105.70 |
| 1 | A | 1087 | G | N9-C1'-C2' | -5.05 | 106.45 | 112.00 |
| 1 | A | 1433 | A | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 1 | A | 13 | U | N1-C1'-C2' | 5.04 | 120.55 | 114.00 |
| 1 | A | 43 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 1 | A | 1319 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | A | 1102 | A | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 1 | A | 985 | C | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 1 | A | 70 | U | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 1 | A | 1062 | U | O4'-C1'-N1 | -5.02 | 104.18 | 108.20 |
| 1 | A | 754 | C | P-O3'-C3' | -5.02 | 113.68 | 119.70 |
| 1 | A | 1320 | C | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 1 | A | 463 | U | C3'-C2'-C1' | 5.00 | 105.50 | 101.50 |
| 1 | A | 109 | A | O3'-P-O5' | -5.00 | 94.50 | 104.00 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 12 | L | 22 | ALA | Peptide |
| 20 | T | 6 | ALA | Peptide |

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32895 | 0 | 44 | 955 | 0 |
| 2 | B | 1705 | 0 | 0 | 63 | 0 |
| 3 | C | 1625 | 0 | 0 | 32 | 0 |
| 4 | D | 1643 | 0 | 0 | 92 | 0 |
| 5 | E | 1106 | 0 | 75 | 80 | 0 |
| 6 | F | 818 | 0 | 0 | 29 | 0 |
| 7 | G | 1182 | 0 | 0 | 27 | 0 |
| 8 | H | 979 | 0 | 0 | 31 | 0 |
| 9 | I | 1022 | 0 | 0 | 33 | 0 |
| 10 | J | 787 | 0 | 0 | 40 | 0 |
| 11 | K | 877 | 0 | 0 | 35 | 0 |
| 12 | L | 955 | 0 | 0 | 31 | 0 |
| 13 | M | 884 | 0 | 0 | 17 | 0 |
| 14 | N | 774 | 0 | 0 | 31 | 0 |
| 15 | O | 714 | 0 | 0 | 25 | 0 |
| 16 | P | 649 | 0 | 0 | 32 | 0 |
| 17 | Q | 649 | 0 | 691 | 137 | 0 |
| 18 | R | 456 | 0 | 0 | 13 | 0 |
| 19 | S | 638 | 0 | 0 | 26 | 0 |
| 20 | T | 665 | 0 | 0 | 28 | 0 |
| 21 | U | 426 | 0 | 0 | 28 | 0 |
| 22 | A | 41 | 0 | 0 | 0 | 0 |
| 22 | N | 2 | 0 | 0 | 0 | 0 |
| 23 | A | 198 | 0 | 0 | 5 | 0 |
| 23 | L | 1 | 0 | 0 | 0 | 0 |
| 23 | N | 7 | 0 | 0 | 0 | 0 |
| 23 | U | 2 | 0 | 0 | 0 | 0 |
| All | All | 51700 | 0 | 810 | 1704 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (1704) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:152:VAL:HB | 5:E:155:LYS:NZ | 1.44 | 1.30 |
| 1:A:1531:A:C8 | 1:A:1531:A:H5' | 1.79 | 1.17 |
| 5:E:153:ALA:HA | 5:E:156:ARG:CB | 1.76 | 1.15 |
| 5:E:155:LYS:HA | 5:E:158:LYS:NZ | 1.62 | 1.12 |
| 17:Q:12:VAL:HG13 | 17:Q:13:SER:H | 1.00 | 1.10 |
| 17:Q:16:MET:HB2 | 17:Q:19:SER:HB3 | 1.31 | 1.07 |
| 5:E:153:ALA:HA | 5:E:156:ARG:HB2 | 1.34 | 1.05 |
| 17:Q:12:VAL:HG11 | 17:Q:21:VAL:CG1 | 1.86 | 1.05 |
| 17:Q:12:VAL:CG1 | 17:Q:21:VAL:HG13 | 1.88 | 1.02 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 17:Q:46:HIS:HB2 | 17:Q:66:LEU:HD12 | 1.42 | 1.01 |
| 1:A:1531:A:H5' | 1:A:1531:A:H8 | 0.88 | 1.01 |
| 5:E:155:LYS:HA | 5:E:158:LYS:HZ2 | 1.26 | 0.99 |
| 17:Q:18:LYS:HA | 17:Q:47:ASP:CB | 1.94 | 0.98 |
| 1:A:1533:C:H3' | 1:A:1534:A:H5'' | 1.43 | 0.98 |
| 17:Q:12:VAL:HG13 | 17:Q:13:SER:N | 1.79 | 0.97 |
| 17:Q:18:LYS:HA | 17:Q:47:ASP:HB2 | 1.45 | 0.95 |
| 17:Q:12:VAL:HG11 | 17:Q:21:VAL:HG13 | 0.95 | 0.95 |
| 17:Q:37:ILE:H | 17:Q:37:ILE:HD12 | 1.33 | 0.94 |
| 1:A:1531:A:C5' | 1:A:1531:A:H8 | 1.81 | 0.92 |
| 17:Q:12:VAL:CG1 | 17:Q:13:SER:H | 1.82 | 0.91 |
| 17:Q:22:VAL:HG21 | 17:Q:60:ILE:HD11 | 1.51 | 0.91 |
| 17:Q:45:VAL:HG21 | 17:Q:60:ILE:CD1 | 2.03 | 0.88 |
| 5:E:152:VAL:HB | 5:E:155:LYS:HZ2 | 1.08 | 0.88 |
| 5:E:155:LYS:HD2 | 5:E:156:ARG:H | 1.35 | 0.88 |
| 5:E:153:ALA:CA | 5:E:156:ARG:HB2 | 2.03 | 0.87 |
| 5:E:156:ARG:O | 5:E:158:LYS:N | 2.08 | 0.87 |
| 5:E:152:VAL:HB | 5:E:155:LYS:HZ1 | 1.33 | 0.86 |
| 1:A:792:A:O2' | 1:A:794:A:N7 | 2.09 | 0.86 |
| 5:E:153:ALA:HA | 5:E:156:ARG:CA | 2.05 | 0.85 |
| 17:Q:45:VAL:HG21 | 17:Q:60:ILE:HD13 | 1.59 | 0.84 |
| 5:E:155:LYS:CD | 5:E:156:ARG:H | 1.89 | 0.84 |
| 17:Q:18:LYS:CA | 17:Q:47:ASP:HB2 | 2.06 | 0.84 |
| 1:A:1202:U:O2' | 1:A:1203:C:C5' | 2.26 | 0.83 |
| 1:A:1533:C:H3' | 1:A:1534:A:C5' | 2.08 | 0.83 |
| 17:Q:74:LEU:HD12 | 17:Q:74:LEU:H | 1.44 | 0.83 |
| 5:E:155:LYS:HA | 5:E:158:LYS:HZ3 | 1.41 | 0.82 |
| 5:E:89:THR:CG2 | 5:E:90:GLY:N | 2.42 | 0.82 |
| 1:A:274:A:O2' | 1:A:275:G:C8 | 2.33 | 0.81 |
| 1:A:430:A:O2' | 1:A:431:A:C5' | 2.29 | 0.80 |
| 11:K:87:GLY:N | 11:K:113:THR:CG2 | 2.44 | 0.80 |
| 5:E:152:VAL:CB | 5:E:155:LYS:HZ2 | 1.92 | 0.80 |
| 17:Q:51:GLU:HG2 | 17:Q:52:CYS:SG | 2.21 | 0.80 |
| 17:Q:6:THR:O | 17:Q:7:LEU:HD12 | 1.82 | 0.79 |
| 5:E:155:LYS:HD2 | 5:E:155:LYS:H | 1.45 | 0.79 |
| 17:Q:11:VAL:HG12 | 17:Q:12:VAL:HG12 | 1.65 | 0.78 |
| 1:A:1533:C:C3' | 1:A:1534:A:H5'' | 2.13 | 0.78 |
| 17:Q:20:ILE:N | 17:Q:47:ASP:OD1 | 2.17 | 0.78 |
| 1:A:184:G:O2' | 1:A:185:U:C6 | 2.36 | 0.78 |
| 1:A:158:G:C2' | 1:A:159:G:C5' | 2.62 | 0.78 |
| 1:A:1381:U:O2' | 1:A:1382:C:C5' | 2.32 | 0.77 |
| 1:A:1239:A:N6 | 1:A:1299:A:N6 | 2.32 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 17:Q:37:ILE:N | 17:Q:37:ILE:HD12 | 1.99 | 0.76 |
| 1:A:1127:G:O2' | 1:A:1128:C:C5' | 2.33 | 0.76 |
| 1:A:184:G:C4 | 1:A:185:U:C5 | 2.73 | 0.76 |
| 1:A:413:G:N2 | 1:A:428:G:O2' | 2.20 | 0.75 |
| 10:J:48:ARG:CG | 10:J:48:ARG:NH1 | 2.50 | 0.75 |
| 1:A:1151:A:C6 | 1:A:1152:A:N6 | 2.54 | 0.75 |
| 17:Q:13:SER:O | 17:Q:20:ILE:HD11 | 1.87 | 0.75 |
| 12:L:49:ARG:CG | 12:L:49:ARG:NH1 | 2.47 | 0.75 |
| 4:D:191:SER:OG | 4:D:192:ALA:N | 2.20 | 0.75 |
| 5:E:153:ALA:CA | 5:E:156:ARG:CB | 2.59 | 0.74 |
| 1:A:397:A:N7 | 1:A:547:A:O2' | 2.20 | 0.74 |
| 5:E:155:LYS:CD | 5:E:156:ARG:N | 2.49 | 0.74 |
| 1:A:558:G:C4 | 1:A:559:A:C2 | 2.75 | 0.74 |
| 1:A:366:A:O2' | 1:A:394:G:N2 | 2.21 | 0.74 |
| 17:Q:20:ILE:HB | 17:Q:47:ASP:OD1 | 1.87 | 0.74 |
| 17:Q:7:LEU:HD23 | 17:Q:24:ILE:CD1 | 2.18 | 0.74 |
| 5:E:149:PRO:O | 5:E:152:VAL:HG22 | 1.88 | 0.73 |
| 1:A:488:C:O2' | 1:A:489:C:C5' | 2.36 | 0.73 |
| 1:A:274:A:O2' | 1:A:275:G:O4' | 2.05 | 0.73 |
| 17:Q:22:VAL:HG21 | 17:Q:60:ILE:CD1 | 2.17 | 0.73 |
| 1:A:558:G:C5 | 1:A:559:A:C2 | 2.76 | 0.72 |
| 1:A:1258:G:O2' | 1:A:1259:C:C6 | 2.43 | 0.72 |
| 11:K:126:ARG:CB | 21:U:33:ARG:NH1 | 2.52 | 0.72 |
| 1:A:1094:G:O2' | 1:A:1095:U:P | 2.47 | 0.72 |
| 5:E:152:VAL:O | 5:E:155:LYS:HD2 | 1.89 | 0.72 |
| 1:A:1151:A:C4 | 1:A:1152:A:N7 | 2.57 | 0.72 |
| 1:A:1348:U:O2' | 1:A:1349:A:C5' | 2.38 | 0.72 |
| 5:E:79:THR:OG1 | 5:E:80:LEU:N | 2.23 | 0.72 |
| 1:A:1162:C:O2' | 1:A:1163:A:O4' | 2.07 | 0.72 |
| 1:A:92:U:O2' | 1:A:93:U:C6 | 2.43 | 0.72 |
| 1:A:93:U:O2' | 1:A:94:G:C5' | 2.38 | 0.72 |
| 5:E:155:LYS:HD3 | 5:E:156:ARG:N | 2.05 | 0.72 |
| 1:A:1167:A:C8 | 1:A:1169:A:N6 | 2.58 | 0.71 |
| 1:A:721:G:C4' | 1:A:722:G:O5' | 2.37 | 0.71 |
| 2:B:22:TRP:O | 2:B:22:TRP:CG | 2.43 | 0.71 |
| 1:A:49:U:O4 | 1:A:365:U:C5 | 2.43 | 0.71 |
| 1:A:1196:A:O2' | 1:A:1197:A:OP2 | 2.08 | 0.71 |
| 4:D:54:LEU:C | 4:D:54:LEU:CD2 | 2.59 | 0.71 |
| 1:A:914:A:N3 | 1:A:915:A:C8 | 2.59 | 0.70 |
| 17:Q:80:LYS:HB2 | 17:Q:80:LYS:NZ | 2.06 | 0.70 |
| 17:Q:69:THR:HG22 | 17:Q:69:THR:O | 1.90 | 0.70 |
| 6:F:52:ASN:O | 6:F:53:LYS:CB | 2.39 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 17:Q:11:VAL:HG12 | 17:Q:12:VAL:N | 2.07 | 0.70 |
| 16:P:28:ARG:CG | 16:P:29:ASN:ND2 | 2.55 | 0.70 |
| 17:Q:49:ASN:O | 17:Q:51:GLU:N | 2.25 | 0.70 |
| 1:A:32:A:C2' | 1:A:33:A:C8 | 2.75 | 0.69 |
| 1:A:923:A:O4' | 1:A:1398:A:C2 | 2.45 | 0.69 |
| 1:A:533:A:OP1 | 23:A:1726:HOH:O | 2.10 | 0.69 |
| 13:M:10:ASP:CG | 13:M:11:HIS:N | 2.46 | 0.69 |
| 17:Q:54:ILE:HD13 | 17:Q:54:ILE:C | 2.12 | 0.69 |
| 17:Q:45:VAL:HG13 | 17:Q:72:TRP:O | 1.93 | 0.69 |
| 1:A:1279:G:C1' | 1:A:1282:C:N4 | 2.56 | 0.69 |
| 21:U:16:ARG:NH1 | 21:U:19:LYS:CG | 2.55 | 0.69 |
| 1:A:428:G:C1' | 1:A:430:A:C8 | 2.75 | 0.68 |
| 1:A:139:A:C5 | 1:A:140:U:C5 | 2.81 | 0.68 |
| 16:P:48:GLU:CG | 16:P:49:GLY:N | 2.56 | 0.68 |
| 1:A:1160:G:O6 | 1:A:1181:G:C6 | 2.46 | 0.68 |
| 17:Q:11:VAL:CG1 | 17:Q:12:VAL:HG12 | 2.23 | 0.68 |
| 4:D:25:ARG:O | 4:D:26:ALA:CB | 2.41 | 0.68 |
| 1:A:914:A:O2' | 1:A:915:A:C5' | 2.42 | 0.68 |
| 1:A:872:A:C2 | 1:A:874:G:C6 | 2.81 | 0.68 |
| 5:E:154:ALA:HB1 | 8:H:65:PHE:CE2 | 2.29 | 0.68 |
| 10:J:57:VAL:CG2 | 10:J:58:ASN:N | 2.55 | 0.67 |
| 14:N:51:PRO:O | 14:N:52:ARG:CB | 2.42 | 0.67 |
| 1:A:204:G:C3' | 1:A:205:A:C5' | 2.72 | 0.67 |
| 8:H:48:PHE:O | 8:H:49:LYS:CB | 2.42 | 0.67 |
| 4:D:33:ILE:O | 4:D:34:GLU:CB | 2.42 | 0.67 |
| 1:A:965:U:C4' | 1:A:969:A:C8 | 2.77 | 0.67 |
| 21:U:9:GLU:CG | 21:U:10:PRO:CD | 2.73 | 0.67 |
| 1:A:439:U:O2' | 1:A:440:C:C5' | 2.43 | 0.67 |
| 20:T:32:LYS:O | 20:T:35:TYR:CD2 | 2.48 | 0.67 |
| 5:E:148:SER:O | 5:E:152:VAL:HG13 | 1.95 | 0.66 |
| 17:Q:80:LYS:HZ2 | 17:Q:80:LYS:HB2 | 1.59 | 0.66 |
| 1:A:1503:A:C8 | 1:A:1531:A:H1' | 2.29 | 0.66 |
| 5:E:155:LYS:HD2 | 5:E:156:ARG:N | 2.10 | 0.66 |
| 1:A:1157:A:C5 | 1:A:1180:A:C6 | 2.83 | 0.66 |
| 6:F:8:PHE:CE1 | 6:F:21:MET:CE | 2.78 | 0.66 |
| 17:Q:80:LYS:N | 17:Q:80:LYS:HD3 | 2.11 | 0.66 |
| 17:Q:18:LYS:C | 17:Q:47:ASP:OD2 | 2.34 | 0.66 |
| 17:Q:55:GLY:HA3 | 17:Q:82:VAL:HG11 | 1.76 | 0.66 |
| 17:Q:45:VAL:HG21 | 17:Q:60:ILE:HD11 | 1.77 | 0.66 |
| 1:A:1363:A:O2' | 1:A:1365:G:N7 | 2.29 | 0.66 |
| 17:Q:7:LEU:HD23 | 17:Q:24:ILE:HD11 | 1.78 | 0.66 |
| 4:D:43:ARG:O | 4:D:45:PRO:CD | 2.44 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:153:ALA:N | 5:E:156:ARG:HB2 | 2.10 | 0.66 |
| 5:E:120:HIS:O | 5:E:121:ASN:CB | 2.44 | 0.66 |
| 1:A:1160:G:N2 | 1:A:1161:C:C2 | 2.64 | 0.66 |
| 2:B:74:ALA:O | 2:B:75:ALA:CB | 2.44 | 0.66 |
| 1:A:1151:A:O2' | 1:A:1152:A:C5' | 2.44 | 0.66 |
| 1:A:338:A:N1 | 1:A:351:G:O6 | 2.29 | 0.66 |
| 16:P:56:ARG:NH1 | 16:P:59:HIS:CD2 | 2.64 | 0.66 |
| 1:A:204:G:C1' | 1:A:465:A:C2 | 2.80 | 0.65 |
| 1:A:1256:A:C1' | 1:A:1258:G:C5 | 2.79 | 0.65 |
| 1:A:1142:G:C2' | 1:A:1143:G:O4' | 2.44 | 0.65 |
| 17:Q:66:LEU:O | 17:Q:67:SER:HB3 | 1.96 | 0.65 |
| 1:A:267:C:O2' | 1:A:268:U:C5' | 2.45 | 0.65 |
| 1:A:1084:G:C5 | 1:A:1085:U:C4 | 2.84 | 0.65 |
| 1:A:1319:A:C8 | 1:A:1323:G:C6 | 2.85 | 0.65 |
| 18:R:63:TYR:CD1 | 18:R:69:TYR:OH | 2.50 | 0.65 |
| 1:A:1367:C:C5' | 10:J:62:ARG:NH1 | 2.60 | 0.65 |
| 1:A:501:C:O2' | 1:A:502:A:C5' | 2.45 | 0.65 |
| 5:E:158:LYS:HE2 | 8:H:63:LYS:NZ | 2.12 | 0.64 |
| 1:A:468:A:O2' | 1:A:469:C:C5' | 2.45 | 0.64 |
| 17:Q:31:PRO:HB2 | 17:Q:32:ILE:HD12 | 1.79 | 0.64 |
| 1:A:430:A:C4 | 1:A:431:A:C8 | 2.85 | 0.64 |
| 1:A:206:C:C2' | 1:A:207:C:O4' | 2.46 | 0.64 |
| 1:A:408:A:C2 | 1:A:435:A:C2 | 2.85 | 0.64 |
| 1:A:914:A:C4 | 1:A:915:A:C8 | 2.86 | 0.64 |
| 1:A:903:G:C5 | 1:A:904:U:C5 | 2.86 | 0.64 |
| 17:Q:45:VAL:CG2 | 17:Q:60:ILE:HD13 | 2.28 | 0.64 |
| 1:A:198:G:O2' | 1:A:199:A:C8 | 2.50 | 0.64 |
| 9:I:37:TYR:CD2 | 9:I:38:PHE:CD2 | 2.85 | 0.64 |
| 1:A:1021:A:C2' | 1:A:1022:A:C5' | 2.76 | 0.64 |
| 12:L:43:LYS:NZ | 12:L:44:PRO:CD | 2.61 | 0.64 |
| 5:E:136:VAL:CG2 | 5:E:136:VAL:O | 2.45 | 0.64 |
| 21:U:7:GLU:CB | 21:U:11:PHE:CE1 | 2.81 | 0.64 |
| 1:A:1138:G:N3 | 1:A:1138:G:C2' | 2.61 | 0.64 |
| 17:Q:48:GLU:OE1 | 17:Q:48:GLU:HA | 1.97 | 0.64 |
| 1:A:1531:A:C8 | 1:A:1531:A:C5' | 2.67 | 0.63 |
| 1:A:255:G:C4 | 1:A:256:U:C5 | 2.86 | 0.63 |
| 6:F:9:MET:CE | 6:F:59:TYR:CE2 | 2.82 | 0.63 |
| 1:A:1358:U:C6 | 1:A:1359:C:C5 | 2.87 | 0.63 |
| 4:D:31:CYS:O | 4:D:32:LYS:CB | 2.46 | 0.63 |
| 9:I:32:ARG:CG | 9:I:36:GLN:CB | 2.76 | 0.63 |
| 1:A:414:A:O2' | 1:A:415:A:C5' | 2.47 | 0.63 |
| 12:L:109:ARG:NH2 | 12:L:116:TYR:CE2 | 2.67 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:937:A:N6 | 1:A:1345:U:O4 | 2.32 | 0.63 |
| 1:A:111:G:O6 | 1:A:330:C:N4 | 2.31 | 0.63 |
| 1:A:487:A:O2' | 1:A:488:C:C5' | 2.47 | 0.62 |
| 4:D:196:GLU:C | 4:D:198:LEU:N | 2.50 | 0.62 |
| 4:D:173:ASP:O | 4:D:174:ALA:CB | 2.46 | 0.62 |
| 3:C:22:PHE:C | 3:C:22:PHE:CD2 | 2.73 | 0.62 |
| 17:Q:20:ILE:H | 17:Q:47:ASP:CG | 2.02 | 0.62 |
| 17:Q:62:GLU:HB2 | 17:Q:72:TRP:CZ2 | 2.34 | 0.62 |
| 1:A:428:G:O4' | 1:A:430:A:C8 | 2.53 | 0.62 |
| 1:A:872:A:C4 | 1:A:874:G:N7 | 2.67 | 0.62 |
| 11:K:34:THR:OG1 | 11:K:39:ASN:N | 2.32 | 0.62 |
| 17:Q:11:VAL:HG12 | 17:Q:12:VAL:CG1 | 2.29 | 0.62 |
| 17:Q:3:LYS:HD2 | 17:Q:3:LYS:O | 1.99 | 0.62 |
| 14:N:90:GLY:O | 14:N:92:ILE:N | 2.32 | 0.62 |
| 1:A:1241:G:O2' | 1:A:1242:G:C8 | 2.52 | 0.62 |
| 1:A:1095:U:O2' | 1:A:1096:C:C5' | 2.47 | 0.62 |
| 2:B:49:PHE:CG | 2:B:212:TYR:OH | 2.53 | 0.62 |
| 1:A:619:U:C2 | 4:D:131:ILE:CD1 | 2.82 | 0.62 |
| 9:I:6:TYR:CG | 9:I:7:GLY:N | 2.68 | 0.62 |
| 1:A:411:A:N6 | 1:A:413:G:N2 | 2.48 | 0.62 |
| 1:A:469:C:O2' | 1:A:470:C:C5' | 2.47 | 0.62 |
| 1:A:1378:C:C5 | 1:A:1379:G:C8 | 2.88 | 0.62 |
| 1:A:977:A:C2' | 1:A:977:A:N3 | 2.62 | 0.62 |
| 1:A:542:G:C2 | 1:A:543:U:C5 | 2.88 | 0.62 |
| 12:L:87:LYS:O | 12:L:88:ASP:CB | 2.46 | 0.62 |
| 1:A:1303:C:C2' | 1:A:1304:G:C8 | 2.83 | 0.61 |
| 1:A:417:G:C6 | 1:A:418:C:C4 | 2.88 | 0.61 |
| 14:N:22:LYS:CG | 14:N:23:ARG:N | 2.63 | 0.61 |
| 1:A:946:A:C2 | 1:A:1236:A:C2 | 2.88 | 0.61 |
| 1:A:1131:G:C2' | 1:A:1132:C:O5' | 2.48 | 0.61 |
| 1:A:697:U:C5 | 1:A:698:G:C8 | 2.87 | 0.61 |
| 17:Q:51:GLU:HG3 | 17:Q:74:LEU:HD21 | 1.82 | 0.61 |
| 21:U:52:VAL:CG1 | 21:U:53:LYS:N | 2.63 | 0.61 |
| 17:Q:28:VAL:O | 17:Q:37:ILE:HD12 | 2.01 | 0.61 |
| 1:A:172:A:C5 | 1:A:174:A:N7 | 2.69 | 0.61 |
| 17:Q:46:HIS:HB2 | 17:Q:66:LEU:CD1 | 2.23 | 0.61 |
| 1:A:1451:U:O2' | 1:A:1452:C:OP1 | 2.19 | 0.61 |
| 13:M:2:ARG:O | 13:M:3:ILE:CG1 | 2.49 | 0.61 |
| 17:Q:10:ARG:O | 17:Q:22:VAL:HG13 | 2.01 | 0.61 |
| 4:D:190:LEU:O | 4:D:191:SER:CB | 2.48 | 0.61 |
| 1:A:438:U:O2' | 1:A:439:U:OP2 | 2.19 | 0.61 |
| 1:A:1070:U:O2 | 1:A:1071:C:C6 | 2.54 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:1468:A:C2' | 1:A:1469:C:C5' | 2.79 | 0.61 |
| 1:A:180:U:C2' | 1:A:181:A:O5' | 2.49 | 0.61 |
| 21:U:39:LYS:N | 21:U:40:PRO:CD | 2.64 | 0.61 |
| 3:C:125:ARG:O | 3:C:126:ARG:CB | 2.49 | 0.60 |
| 8:H:124:ILE:CG1 | 8:H:124:ILE:O | 2.49 | 0.60 |
| 1:A:266:G:O3' | 17:Q:68:LYS:HB2 | 2.01 | 0.60 |
| 1:A:874:G:O2' | 1:A:875:U:C5' | 2.50 | 0.60 |
| 21:U:10:PRO:O | 21:U:11:PHE:CB | 2.49 | 0.60 |
| 5:E:81:GLN:NE2 | 5:E:81:GLN:N | 2.49 | 0.60 |
| 17:Q:60:ILE:CG2 | 17:Q:72:TRP:HE3 | 2.13 | 0.60 |
| 1:A:500:G:C6 | 1:A:501:C:N4 | 2.69 | 0.60 |
| 4:D:2:ARG:NH2 | 4:D:114:ARG:CD | 2.65 | 0.60 |
| 19:S:51:HIS:CD2 | 19:S:53:GLY:N | 2.69 | 0.60 |
| 1:A:86:G:N2 | 1:A:87:C:N4 | 2.50 | 0.60 |
| 17:Q:7:LEU:HD22 | 17:Q:72:TRP:CH2 | 2.36 | 0.60 |
| 1:A:1064:G:N2 | 1:A:1190:G:O2' | 2.35 | 0.60 |
| 1:A:120:A:C5 | 1:A:122:G:C6 | 2.90 | 0.60 |
| 10:J:84:VAL:CG1 | 10:J:85:ASP:N | 2.64 | 0.60 |
| 15:O:63:ARG:NH1 | 15:O:67:ASP:OD1 | 2.34 | 0.60 |
| 5:E:153:ALA:HA | 5:E:156:ARG:N | 2.15 | 0.60 |
| 1:A:198:G:O2' | 1:A:199:A:C5' | 2.49 | 0.60 |
| 1:A:92:U:O2' | 1:A:93:U:C5' | 2.50 | 0.60 |
| 16:P:10:GLY:O | 16:P:11:ALA:CB | 2.49 | 0.60 |
| 9:I:100:ALA:CB | 9:I:102:PHE:CE2 | 2.84 | 0.60 |
| 1:A:468:A:C2 | 1:A:469:C:N4 | 2.70 | 0.60 |
| 17:Q:58:VAL:CG2 | 17:Q:59:GLU:N | 2.65 | 0.60 |
| 1:A:1095:U:O2' | 1:A:1096:C:O4' | 2.20 | 0.59 |
| 1:A:1283:U:O2' | 1:A:1284:C:C6 | 2.55 | 0.59 |
| 14:N:50:LEU:O | 14:N:52:ARG:N | 2.35 | 0.59 |
| 1:A:511:C:O2' | 1:A:512:U:C5' | 2.50 | 0.59 |
| 2:B:163:ILE:CG2 | 2:B:164:ASP:N | 2.64 | 0.59 |
| 5:E:156:ARG:C | 5:E:158:LYS:H | 2.05 | 0.59 |
| 1:A:427:U:C4 | 1:A:428:G:C6 | 2.89 | 0.59 |
| 1:A:1152:A:C2' | 1:A:1153:G:C8 | 2.85 | 0.59 |
| 1:A:489:C:C2' | 1:A:490:C:C5' | 2.80 | 0.59 |
| 1:A:94:G:C4' | 1:A:95:C:O5' | 2.49 | 0.59 |
| 1:A:1469:C:C6 | 1:A:1469:C:C3' | 2.85 | 0.59 |
| 1:A:642:A:O2' | 1:A:643:C:C5' | 2.50 | 0.59 |
| 1:A:701:U:O2' | 1:A:702:A:OP2 | 2.19 | 0.59 |
| 12:L:24:GLU:CB | 12:L:26:CYS:SG | 2.90 | 0.59 |
| 1:A:15:G:C5 | 1:A:1396:A:C2 | 2.90 | 0.59 |
| 1:A:977:A:C8 | 1:A:1223:C:C2 | 2.90 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 17:Q:14:ASP:O | 17:Q:16:MET:HG2 | 2.03 | 0.59 |
| 11:K:51:PHE:N | 11:K:51:PHE:CD2 | 2.69 | 0.59 |
| 1:A:1382:C:O2' | 1:A:1383:C:C5' | 2.50 | 0.59 |
| 1:A:968:A:C4' | 1:A:969:A:OP2 | 2.50 | 0.59 |
| 16:P:79:ASN:O | 16:P:80:LYS:CB | 2.51 | 0.59 |
| 1:A:1158:C:O2 | 1:A:1158:C:C2' | 2.51 | 0.59 |
| 1:A:1053:G:O2' | 1:A:1054:C:OP2 | 2.20 | 0.59 |
| 1:A:569:C:C5' | 1:A:570:G:OP1 | 2.51 | 0.59 |
| 1:A:842:U:C3' | 1:A:843:U:C5' | 2.80 | 0.59 |
| 1:A:489:C:O2' | 1:A:490:C:C5' | 2.50 | 0.59 |
| 11:K:124:LYS:NZ | 21:U:33:ARG:NH2 | 2.51 | 0.59 |
| 4:D:195:ASN:O | 4:D:196:GLU:CG | 2.51 | 0.59 |
| 1:A:667:G:C4' | 15:O:50:HIS:ND1 | 2.66 | 0.59 |
| 11:K:126:ARG:N | 21:U:33:ARG:NH2 | 2.51 | 0.59 |
| 17:Q:35:LYS:HG2 | 17:Q:36:PHE:N | 2.18 | 0.59 |
| 1:A:616:G:C2 | 1:A:625:U:O2 | 2.56 | 0.59 |
| 10:J:18:ILE:O | 10:J:22:THR:N | 2.35 | 0.59 |
| 13:M:113:LYS:N | 13:M:114:PRO:CD | 2.66 | 0.58 |
| 5:E:149:PRO:CA | 5:E:152:VAL:HG13 | 2.33 | 0.58 |
| 1:A:15:G:N7 | 1:A:1396:A:C2 | 2.71 | 0.58 |
| 10:J:52:LEU:CD2 | 10:J:62:ARG:CG | 2.80 | 0.58 |
| 1:A:1303:C:O2' | 1:A:1304:G:C5' | 2.52 | 0.58 |
| 15:O:16:ARG:O | 15:O:17:ASP:CB | 2.51 | 0.58 |
| 1:A:1319:A:N7 | 1:A:1323:G:C6 | 2.71 | 0.58 |
| 1:A:1449:C:C2' | 1:A:1450:U:C5' | 2.81 | 0.58 |
| 1:A:1055:A:N6 | 1:A:1206:G:C5 | 2.72 | 0.58 |
| 1:A:1184:G:O2' | 1:A:1185:G:C5' | 2.51 | 0.58 |
| 7:G:12:LEU:CD2 | 7:G:12:LEU:N | 2.66 | 0.58 |
| 1:A:91:U:O2' | 1:A:92:U:O4' | 2.21 | 0.58 |
| 1:A:920:U:O4' | 1:A:1080:A:C2 | 2.57 | 0.58 |
| 1:A:462:G:C5' | 1:A:463:U:OP2 | 2.51 | 0.58 |
| 10:J:15:HIS:CG | 10:J:16:ARG:N | 2.71 | 0.58 |
| 1:A:1160:G:O6 | 1:A:1181:G:O6 | 2.22 | 0.58 |
| 1:A:89:U:O2' | 1:A:90:C:C5' | 2.52 | 0.58 |
| 1:A:414:A:C2' | 1:A:415:A:C8 | 2.87 | 0.58 |
| 1:A:575:G:C6 | 1:A:821:G:N7 | 2.72 | 0.58 |
| 20:T:2:ASN:O | 20:T:3:ILE:C | 2.41 | 0.58 |
| 17:Q:48:GLU:O | 17:Q:49:ASN:ND2 | 2.37 | 0.58 |
| 1:A:450:G:N7 | 1:A:481:G:O6 | 2.37 | 0.58 |
| 16:P:73:ALA:O | 16:P:77:GLU:CB | 2.52 | 0.58 |
| 1:A:126:G:C2' | 1:A:127:G:O5' | 2.51 | 0.58 |
| 5:E:109:ALA:O | 5:E:110:MET:CB | 2.52 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:17:HIS:CD2 | 2:B:202:ASN:ND2 | 2.72 | 0.58 |
| 17:Q:18:LYS:HA | 17:Q:47:ASP:HB3 | 1.81 | 0.58 |
| 11:K:21:HIS:CD2 | 11:K:34:THR:CG2 | 2.86 | 0.58 |
| 1:A:972:C:O2' | 1:A:973:G:O5' | 2.22 | 0.58 |
| 2:B:139:GLU:O | 2:B:143:LEU:CD2 | 2.52 | 0.58 |
| 1:A:209:U:C5' | 1:A:210:C:OP2 | 2.52 | 0.58 |
| 17:Q:74:LEU:HD12 | 17:Q:74:LEU:N | 2.13 | 0.58 |
| 1:A:110:C:O2' | 1:A:111:G:O4' | 2.21 | 0.58 |
| 1:A:652:U:O2' | 1:A:653:U:O5' | 2.22 | 0.58 |
| 4:D:75:TYR:C | 4:D:75:TYR:CD1 | 2.77 | 0.58 |
| 17:Q:27:PHE:O | 17:Q:28:VAL:HG12 | 2.03 | 0.58 |
| 1:A:1129:C:C5' | 9:I:17:ARG:NH2 | 2.67 | 0.57 |
| 1:A:1153:G:O2' | 1:A:1154:G:O5' | 2.22 | 0.57 |
| 1:A:559:A:C4' | 1:A:560:A:O5' | 2.52 | 0.57 |
| 13:M:10:ASP:OD1 | 13:M:11:HIS:N | 2.37 | 0.57 |
| 1:A:1432:G:O2' | 1:A:1433:A:OP2 | 2.22 | 0.57 |
| 1:A:563:A:C8 | 1:A:567:G:O4' | 2.56 | 0.57 |
| 17:Q:80:LYS:H | 17:Q:80:LYS:HZ2 | 1.52 | 0.57 |
| 12:L:43:LYS:CB | 12:L:44:PRO:CD | 2.81 | 0.57 |
| 1:A:274:A:O2' | 1:A:275:G:C5' | 2.52 | 0.57 |
| 12:L:27:PRO:CB | 12:L:28:GLN:OE1 | 2.52 | 0.57 |
| 5:E:148:SER:O | 5:E:152:VAL:N | 2.37 | 0.57 |
| 1:A:94:G:C4' | 1:A:95:C:C5' | 2.81 | 0.57 |
| 1:A:981:U:C2 | 1:A:982:U:C5 | 2.92 | 0.57 |
| 1:A:1242:G:C5 | 1:A:1243:C:C5 | 2.92 | 0.57 |
| 4:D:52:VAL:CG2 | 4:D:53:GLN:N | 2.66 | 0.57 |
| 1:A:144:G:C4 | 1:A:179:A:C2 | 2.92 | 0.57 |
| 1:A:1394:A:N1 | 1:A:1500:A:O2' | 2.36 | 0.57 |
| 1:A:330:C:C5' | 1:A:330:C:C6 | 2.87 | 0.57 |
| 1:A:1012:A:N6 | 1:A:1013:G:C6 | 2.73 | 0.57 |
| 8:H:46:GLU:O | 8:H:47:ASP:CB | 2.51 | 0.57 |
| 1:A:1046:A:O2' | 1:A:1047:G:C5' | 2.52 | 0.57 |
| 1:A:71:A:O2' | 1:A:72:A:O5' | 2.22 | 0.57 |
| 1:A:1227:A:O2' | 1:A:1228:C:O5' | 2.22 | 0.57 |
| 1:A:1055:A:N6 | 1:A:1206:G:C6 | 2.73 | 0.57 |
| 1:A:982:U:C4' | 1:A:983:A:O5' | 2.53 | 0.57 |
| 1:A:572:A:C5' | 1:A:573:A:OP2 | 2.53 | 0.57 |
| 1:A:542:G:C2 | 1:A:543:U:C4 | 2.93 | 0.57 |
| 1:A:1091:U:C2 | 1:A:1095:U:N3 | 2.72 | 0.57 |
| 1:A:1181:G:O2' | 1:A:1182:G:C4 | 2.58 | 0.57 |
| 1:A:76:G:N1 | 1:A:95:C:N4 | 2.52 | 0.57 |
| 1:A:198:G:C4 | 1:A:199:A:N7 | 2.72 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:104:ILE:O | 5:E:104:ILE:CG2 | 2.53 | 0.57 |
| 5:E:152:VAL:O | 5:E:154:ALA:N | 2.37 | 0.57 |
| 1:A:842:U:O2' | 1:A:846:G:N1 | 2.38 | 0.57 |
| 1:A:57:G:C5 | 1:A:58:C:C4 | 2.93 | 0.57 |
| 4:D:16:THR:CG2 | 4:D:17:ASP:N | 2.67 | 0.57 |
| 1:A:566:G:C4' | 1:A:567:G:OP1 | 2.53 | 0.56 |
| 4:D:124:VAL:O | 4:D:126:GLY:N | 2.38 | 0.56 |
| 3:C:146:LYS:CB | 3:C:202:PHE:CD2 | 2.87 | 0.56 |
| 1:A:545:C:C2' | 1:A:546:A:C5' | 2.83 | 0.56 |
| 1:A:807:A:C5 | 1:A:808:C:C5 | 2.93 | 0.56 |
| 5:E:81:GLN:NE2 | 5:E:146:MET:SD | 2.79 | 0.56 |
| 17:Q:16:MET:HE2 | 17:Q:20:ILE:HD12 | 1.86 | 0.56 |
| 1:A:1167:A:N7 | 1:A:1169:A:N6 | 2.52 | 0.56 |
| 16:P:29:ASN:N | 16:P:29:ASN:ND2 | 2.53 | 0.56 |
| 1:A:1279:G:C2' | 1:A:1279:G:N3 | 2.68 | 0.56 |
| 1:A:1064:G:O2' | 1:A:1190:G:N2 | 2.38 | 0.56 |
| 1:A:687:A:C2 | 1:A:704:A:C5 | 2.94 | 0.56 |
| 1:A:108:G:C2' | 1:A:109:A:OP1 | 2.50 | 0.56 |
| 1:A:328:C:O2 | 1:A:328:C:C2' | 2.51 | 0.56 |
| 1:A:1152:A:C4 | 1:A:1153:G:N7 | 2.73 | 0.56 |
| 13:M:45:SER:O | 13:M:46:GLU:CB | 2.53 | 0.56 |
| 2:B:186:VAL:N | 2:B:199:ILE:O | 2.39 | 0.56 |
| 1:A:495:A:C4' | 1:A:496:A:O5' | 2.54 | 0.56 |
| 17:Q:20:ILE:CB | 17:Q:47:ASP:OD1 | 2.51 | 0.56 |
| 17:Q:54:ILE:HD13 | 17:Q:54:ILE:O | 2.06 | 0.56 |
| 1:A:414:A:C4 | 1:A:415:A:C8 | 2.94 | 0.56 |
| 1:A:996:A:C2 | 1:A:1046:A:C5' | 2.88 | 0.56 |
| 1:A:55:A:C4 | 1:A:56:U:C6 | 2.93 | 0.56 |
| 19:S:79:TYR:CG | 19:S:80:ARG:N | 2.73 | 0.56 |
| 17:Q:18:LYS:CB | 17:Q:47:ASP:HB2 | 2.35 | 0.56 |
| 2:B:20:ARG:O | 2:B:21:TYR:C | 2.44 | 0.56 |
| 1:A:1319:A:C5 | 1:A:1323:G:C4 | 2.94 | 0.56 |
| 1:A:1410:A:C2' | 1:A:1411:C:O5' | 2.53 | 0.56 |
| 1:A:900:A:N1 | 1:A:901:A:C2 | 2.74 | 0.56 |
| 1:A:192:A:C5 | 1:A:193:C:C5 | 2.93 | 0.56 |
| 1:A:1231:G:C6 | 1:A:1232:U:C4 | 2.94 | 0.56 |
| 6:F:93:LYS:O | 6:F:94:HIS:CB | 2.53 | 0.56 |
| 1:A:1225:A:C2' | 1:A:1226:C:C5 | 2.88 | 0.56 |
| 17:Q:80:LYS:HZ2 | 17:Q:80:LYS:CB | 2.17 | 0.56 |
| 1:A:197:A:O2' | 1:A:198:G:C8 | 2.58 | 0.56 |
| 1:A:483:C:O2 | 16:P:13:LYS:NZ | 2.39 | 0.56 |
| 4:D:122:ILE:N | 4:D:122:ILE:CD1 | 2.67 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 10:J:14:ASP:CB | 10:J:17:LEU:CB | 2.84 | 0.56 |
| 1:A:1157:A:C6 | 1:A:1180:A:C5 | 2.94 | 0.56 |
| 1:A:1061:G:C6 | 1:A:1197:A:C2 | 2.94 | 0.56 |
| 1:A:495:A:C2 | 1:A:496:A:N6 | 2.74 | 0.56 |
| 1:A:771:G:C4 | 1:A:809:G:N2 | 2.74 | 0.56 |
| 1:A:1167:A:N7 | 1:A:1169:A:C6 | 2.73 | 0.56 |
| 1:A:1358:U:C5 | 1:A:1359:C:C4 | 2.94 | 0.56 |
| 11:K:39:ASN:O | 11:K:40:ALA:CB | 2.54 | 0.56 |
| 1:A:686:U:O2' | 1:A:687:A:C8 | 2.59 | 0.56 |
| 1:A:1210:C:C2' | 1:A:1211:U:C5' | 2.84 | 0.56 |
| 1:A:243:A:C2 | 1:A:246:A:C8 | 2.94 | 0.56 |
| 9:I:82:ILE:O | 9:I:86:LEU:N | 2.39 | 0.56 |
| 18:R:50:TYR:O | 18:R:54:LEU:N | 2.39 | 0.56 |
| 1:A:523:A:C2 | 1:A:527:G:O6 | 2.59 | 0.55 |
| 12:L:72:ASN:OD1 | 12:L:104:SER:CB | 2.54 | 0.55 |
| 1:A:486:U:C5' | 1:A:486:U:C6 | 2.89 | 0.55 |
| 1:A:453:G:C6 | 1:A:454:G:C5 | 2.94 | 0.55 |
| 1:A:1320:C:O2' | 1:A:1321:U:O4' | 2.25 | 0.55 |
| 1:A:198:G:C6 | 1:A:220:G:C2 | 2.94 | 0.55 |
| 4:D:172:VAL:CG1 | 4:D:173:ASP:N | 2.67 | 0.55 |
| 2:B:202:ASN:ND2 | 2:B:205:ALA:CB | 2.69 | 0.55 |
| 4:D:12:ARG:NH1 | 4:D:36:ALA:O | 2.38 | 0.55 |
| 5:E:121:ASN:ND2 | 5:E:122:VAL:N | 2.54 | 0.55 |
| 1:A:80:A:C2 | 1:A:90:C:N3 | 2.74 | 0.55 |
| 1:A:87:C:O2' | 1:A:88:U:O4' | 2.24 | 0.55 |
| 1:A:455:G:C2 | 1:A:478:A:C2 | 2.94 | 0.55 |
| 20:T:33:LYS:CE | 20:T:33:LYS:N | 2.70 | 0.55 |
| 1:A:486:U:O2' | 1:A:487:A:C5' | 2.54 | 0.55 |
| 17:Q:44:HIS:HD2 | 17:Q:69:THR:HG22 | 1.71 | 0.55 |
| 6:F:3:HIS:N | 6:F:92:THR:CG2 | 2.70 | 0.55 |
| 3:C:10:ARG:O | 3:C:13:ILE:N | 2.39 | 0.55 |
| 14:N:60:ARG:O | 14:N:61:ASN:CB | 2.54 | 0.55 |
| 1:A:251:G:N1 | 1:A:266:G:C6 | 2.75 | 0.55 |
| 1:A:502:A:C2 | 1:A:544:G:C2 | 2.94 | 0.55 |
| 11:K:34:THR:OG1 | 11:K:40:ALA:N | 2.40 | 0.55 |
| 1:A:913:A:O2' | 1:A:914:A:OP2 | 2.25 | 0.55 |
| 1:A:495:A:C2 | 1:A:496:A:C6 | 2.94 | 0.55 |
| 1:A:1494:G:C2 | 1:A:1495:U:C5 | 2.94 | 0.55 |
| 9:I:98:ARG:CG | 9:I:103:VAL:CG2 | 2.84 | 0.55 |
| 5:E:153:ALA:O | 5:E:156:ARG:O | 2.25 | 0.55 |
| 16:P:19:VAL:CG1 | 16:P:37:GLY:C | 2.75 | 0.55 |
| 1:A:1284:C:C6 | 1:A:1285:A:N7 | 2.75 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:173:U:C2 | 1:A:197:A:C2 | 2.95 | 0.55 |
| 14:N:19:TYR:O | 14:N:22:LYS:CB | 2.54 | 0.55 |
| 4:D:2:ARG:CB | 4:D:4:LEU:CD1 | 2.84 | 0.55 |
| 1:A:1399:C:O2 | 1:A:1401:G:C5 | 2.60 | 0.55 |
| 5:E:45:VAL:CG2 | 5:E:117:ALA:CB | 2.85 | 0.55 |
| 16:P:23:ASP:O | 16:P:25:ARG:N | 2.40 | 0.55 |
| 4:D:19:PHE:CD1 | 4:D:19:PHE:N | 2.75 | 0.55 |
| 1:A:74:A:O2' | 1:A:75:G:O4' | 2.23 | 0.55 |
| 6:F:37:HIS:ND1 | 6:F:95:ALA:CB | 2.70 | 0.55 |
| 1:A:1306:A:C6 | 1:A:1307:U:C2 | 2.95 | 0.54 |
| 1:A:1032:G:N2 | 1:A:1033:G:C8 | 2.75 | 0.54 |
| 11:K:13:LYS:O | 11:K:14:GLN:CB | 2.55 | 0.54 |
| 3:C:106:ARG:O | 3:C:106:ARG:CG | 2.54 | 0.54 |
| 17:Q:60:ILE:CG2 | 17:Q:72:TRP:CE3 | 2.90 | 0.54 |
| 1:A:1167:A:C8 | 1:A:1169:A:C6 | 2.96 | 0.54 |
| 11:K:109:ILE:CG2 | 11:K:110:THR:N | 2.70 | 0.54 |
| 6:F:55:HIS:O | 6:F:56:LYS:CB | 2.55 | 0.54 |
| 1:A:657:U:O2 | 15:O:21:THR:CG2 | 2.54 | 0.54 |
| 17:Q:15:LYS:HD2 | 17:Q:15:LYS:C | 2.27 | 0.54 |
| 1:A:184:G:O2' | 1:A:185:U:O5' | 2.25 | 0.54 |
| 1:A:1253:G:N1 | 1:A:1285:A:N6 | 2.55 | 0.54 |
| 1:A:795:C:C5' | 1:A:796:C:OP2 | 2.55 | 0.54 |
| 1:A:935:A:O2' | 1:A:936:C:O4' | 2.25 | 0.54 |
| 17:Q:7:LEU:HD22 | 17:Q:72:TRP:CZ3 | 2.42 | 0.54 |
| 16:P:28:ARG:NE | 16:P:29:ASN:ND2 | 2.55 | 0.54 |
| 1:A:1319:A:C4' | 1:A:1320:C:OP1 | 2.55 | 0.54 |
| 1:A:414:A:N3 | 1:A:415:A:C8 | 2.75 | 0.54 |
| 4:D:194:ILE:O | 4:D:194:ILE:CG1 | 2.54 | 0.54 |
| 1:A:74:A:C6 | 1:A:97:G:O6 | 2.60 | 0.54 |
| 17:Q:58:VAL:HG22 | 17:Q:59:GLU:N | 2.22 | 0.54 |
| 12:L:23:LEU:CB | 12:L:58:ASN:ND2 | 2.70 | 0.54 |
| 1:A:1429:A:C2 | 1:A:1472:U:C2 | 2.96 | 0.54 |
| 15:O:81:ILE:O | 15:O:85:GLY:N | 2.40 | 0.54 |
| 17:Q:13:SER:O | 17:Q:20:ILE:CD1 | 2.56 | 0.54 |
| 4:D:151:GLN:O | 4:D:152:SER:C | 2.45 | 0.54 |
| 1:A:1159:U:N3 | 1:A:1182:G:C5 | 2.75 | 0.54 |
| 1:A:496:A:N3 | 1:A:496:A:C2' | 2.71 | 0.54 |
| 17:Q:4:ILE:HD12 | 17:Q:4:ILE:N | 2.23 | 0.54 |
| 1:A:991:U:C4' | 1:A:992:U:OP1 | 2.56 | 0.54 |
| 1:A:1261:A:N1 | 1:A:1274:A:C2 | 2.75 | 0.54 |
| 3:C:2:GLN:N | 3:C:2:GLN:OE1 | 2.41 | 0.54 |
| 1:A:466:A:C5' | 1:A:467:U:OP2 | 2.56 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 16:P:59:HIS:CE1 | 16:P:63:GLN:NE2 | 2.76 | 0.54 |
| 3:C:13:ILE:O | 3:C:15:LYS:N | 2.40 | 0.54 |
| 2:B:15:PHE:CD1 | 2:B:16:GLY:N | 2.76 | 0.54 |
| 11:K:71:ASP:OD1 | 11:K:72:ALA:N | 2.41 | 0.54 |
| 1:A:694:A:C2' | 1:A:695:A:O5' | 2.55 | 0.54 |
| 5:E:148:SER:O | 5:E:152:VAL:CG1 | 2.56 | 0.54 |
| 17:Q:73:THR:HG22 | 17:Q:74:LEU:N | 2.22 | 0.54 |
| 1:A:1203:C:O2' | 1:A:1204:A:C5' | 2.56 | 0.54 |
| 1:A:668:G:O2' | 15:O:45:HIS:CD2 | 2.61 | 0.54 |
| 1:A:614:C:C2' | 1:A:615:G:O5' | 2.55 | 0.54 |
| 1:A:1087:G:O2' | 1:A:1088:G:C5' | 2.56 | 0.54 |
| 17:Q:14:ASP:O | 17:Q:16:MET:SD | 2.66 | 0.54 |
| 17:Q:79:GLU:C | 17:Q:80:LYS:HD3 | 2.28 | 0.54 |
| 1:A:1152:A:O2' | 1:A:1153:G:C8 | 2.61 | 0.54 |
| 1:A:66:A:O4' | 1:A:173:U:C4 | 2.61 | 0.54 |
| 1:A:1227:A:N3 | 1:A:1227:A:C2' | 2.70 | 0.54 |
| 2:B:163:ILE:O | 2:B:185:ILE:CG1 | 2.56 | 0.54 |
| 1:A:1306:A:C2' | 1:A:1307:U:C5' | 2.85 | 0.54 |
| 15:O:23:SER:O | 15:O:24:THR:C | 2.45 | 0.54 |
| 9:I:56:MET:SD | 9:I:57:VAL:N | 2.81 | 0.54 |
| 4:D:35:GLN:O | 4:D:36:ALA:CB | 2.55 | 0.53 |
| 1:A:1196:A:O2' | 1:A:1197:A:P | 2.66 | 0.53 |
| 1:A:174:A:O2' | 1:A:175:C:C5' | 2.56 | 0.53 |
| 16:P:40:ASN:OD1 | 16:P:42:ILE:N | 2.41 | 0.53 |
| 20:T:2:ASN:O | 20:T:4:LYS:N | 2.41 | 0.53 |
| 1:A:1087:G:O2' | 1:A:1088:G:C8 | 2.61 | 0.53 |
| 1:A:1506:U:C3' | 23:A:1677:HOH:O | 2.55 | 0.53 |
| 5:E:153:ALA:O | 5:E:154:ALA:C | 2.46 | 0.53 |
| 7:G:144:ALA:C | 7:G:146:ALA:N | 2.61 | 0.53 |
| 1:A:369:G:OP2 | 1:A:388:G:N1 | 2.41 | 0.53 |
| 5:E:155:LYS:HD2 | 5:E:155:LYS:N | 2.16 | 0.53 |
| 1:A:275:G:N3 | 1:A:276:G:C8 | 2.76 | 0.53 |
| 1:A:1381:U:O2' | 1:A:1382:C:C6 | 2.61 | 0.53 |
| 1:A:1157:A:C2 | 1:A:1181:G:C4 | 2.96 | 0.53 |
| 4:D:170:LEU:CD1 | 4:D:170:LEU:N | 2.70 | 0.53 |
| 1:A:82:G:N2 | 1:A:84:U:C4 | 2.77 | 0.53 |
| 1:A:1134:G:O6 | 1:A:1141:C:N4 | 2.41 | 0.53 |
| 11:K:69:CYS:O | 11:K:73:VAL:CG2 | 2.56 | 0.53 |
| 9:I:51:LEU:CB | 9:I:56:MET:CG | 2.87 | 0.53 |
| 2:B:132:GLU:O | 2:B:136:ARG:CB | 2.56 | 0.53 |
| 1:A:1531:A:O2' | 1:A:1532:U:H5' | 2.09 | 0.53 |
| 1:A:1258:G:N3 | 1:A:1259:C:C5 | 2.76 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:903:G:C4 | 1:A:904:U:C5 | 2.96 | 0.53 |
| 4:D:99:ASN:OD1 | 4:D:110:ARG:NH1 | 2.41 | 0.53 |
| 1:A:60:A:C4' | 1:A:61:G:O5' | 2.57 | 0.53 |
| 2:B:9:LEU:CD1 | 2:B:42:LEU:CD1 | 2.87 | 0.53 |
| 1:A:1153:G:C2 | 1:A:1154:G:C8 | 2.97 | 0.53 |
| 1:A:914:A:O2' | 1:A:915:A:O4' | 2.27 | 0.53 |
| 1:A:1046:A:C2' | 1:A:1047:G:O5' | 2.57 | 0.53 |
| 4:D:149:LYS:O | 4:D:151:GLN:OE1 | 2.27 | 0.53 |
| 1:A:82:G:N2 | 1:A:84:U:N3 | 2.57 | 0.53 |
| 1:A:259:G:C4 | 1:A:260:G:C8 | 2.97 | 0.53 |
| 16:P:43:ALA:O | 16:P:44:SER:OG | 2.27 | 0.53 |
| 20:T:82:ILE:CD1 | 20:T:83:ASN:N | 2.72 | 0.53 |
| 5:E:148:SER:O | 5:E:152:VAL:CA | 2.57 | 0.53 |
| 17:Q:60:ILE:HG22 | 17:Q:72:TRP:CE3 | 2.43 | 0.53 |
| 1:A:1070:U:C2 | 1:A:1071:C:C5 | 2.97 | 0.53 |
| 1:A:667:G:OP1 | 1:A:732:C:O2' | 2.27 | 0.53 |
| 1:A:1078:U:O4' | 5:E:88:HIS:CE1 | 2.62 | 0.53 |
| 17:Q:46:HIS:CD2 | 17:Q:48:GLU:H | 2.27 | 0.53 |
| 1:A:1277:C:O2' | 1:A:1279:G:C8 | 2.62 | 0.53 |
| 15:O:3:SER:O | 15:O:6:ALA:N | 2.42 | 0.53 |
| 4:D:164:ARG:O | 4:D:166:LYS:N | 2.41 | 0.53 |
| 1:A:679:C:O2 | 1:A:712:A:C2 | 2.61 | 0.53 |
| 14:N:79:SER:O | 14:N:81:ILE:N | 2.42 | 0.53 |
| 1:A:1299:A:C8 | 1:A:1301:U:C1' | 2.91 | 0.52 |
| 1:A:11:G:C5 | 1:A:12:U:C5 | 2.96 | 0.52 |
| 1:A:790:A:C6 | 1:A:791:G:C6 | 2.97 | 0.52 |
| 20:T:16:ALA:O | 20:T:17:ARG:C | 2.48 | 0.52 |
| 4:D:160:LEU:CD2 | 4:D:161:ALA:N | 2.73 | 0.52 |
| 1:A:1084:G:C6 | 1:A:1085:U:O4 | 2.62 | 0.52 |
| 1:A:1323:G:O2' | 1:A:1324:A:C8 | 2.62 | 0.52 |
| 1:A:1060:U:C5 | 3:C:1:GLY:CA | 2.93 | 0.52 |
| 12:L:33:CYS:CA | 12:L:53:ARG:O | 2.57 | 0.52 |
| 14:N:40:ARG:NH1 | 14:N:44:VAL:CG2 | 2.72 | 0.52 |
| 1:A:74:A:C2 | 1:A:75:G:C4 | 2.98 | 0.52 |
| 17:Q:40:THR:HG22 | 17:Q:41:THR:N | 2.25 | 0.52 |
| 1:A:748:G:C6 | 1:A:749:A:C6 | 2.98 | 0.52 |
| 1:A:275:G:O2' | 1:A:276:G:C5' | 2.58 | 0.52 |
| 1:A:984:C:N3 | 1:A:1222:G:C2 | 2.77 | 0.52 |
| 2:B:209:VAL:CG2 | 2:B:210:THR:N | 2.72 | 0.52 |
| 3:C:6:PRO:CG | 3:C:183:TYR:CD2 | 2.92 | 0.52 |
| 1:A:1508:A:C2' | 1:A:1509:C:O5' | 2.57 | 0.52 |
| 1:A:292:G:C2 | 1:A:309:A:C2 | 2.97 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:451:A:C1' | 1:A:452:A:N7 | 2.72 | 0.52 |
| 19:S:33:TRP:NE1 | 19:S:51:HIS:ND1 | 2.58 | 0.52 |
| 1:A:44:A:OP2 | 16:P:12:LYS:NZ | 2.43 | 0.52 |
| 1:A:152:A:N6 | 1:A:170:U:C2 | 2.78 | 0.52 |
| 19:S:45:GLY:N | 19:S:61:VAL:CG2 | 2.72 | 0.52 |
| 11:K:30:ILE:CD1 | 11:K:30:ILE:C | 2.78 | 0.52 |
| 21:U:19:LYS:CA | 21:U:19:LYS:CE | 2.87 | 0.52 |
| 1:A:1358:U:C6 | 1:A:1359:C:C6 | 2.98 | 0.52 |
| 10:J:19:ASP:N | 10:J:19:ASP:OD1 | 2.41 | 0.52 |
| 15:O:15:GLY:O | 15:O:17:ASP:N | 2.43 | 0.52 |
| 1:A:693:G:C2' | 1:A:694:A:C5' | 2.88 | 0.52 |
| 21:U:3:ILE:CA | 21:U:19:LYS:NZ | 2.73 | 0.52 |
| 4:D:147:LYS:O | 4:D:148:ALA:C | 2.49 | 0.52 |
| 3:C:95:GLY:O | 3:C:96:VAL:CG1 | 2.58 | 0.52 |
| 2:B:46:VAL:CB | 2:B:47:PRO:CD | 2.88 | 0.52 |
| 3:C:166:TRP:N | 3:C:166:TRP:CE3 | 2.78 | 0.52 |
| 1:A:922:G:C6 | 1:A:923:A:C6 | 2.97 | 0.52 |
| 1:A:438:U:O2' | 1:A:439:U:P | 2.68 | 0.52 |
| 4:D:131:ILE:O | 4:D:133:SER:N | 2.43 | 0.52 |
| 1:A:322:C:O2' | 20:T:17:ARG:CG | 2.58 | 0.52 |
| 4:D:28:ASP:C | 4:D:29:THR:O | 2.47 | 0.52 |
| 2:B:81:ASP:OD1 | 2:B:83:ALA:N | 2.43 | 0.52 |
| 12:L:121:PRO:O | 12:L:122:LYS:C | 2.48 | 0.52 |
| 1:A:1480:A:C6 | 1:A:1481:U:N3 | 2.78 | 0.52 |
| 1:A:582:C:C2 | 1:A:583:A:C8 | 2.98 | 0.52 |
| 1:A:486:U:C2' | 1:A:487:A:C5' | 2.88 | 0.51 |
| 4:D:196:GLU:O | 4:D:198:LEU:N | 2.42 | 0.51 |
| 1:A:652:U:O2' | 1:A:653:U:P | 2.67 | 0.51 |
| 1:A:1251:A:C2' | 1:A:1252:A:C8 | 2.93 | 0.51 |
| 8:H:8:ASP:O | 8:H:9:MET:C | 2.48 | 0.51 |
| 13:M:95:PRO:CG | 13:M:101:THR:CG2 | 2.88 | 0.51 |
| 5:E:152:VAL:O | 5:E:155:LYS:CD | 2.58 | 0.51 |
| 2:B:9:LEU:CD2 | 2:B:11:ALA:N | 2.73 | 0.51 |
| 1:A:829:G:C6 | 1:A:858:G:C2 | 2.99 | 0.51 |
| 1:A:39:G:C4 | 1:A:40:C:C5 | 2.99 | 0.51 |
| 1:A:198:G:O2' | 1:A:199:A:O5' | 2.27 | 0.51 |
| 4:D:147:LYS:CD | 4:D:147:LYS:N | 2.74 | 0.51 |
| 1:A:466:A:C4' | 1:A:467:U:OP2 | 2.57 | 0.51 |
| 1:A:1319:A:C5 | 1:A:1323:G:C5 | 2.98 | 0.51 |
| 1:A:1241:G:C2 | 1:A:1242:G:C5 | 2.99 | 0.51 |
| 11:K:15:VAL:CG1 | 11:K:78:ILE:CG2 | 2.88 | 0.51 |
| 4:D:193:ASP:N | 4:D:193:ASP:OD1 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 17:Q:11:VAL:HG23 | 17:Q:56:ASP:O | 2.10 | 0.51 |
| 1:A:468:A:C2 | 1:A:469:C:C5 | 2.98 | 0.51 |
| 1:A:199:A:O2' | 1:A:200:G:O4' | 2.28 | 0.51 |
| 14:N:40:ARG:NH1 | 14:N:44:VAL:CG1 | 2.73 | 0.51 |
| 1:A:895:G:C6 | 1:A:896:C:C4 | 2.99 | 0.51 |
| 1:A:1048:G:OP1 | 14:N:3:GLN:N | 2.43 | 0.51 |
| 5:E:24:VAL:O | 5:E:25:LYS:C | 2.49 | 0.51 |
| 4:D:188:SER:O | 4:D:190:LEU:N | 2.43 | 0.51 |
| 1:A:71:A:C8 | 1:A:100:G:C2 | 2.98 | 0.51 |
| 1:A:771:G:C4 | 1:A:772:U:C5 | 2.99 | 0.51 |
| 1:A:1101:A:C8 | 2:B:170:ILE:CG2 | 2.94 | 0.51 |
| 5:E:152:VAL:HB | 5:E:155:LYS:CE | 2.36 | 0.51 |
| 1:A:1161:C:O2' | 1:A:1162:C:C6 | 2.63 | 0.51 |
| 1:A:198:G:C2' | 1:A:199:A:C8 | 2.93 | 0.51 |
| 1:A:1336:C:O2' | 1:A:1337:G:OP2 | 2.28 | 0.51 |
| 7:G:79:VAL:CG1 | 7:G:80:GLY:N | 2.74 | 0.51 |
| 1:A:1160:G:O2' | 1:A:1161:C:O5' | 2.28 | 0.51 |
| 15:O:45:HIS:O | 15:O:47:LYS:N | 2.44 | 0.51 |
| 8:H:9:MET:CE | 8:H:32:LYS:CA | 2.89 | 0.51 |
| 14:N:63:CYS:SG | 14:N:66:THR:OG1 | 2.69 | 0.51 |
| 1:A:428:G:O3' | 4:D:12:ARG:NH2 | 2.44 | 0.51 |
| 16:P:48:GLU:OE1 | 16:P:49:GLY:N | 2.44 | 0.51 |
| 1:A:204:G:C2 | 1:A:465:A:C5 | 2.99 | 0.51 |
| 1:A:468:A:N1 | 1:A:469:C:N4 | 2.58 | 0.51 |
| 1:A:408:A:C2 | 1:A:435:A:N3 | 2.79 | 0.51 |
| 1:A:1124:G:OP1 | 10:J:37:ARG:C | 2.48 | 0.51 |
| 1:A:421:U:C6 | 1:A:421:U:C3' | 2.94 | 0.51 |
| 5:E:112:ALA:O | 5:E:113:VAL:C | 2.49 | 0.51 |
| 1:A:736:C:OP1 | 18:R:60:ARG:NH1 | 2.44 | 0.51 |
| 1:A:1284:C:C6 | 1:A:1285:A:C8 | 2.99 | 0.51 |
| 2:B:209:VAL:O | 2:B:211:LEU:N | 2.44 | 0.51 |
| 1:A:261:U:OP2 | 20:T:73:ARG:NH2 | 2.44 | 0.51 |
| 1:A:1533:C:O5' | 1:A:1533:C:H6 | 1.93 | 0.50 |
| 1:A:1152:A:C2 | 1:A:1153:G:C5 | 2.99 | 0.50 |
| 1:A:1324:A:C5 | 1:A:1325:C:C5 | 2.99 | 0.50 |
| 1:A:667:G:C4' | 15:O:50:HIS:CE1 | 2.94 | 0.50 |
| 1:A:983:A:O2' | 1:A:984:C:C5' | 2.59 | 0.50 |
| 1:A:687:A:N1 | 1:A:704:A:C5 | 2.79 | 0.50 |
| 4:D:3:TYR:CE2 | 4:D:5:GLY:O | 2.65 | 0.50 |
| 11:K:43:TRP:CE3 | 11:K:43:TRP:C | 2.85 | 0.50 |
| 3:C:152:VAL:CG2 | 3:C:152:VAL:O | 2.59 | 0.50 |
| 10:J:47:GLU:OE2 | 14:N:75:LYS:NZ | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 17:Q:73:THR:HG22 | 17:Q:74:LEU:H | 1.76 | 0.50 |
| 4:D:117:VAL:CA | 4:D:122:ILE:CD1 | 2.89 | 0.50 |
| 1:A:1494:G:C2 | 1:A:1495:U:C6 | 2.99 | 0.50 |
| 12:L:74:GLN:O | 12:L:75:GLU:C | 2.49 | 0.50 |
| 12:L:86:VAL:CG1 | 12:L:86:VAL:O | 2.59 | 0.50 |
| 17:Q:80:LYS:N | 17:Q:80:LYS:HZ2 | 2.09 | 0.50 |
| 1:A:121:U:O2' | 1:A:122:G:OP1 | 2.28 | 0.50 |
| 1:A:747:A:C5' | 1:A:748:G:OP2 | 2.59 | 0.50 |
| 1:A:9:G:C2 | 1:A:10:A:C8 | 2.99 | 0.50 |
| 17:Q:56:ASP:OD2 | 17:Q:80:LYS:HA | 2.12 | 0.50 |
| 1:A:75:G:C5 | 1:A:76:G:C8 | 2.98 | 0.50 |
| 1:A:674:G:C4' | 18:R:69:TYR:CD1 | 2.95 | 0.50 |
| 1:A:864:A:C3' | 1:A:865:A:C8 | 2.94 | 0.50 |
| 3:C:33:ASP:O | 3:C:37:LYS:CB | 2.60 | 0.50 |
| 16:P:16:PHE:C | 16:P:16:PHE:CD1 | 2.84 | 0.50 |
| 1:A:267:C:C5 | 1:A:268:U:C5 | 3.00 | 0.50 |
| 4:D:34:GLU:O | 4:D:36:ALA:N | 2.44 | 0.50 |
| 1:A:1256:A:C4 | 1:A:1258:G:C6 | 3.00 | 0.50 |
| 1:A:1091:U:O2 | 1:A:1093:A:C8 | 2.65 | 0.50 |
| 1:A:417:G:C5 | 1:A:418:C:C4 | 3.00 | 0.50 |
| 1:A:1294:G:C6 | 1:A:1295:U:C4 | 3.00 | 0.50 |
| 1:A:587:G:N2 | 1:A:755:G:C5 | 2.79 | 0.50 |
| 20:T:53:MET:CE | 20:T:57:VAL:CG2 | 2.90 | 0.50 |
| 17:Q:16:MET:HE3 | 17:Q:21:VAL:HG12 | 1.94 | 0.50 |
| 17:Q:49:ASN:ND2 | 17:Q:49:ASN:O | 2.44 | 0.50 |
| 1:A:1346:A:O4' | 1:A:1348:U:C6 | 2.63 | 0.50 |
| 1:A:875:U:O2' | 8:H:14:ARG:NH1 | 2.45 | 0.50 |
| 1:A:652:U:C4 | 1:A:752:G:N3 | 2.79 | 0.50 |
| 16:P:4:ILE:O | 16:P:68:SER:OG | 2.29 | 0.50 |
| 7:G:27:ASN:OD1 | 7:G:35:LYS:NZ | 2.44 | 0.50 |
| 1:A:1387:G:C6 | 1:A:1388:C:N4 | 2.80 | 0.50 |
| 1:A:469:C:O2' | 1:A:470:C:O4' | 2.30 | 0.50 |
| 1:A:506:G:C6 | 1:A:507:C:C4 | 3.00 | 0.50 |
| 1:A:1269:A:C2 | 1:A:1312:G:N3 | 2.80 | 0.50 |
| 19:S:64:GLU:CD | 19:S:64:GLU:N | 2.65 | 0.50 |
| 1:A:877:G:N3 | 8:H:1:SER:N | 2.59 | 0.50 |
| 1:A:1134:G:N1 | 1:A:1141:C:C4 | 2.80 | 0.50 |
| 1:A:1143:G:N3 | 1:A:1144:G:C8 | 2.80 | 0.50 |
| 1:A:1052:U:C5' | 1:A:1053:G:OP2 | 2.60 | 0.50 |
| 1:A:61:G:C2' | 1:A:62:U:C6 | 2.95 | 0.50 |
| 1:A:908:A:C2 | 1:A:909:A:C4 | 3.00 | 0.50 |
| 1:A:27:G:C5 | 1:A:557:G:C2 | 3.00 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:596:A:C6 | 1:A:645:G:C2 | 3.00 | 0.50 |
| 19:S:62:THR:CG2 | 19:S:63:ASP:N | 2.75 | 0.50 |
| 3:C:156:LEU:CD1 | 3:C:156:LEU:N | 2.75 | 0.50 |
| 17:Q:18:LYS:HB3 | 17:Q:47:ASP:HB2 | 1.93 | 0.49 |
| 17:Q:54:ILE:C | 17:Q:54:ILE:CD1 | 2.77 | 0.49 |
| 1:A:462:G:C8 | 1:A:463:U:C5 | 2.99 | 0.49 |
| 1:A:568:G:O2' | 1:A:574:A:N1 | 2.44 | 0.49 |
| 1:A:355:C:O4' | 1:A:388:G:O2' | 2.30 | 0.49 |
| 1:A:19:A:N3 | 1:A:917:G:C2 | 2.80 | 0.49 |
| 1:A:1202:U:C5 | 1:A:1203:C:C5 | 3.00 | 0.49 |
| 1:A:1453:G:O2' | 1:A:1454:G:O5' | 2.30 | 0.49 |
| 1:A:1079:G:N2 | 1:A:1080:A:C2 | 2.80 | 0.49 |
| 20:T:33:LYS:CE | 20:T:33:LYS:CA | 2.90 | 0.49 |
| 7:G:146:ALA:C | 7:G:148:LYS:N | 2.64 | 0.49 |
| 1:A:160:A:O2' | 1:A:344:A:C6 | 2.64 | 0.49 |
| 17:Q:49:ASN:O | 17:Q:50:ASN:C | 2.50 | 0.49 |
| 1:A:87:C:O2' | 1:A:88:U:O5' | 2.30 | 0.49 |
| 1:A:212:G:C2 | 1:A:213:G:C5 | 3.00 | 0.49 |
| 1:A:868:C:N4 | 1:A:869:G:C2 | 2.80 | 0.49 |
| 1:A:263:A:P | 20:T:73:ARG:NH1 | 2.85 | 0.49 |
| 11:K:85:VAL:CG1 | 11:K:92:ARG:NH1 | 2.75 | 0.49 |
| 1:A:203:G:C2 | 1:A:215:C:N3 | 2.80 | 0.49 |
| 1:A:203:G:O2' | 1:A:466:A:C2 | 2.66 | 0.49 |
| 1:A:587:G:C2 | 1:A:755:G:C6 | 3.00 | 0.49 |
| 2:B:187:ASP:OD1 | 2:B:188:THR:N | 2.45 | 0.49 |
| 9:I:8:THR:O | 9:I:81:GLY:CA | 2.61 | 0.49 |
| 2:B:22:TRP:CD1 | 2:B:22:TRP:O | 2.65 | 0.49 |
| 11:K:109:ILE:CG2 | 21:U:16:ARG:NE | 2.75 | 0.49 |
| 2:B:49:PHE:CD1 | 2:B:49:PHE:C | 2.86 | 0.49 |
| 12:L:23:LEU:O | 12:L:25:ALA:N | 2.46 | 0.49 |
| 1:A:1055:A:C6 | 1:A:1206:G:C5 | 3.00 | 0.49 |
| 5:E:103:GLY:O | 5:E:104:ILE:CG2 | 2.60 | 0.49 |
| 1:A:55:A:C5 | 1:A:56:U:C5 | 2.99 | 0.49 |
| 1:A:1101:A:N7 | 2:B:170:ILE:CG2 | 2.76 | 0.49 |
| 1:A:262:A:C6 | 1:A:263:A:C6 | 3.00 | 0.49 |
| 1:A:958:A:C6 | 1:A:959:A:N1 | 2.80 | 0.49 |
| 1:A:8:A:N6 | 4:D:201:GLU:O | 2.45 | 0.49 |
| 17:Q:16:MET:CG | 17:Q:20:ILE:HD13 | 2.42 | 0.49 |
| 1:A:1157:A:C6 | 1:A:1180:A:C6 | 3.00 | 0.49 |
| 1:A:1162:C:C2' | 1:A:1163:A:C8 | 2.96 | 0.49 |
| 1:A:77:A:N6 | 1:A:90:C:C4 | 2.80 | 0.49 |
| 1:A:499:A:O2' | 1:A:500:G:C8 | 2.66 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:415:A:C2' | 1:A:416:G:C8 | 2.95 | 0.49 |
| 1:A:684:U:C1' | 11:K:39:ASN:O | 2.60 | 0.49 |
| 1:A:148:G:N2 | 1:A:175:C:O2 | 2.46 | 0.49 |
| 10:J:80:THR:O | 10:J:82:LYS:N | 2.45 | 0.49 |
| 1:A:983:A:N3 | 1:A:983:A:C2' | 2.75 | 0.49 |
| 8:H:82:LEU:CD1 | 8:H:84:ILE:CD1 | 2.90 | 0.49 |
| 1:A:562:U:C4 | 1:A:884:U:C6 | 3.01 | 0.49 |
| 1:A:855:U:OP2 | 1:A:871:U:N3 | 2.46 | 0.49 |
| 11:K:125:LYS:C | 21:U:33:ARG:NH1 | 2.66 | 0.49 |
| 11:K:125:LYS:C | 21:U:33:ARG:NH2 | 2.66 | 0.49 |
| 1:A:914:A:C2 | 1:A:915:A:C8 | 3.01 | 0.49 |
| 20:T:56:ILE:CG2 | 20:T:57:VAL:N | 2.76 | 0.49 |
| 1:A:1264:U:O2 | 1:A:1272:G:C2 | 2.65 | 0.49 |
| 1:A:1098:C:C2 | 1:A:1099:G:C8 | 3.00 | 0.49 |
| 1:A:1127:G:C2' | 1:A:1128:C:C5' | 2.91 | 0.49 |
| 8:H:48:PHE:N | 8:H:48:PHE:CD1 | 2.81 | 0.49 |
| 1:A:1319:A:C8 | 1:A:1323:G:C5 | 3.00 | 0.49 |
| 1:A:545:C:C5' | 4:D:68:GLU:CG | 2.91 | 0.49 |
| 1:A:198:G:N3 | 1:A:199:A:C8 | 2.81 | 0.49 |
| 4:D:172:VAL:O | 4:D:173:ASP:CB | 2.60 | 0.49 |
| 1:A:1077:G:N1 | 1:A:1081:A:C6 | 2.80 | 0.49 |
| 17:Q:54:ILE:HG12 | 17:Q:55:GLY:N | 2.28 | 0.49 |
| 1:A:469:C:C2' | 1:A:470:C:C6 | 2.96 | 0.49 |
| 1:A:563:A:N3 | 1:A:563:A:C2' | 2.75 | 0.49 |
| 1:A:984:C:O2' | 1:A:985:C:C5' | 2.61 | 0.49 |
| 4:D:47:LEU:CD2 | 4:D:52:VAL:CG1 | 2.91 | 0.49 |
| 9:I:88:GLU:CG | 9:I:89:TYR:N | 2.76 | 0.49 |
| 6:F:41:ASP:OD2 | 6:F:58:HIS:NE2 | 2.45 | 0.49 |
| 1:A:1288:A:C6 | 1:A:1289:A:C5 | 3.01 | 0.49 |
| 7:G:83:THR:O | 7:G:84:TYR:C | 2.50 | 0.49 |
| 1:A:461:A:C3' | 1:A:461:A:N3 | 2.76 | 0.49 |
| 1:A:849:G:C6 | 1:A:850:U:C4 | 3.00 | 0.49 |
| 3:C:139:ASN:C | 3:C:139:ASN:ND2 | 2.66 | 0.49 |
| 9:I:9:GLY:CA | 9:I:80:HIS:CD2 | 2.96 | 0.49 |
| 1:A:131:A:O2' | 1:A:132:C:O4' | 2.31 | 0.49 |
| 1:A:429:U:C1' | 1:A:430:A:C5' | 2.91 | 0.48 |
| 1:A:75:G:C2 | 1:A:96:U:N3 | 2.81 | 0.48 |
| 1:A:701:U:O2 | 1:A:701:U:C2' | 2.61 | 0.48 |
| 1:A:210:C:C4' | 1:A:211:G:N2 | 2.76 | 0.48 |
| 1:A:567:G:O2' | 1:A:568:G:O5' | 2.31 | 0.48 |
| 1:A:596:A:N3 | 1:A:597:G:C8 | 2.80 | 0.48 |
| 1:A:1108:G:C5 | 1:A:1109:C:C6 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 6:F:7:VAL:CG2 | 6:F:7:VAL:O | 2.61 | 0.48 |
| 4:D:36:ALA:C | 4:D:38:GLY:N | 2.66 | 0.48 |
| 1:A:1128:C:O2' | 1:A:1129:C:C5' | 2.60 | 0.48 |
| 1:A:1157:A:N7 | 1:A:1180:A:C6 | 2.81 | 0.48 |
| 1:A:1157:A:N7 | 1:A:1180:A:N6 | 2.61 | 0.48 |
| 1:A:1501:C:N3 | 1:A:1504:G:C6 | 2.81 | 0.48 |
| 1:A:1429:A:C2 | 1:A:1472:U:N3 | 2.81 | 0.48 |
| 1:A:1421:G:C2 | 1:A:1422:G:C8 | 3.01 | 0.48 |
| 2:B:67:LEU:CD2 | 2:B:91:VAL:CG2 | 2.91 | 0.48 |
| 5:E:44:ARG:CA | 5:E:71:ILE:O | 2.61 | 0.48 |
| 5:E:139:THR:O | 5:E:140:ILE:C | 2.50 | 0.48 |
| 17:Q:13:SER:O | 17:Q:16:MET:SD | 2.71 | 0.48 |
| 6:F:86:ARG:CZ | 18:R:63:TYR:CB | 2.91 | 0.48 |
| 4:D:2:ARG:CZ | 4:D:114:ARG:CD | 2.91 | 0.48 |
| 15:O:63:ARG:NH1 | 15:O:87:ARG:NH2 | 2.61 | 0.48 |
| 1:A:1494:G:N3 | 1:A:1495:U:C6 | 2.82 | 0.48 |
| 1:A:1234:C:C2' | 1:A:1235:U:C5' | 2.90 | 0.48 |
| 5:E:14:LEU:CD1 | 5:E:14:LEU:O | 2.61 | 0.48 |
| 1:A:182:A:O2' | 1:A:184:G:N7 | 2.46 | 0.48 |
| 1:A:452:A:N6 | 1:A:480:U:C2 | 2.81 | 0.48 |
| 1:A:44:A:C2 | 1:A:399:G:C2 | 3.02 | 0.48 |
| 1:A:11:G:C6 | 1:A:12:U:C4 | 3.01 | 0.48 |
| 8:H:1:SER:O | 8:H:3:GLN:N | 2.46 | 0.48 |
| 1:A:586:C:O2' | 8:H:3:GLN:NE2 | 2.46 | 0.48 |
| 3:C:144:GLY:O | 3:C:145:ALA:CB | 2.60 | 0.48 |
| 17:Q:82:VAL:HG22 | 17:Q:82:VAL:OXT | 2.13 | 0.48 |
| 1:A:1258:G:O2' | 1:A:1259:C:C5' | 2.62 | 0.48 |
| 4:D:133:SER:O | 4:D:134:TYR:C | 2.49 | 0.48 |
| 1:A:1191:A:C2 | 1:A:1192:C:C4 | 3.01 | 0.48 |
| 14:N:29:ILE:CG2 | 14:N:34:ASN:ND2 | 2.77 | 0.48 |
| 1:A:819:A:N7 | 1:A:1529:G:C2 | 2.81 | 0.48 |
| 1:A:1016:A:C8 | 1:A:1017:U:C1' | 2.97 | 0.48 |
| 16:P:23:ASP:O | 16:P:24:SER:C | 2.51 | 0.48 |
| 14:N:44:VAL:CG2 | 14:N:45:LEU:N | 2.75 | 0.48 |
| 4:D:89:LEU:CD2 | 4:D:199:ILE:CD1 | 2.92 | 0.48 |
| 10:J:53:ILE:CG1 | 14:N:84:ARG:CZ | 2.91 | 0.48 |
| 5:E:152:VAL:CB | 5:E:155:LYS:NZ | 2.41 | 0.48 |
| 1:A:1150:A:O2' | 10:J:42:LEU:C | 2.51 | 0.48 |
| 1:A:1151:A:N6 | 1:A:1152:A:N6 | 2.61 | 0.48 |
| 6:F:86:ARG:CD | 18:R:63:TYR:O | 2.62 | 0.48 |
| 1:A:542:G:N3 | 1:A:543:U:C5 | 2.81 | 0.48 |
| 7:G:83:THR:O | 7:G:85:GLN:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:410:G:OP2 | 4:D:21:LYS:CE | 2.61 | 0.48 |
| 20:T:66:ILE:O | 20:T:67:HIS:O | 2.32 | 0.48 |
| 10:J:33:GLY:O | 10:J:34:ALA:CB | 2.61 | 0.48 |
| 17:Q:15:LYS:HD2 | 17:Q:16:MET:N | 2.28 | 0.48 |
| 11:K:125:LYS:O | 21:U:33:ARG:NH1 | 2.46 | 0.48 |
| 1:A:1157:A:C1' | 1:A:1181:G:C2 | 2.97 | 0.48 |
| 11:K:109:ILE:O | 11:K:110:THR:CG2 | 2.61 | 0.48 |
| 1:A:1317:C:C3' | 1:A:1317:C:C6 | 2.97 | 0.48 |
| 1:A:1322:C:O2' | 1:A:1323:G:C5' | 2.61 | 0.48 |
| 1:A:500:G:C4 | 1:A:501:C:C5 | 3.01 | 0.48 |
| 1:A:515:G:N1 | 1:A:537:G:C6 | 2.82 | 0.48 |
| 1:A:1387:G:C4 | 1:A:1388:C:C5 | 3.02 | 0.48 |
| 10:J:63:ASP:OD2 | 14:N:97:LYS:NZ | 2.47 | 0.48 |
| 1:A:137:U:C2' | 1:A:137:U:O2 | 2.60 | 0.48 |
| 1:A:92:U:C2' | 1:A:93:U:C6 | 2.96 | 0.48 |
| 1:A:903:G:C4 | 1:A:904:U:C6 | 3.02 | 0.48 |
| 1:A:480:U:C5' | 1:A:481:G:OP2 | 2.62 | 0.48 |
| 1:A:192:A:C6 | 1:A:193:C:C4 | 3.02 | 0.48 |
| 8:H:1:SER:C | 8:H:3:GLN:N | 2.66 | 0.48 |
| 1:A:765:G:N1 | 1:A:812:G:O2' | 2.46 | 0.48 |
| 3:C:154:GLY:O | 3:C:195:ILE:CG1 | 2.61 | 0.48 |
| 5:E:94:PHE:O | 5:E:94:PHE:CD1 | 2.67 | 0.48 |
| 8:H:76:ARG:NE | 8:H:78:SER:O | 2.47 | 0.48 |
| 1:A:792:A:N3 | 1:A:794:A:C5 | 2.82 | 0.48 |
| 1:A:466:A:O2' | 1:A:467:U:C5 | 2.67 | 0.48 |
| 1:A:1141:C:O2 | 1:A:1142:G:C8 | 2.67 | 0.48 |
| 2:B:56:LEU:CD1 | 2:B:220:VAL:CG2 | 2.91 | 0.48 |
| 1:A:977:A:C3' | 1:A:1362:A:N6 | 2.76 | 0.48 |
| 1:A:687:A:C6 | 1:A:704:A:N7 | 2.82 | 0.48 |
| 1:A:752:G:O2' | 1:A:753:A:P | 2.71 | 0.48 |
| 20:T:18:LYS:O | 20:T:19:HIS:C | 2.52 | 0.48 |
| 19:S:30:LEU:O | 19:S:49:ALA:CB | 2.61 | 0.48 |
| 3:C:174:LEU:O | 3:C:174:LEU:CD1 | 2.62 | 0.48 |
| 1:A:429:U:C4' | 1:A:430:A:O5' | 2.62 | 0.47 |
| 1:A:1152:A:O2' | 1:A:1153:G:C5' | 2.62 | 0.47 |
| 1:A:338:A:C6 | 1:A:351:G:O6 | 2.66 | 0.47 |
| 1:A:520:A:C2 | 1:A:536:C:O2 | 2.67 | 0.47 |
| 1:A:619:U:O2 | 4:D:130:ASN:N | 2.47 | 0.47 |
| 1:A:1501:C:C4 | 1:A:1504:G:C5 | 3.02 | 0.47 |
| 2:B:9:LEU:CD2 | 2:B:11:ALA:CB | 2.92 | 0.47 |
| 1:A:292:G:N2 | 1:A:309:A:C4 | 2.82 | 0.47 |
| 16:P:16:PHE:O | 16:P:16:PHE:CD1 | 2.67 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:889:A:N6 | 1:A:908:A:OP2 | 2.47 | 0.47 |
| 13:M:106:ARG:NH2 | 13:M:112:ARG:CB | 2.77 | 0.47 |
| 1:A:1299:A:C2' | 1:A:1299:A:N3 | 2.77 | 0.47 |
| 1:A:374:A:OP1 | 1:A:452:A:N1 | 2.47 | 0.47 |
| 19:S:79:TYR:O | 19:S:80:ARG:CB | 2.61 | 0.47 |
| 7:G:121:ASN:O | 7:G:125:ASP:CB | 2.62 | 0.47 |
| 11:K:28:ASN:OD1 | 11:K:29:THR:N | 2.47 | 0.47 |
| 1:A:792:A:C4' | 1:A:793:U:O5' | 2.62 | 0.47 |
| 1:A:1203:C:O2' | 1:A:1204:A:O4' | 2.33 | 0.47 |
| 1:A:1258:G:C4 | 1:A:1259:C:C5 | 3.02 | 0.47 |
| 1:A:468:A:N3 | 1:A:469:C:C5 | 2.83 | 0.47 |
| 20:T:35:TYR:CG | 20:T:36:ALA:N | 2.83 | 0.47 |
| 1:A:66:A:N3 | 1:A:66:A:C2' | 2.76 | 0.47 |
| 10:J:18:ILE:CG2 | 10:J:19:ASP:N | 2.77 | 0.47 |
| 1:A:125:U:C2' | 1:A:126:G:C5' | 2.92 | 0.47 |
| 9:I:65:THR:CG2 | 9:I:66:VAL:N | 2.76 | 0.47 |
| 1:A:716:A:C6 | 1:A:717:U:N3 | 2.82 | 0.47 |
| 7:G:26:VAL:CG1 | 7:G:42:VAL:CG2 | 2.93 | 0.47 |
| 21:U:13:VAL:CG1 | 21:U:15:LEU:CG | 2.91 | 0.47 |
| 3:C:54:ILE:CD1 | 3:C:54:ILE:C | 2.82 | 0.47 |
| 1:A:15:G:C4 | 1:A:16:A:C8 | 3.03 | 0.47 |
| 1:A:257:G:C2' | 1:A:258:G:O5' | 2.62 | 0.47 |
| 20:T:43:LYS:CB | 20:T:86:ALA:CB | 2.92 | 0.47 |
| 7:G:23:ALA:O | 7:G:26:VAL:CG2 | 2.62 | 0.47 |
| 1:A:1328:C:C4 | 1:A:1329:A:N7 | 2.83 | 0.47 |
| 10:J:28:THR:CG2 | 10:J:28:THR:O | 2.62 | 0.47 |
| 17:Q:27:PHE:HA | 17:Q:37:ILE:O | 2.15 | 0.47 |
| 1:A:1130:A:C5 | 1:A:1146:A:C6 | 3.03 | 0.47 |
| 1:A:1152:A:N3 | 1:A:1153:G:C8 | 2.83 | 0.47 |
| 1:A:16:A:O2' | 1:A:17:U:C5' | 2.62 | 0.47 |
| 16:P:11:ALA:O | 16:P:12:LYS:C | 2.53 | 0.47 |
| 1:A:653:U:O2' | 1:A:654:G:C5' | 2.62 | 0.47 |
| 3:C:10:ARG:O | 3:C:13:ILE:O | 2.32 | 0.47 |
| 1:A:1058:G:C5 | 1:A:1059:C:C5 | 3.02 | 0.47 |
| 4:D:1:ALA:O | 4:D:67:LEU:CD1 | 2.63 | 0.47 |
| 9:I:21:LYS:O | 9:I:61:ASP:N | 2.47 | 0.47 |
| 10:J:49:PHE:CE1 | 14:N:76:PHE:CZ | 3.02 | 0.47 |
| 1:A:274:A:O2' | 1:A:275:G:O5' | 2.32 | 0.47 |
| 10:J:48:ARG:NH1 | 10:J:66:GLU:OE1 | 2.48 | 0.47 |
| 1:A:1053:G:C6 | 1:A:1199:U:C2 | 3.03 | 0.47 |
| 1:A:982:U:C2 | 1:A:983:A:N1 | 2.82 | 0.47 |
| 1:A:1430:A:C2 | 1:A:1471:U:C2 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 20:T:14:GLU:OE2 | 20:T:17:ARG:NE | 2.47 | 0.47 |
| 3:C:31:ASN:O | 3:C:35:ASP:N | 2.48 | 0.47 |
| 12:L:4:ASN:ND2 | 12:L:8:ARG:NH1 | 2.62 | 0.47 |
| 1:A:827:U:N3 | 1:A:870:U:C2 | 2.82 | 0.47 |
| 17:Q:51:GLU:O | 17:Q:52:CYS:O | 2.32 | 0.47 |
| 1:A:159:G:N2 | 1:A:162:A:OP2 | 2.48 | 0.47 |
| 4:D:13:ARG:CG | 4:D:55:ARG:NH2 | 2.78 | 0.47 |
| 1:A:545:C:C2' | 1:A:545:C:O2 | 2.62 | 0.47 |
| 4:D:56:GLU:OE2 | 4:D:195:ASN:N | 2.48 | 0.47 |
| 6:F:46:GLN:NE2 | 6:F:56:LYS:CG | 2.78 | 0.47 |
| 9:I:49:GLN:O | 9:I:51:LEU:N | 2.47 | 0.47 |
| 1:A:152:A:C8 | 1:A:153:C:C5 | 3.02 | 0.47 |
| 20:T:27:MET:CE | 20:T:57:VAL:CG2 | 2.93 | 0.47 |
| 20:T:57:VAL:CG1 | 20:T:71:ALA:CB | 2.93 | 0.47 |
| 1:A:1077:G:N2 | 1:A:1081:A:C4 | 2.83 | 0.47 |
| 1:A:951:G:N3 | 1:A:970:C:O2' | 2.48 | 0.47 |
| 1:A:201:G:N2 | 1:A:217:C:O2 | 2.47 | 0.47 |
| 1:A:1028:C:C2 | 1:A:1034:G:C4 | 3.03 | 0.47 |
| 1:A:1371:G:C5 | 1:A:1372:U:C4 | 3.03 | 0.47 |
| 1:A:1162:C:O2' | 1:A:1163:A:C5' | 2.63 | 0.47 |
| 1:A:1053:G:O2' | 1:A:1054:C:P | 2.73 | 0.47 |
| 1:A:1013:G:N2 | 1:A:1016:A:OP2 | 2.47 | 0.47 |
| 1:A:441:A:C2 | 1:A:497:G:C6 | 3.03 | 0.47 |
| 7:G:128:GLU:O | 7:G:129:ASN:C | 2.53 | 0.47 |
| 1:A:1521:C:C2' | 1:A:1522:U:O5' | 2.62 | 0.47 |
| 1:A:1161:C:O2' | 1:A:1162:C:C5' | 2.63 | 0.47 |
| 2:B:72:LYS:O | 2:B:74:ALA:N | 2.48 | 0.47 |
| 1:A:255:G:C5 | 1:A:256:U:C5 | 3.03 | 0.47 |
| 1:A:1454:G:N2 | 1:A:1455:G:C4 | 2.82 | 0.47 |
| 1:A:86:G:C2 | 1:A:87:C:N4 | 2.82 | 0.47 |
| 1:A:596:A:N6 | 1:A:645:G:N1 | 2.62 | 0.47 |
| 9:I:27:ILE:CD1 | 9:I:27:ILE:N | 2.77 | 0.47 |
| 1:A:1151:A:O2' | 1:A:1152:A:C8 | 2.68 | 0.47 |
| 21:U:9:GLU:CB | 21:U:10:PRO:CD | 2.92 | 0.47 |
| 14:N:42:ASN:O | 14:N:44:VAL:N | 2.48 | 0.47 |
| 9:I:89:TYR:O | 9:I:90:ASP:CB | 2.63 | 0.47 |
| 1:A:1126:U:C6 | 1:A:1281:C:N3 | 2.83 | 0.47 |
| 1:A:224:U:C2 | 1:A:225:C:C5 | 3.03 | 0.47 |
| 17:Q:80:LYS:CD | 17:Q:80:LYS:N | 2.78 | 0.46 |
| 1:A:184:G:N3 | 1:A:185:U:C5 | 2.82 | 0.46 |
| 1:A:1159:U:N3 | 1:A:1182:G:C4 | 2.83 | 0.46 |
| 1:A:373:A:O2' | 1:A:374:A:C5' | 2.62 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1508:A:O2' | 1:A:1509:C:C5' | 2.63 | 0.46 |
| 1:A:607:A:C6 | 1:A:608:A:C6 | 3.03 | 0.46 |
| 7:G:96:ASN:N | 7:G:96:ASN:OD1 | 2.48 | 0.46 |
| 1:A:791:G:C6 | 1:A:792:A:N7 | 2.84 | 0.46 |
| 1:A:1169:A:C2 | 1:A:1170:A:C4 | 3.03 | 0.46 |
| 1:A:197:A:O2' | 1:A:198:G:O4' | 2.34 | 0.46 |
| 1:A:1429:A:N1 | 1:A:1472:U:C4 | 2.83 | 0.46 |
| 1:A:1124:G:C3' | 1:A:1145:A:N6 | 2.77 | 0.46 |
| 1:A:1007:U:C2' | 1:A:1008:U:C5' | 2.93 | 0.46 |
| 3:C:59:PRO:O | 3:C:60:ALA:C | 2.54 | 0.46 |
| 11:K:109:ILE:O | 21:U:5:VAL:N | 2.49 | 0.46 |
| 19:S:33:TRP:O | 19:S:35:ARG:N | 2.48 | 0.46 |
| 1:A:1080:A:OP1 | 5:E:51:LYS:CE | 2.64 | 0.46 |
| 1:A:62:U:O3' | 1:A:384:G:N2 | 2.49 | 0.46 |
| 6:F:38:ARG:CG | 6:F:39:LEU:N | 2.77 | 0.46 |
| 18:R:44:THR:OG1 | 18:R:46:THR:CG2 | 2.63 | 0.46 |
| 1:A:551:U:C2' | 1:A:552:U:O5' | 2.63 | 0.46 |
| 1:A:1024:G:C5 | 1:A:1025:U:C5 | 3.04 | 0.46 |
| 1:A:49:U:C4 | 1:A:364:A:C6 | 3.04 | 0.46 |
| 11:K:126:ARG:CA | 21:U:33:ARG:NH1 | 2.78 | 0.46 |
| 1:A:978:A:O4' | 1:A:1322:C:C6 | 2.68 | 0.46 |
| 19:S:80:ARG:CG | 19:S:80:ARG:O | 2.63 | 0.46 |
| 4:D:147:LYS:O | 4:D:149:LYS:N | 2.48 | 0.46 |
| 7:G:144:ALA:O | 7:G:146:ALA:N | 2.48 | 0.46 |
| 20:T:73:ARG:O | 20:T:77:ASN:ND2 | 2.49 | 0.46 |
| 16:P:7:ALA:O | 16:P:9:HIS:CD2 | 2.68 | 0.46 |
| 14:N:86:ALA:O | 14:N:91:GLU:CB | 2.63 | 0.46 |
| 1:A:555:U:C2' | 1:A:556:C:O5' | 2.64 | 0.46 |
| 6:F:71:ILE:CG2 | 6:F:72:ASP:N | 2.78 | 0.46 |
| 5:E:155:LYS:CA | 5:E:158:LYS:NZ | 2.55 | 0.46 |
| 17:Q:65:PRO:C | 17:Q:66:LEU:HD23 | 2.36 | 0.46 |
| 1:A:1180:A:C5' | 1:A:1181:G:OP2 | 2.63 | 0.46 |
| 1:A:204:G:N3 | 1:A:465:A:C2 | 2.84 | 0.46 |
| 1:A:198:G:O6 | 1:A:220:G:C6 | 2.69 | 0.46 |
| 1:A:957:U:O2 | 1:A:959:A:C8 | 2.69 | 0.46 |
| 1:A:1328:C:C2 | 1:A:1329:A:C8 | 3.04 | 0.46 |
| 4:D:168:THR:CG2 | 4:D:183:ARG:NH2 | 2.79 | 0.46 |
| 2:B:118:THR:O | 2:B:119:GLN:CB | 2.64 | 0.46 |
| 12:L:71:HIS:C | 12:L:71:HIS:ND1 | 2.68 | 0.46 |
| 1:A:791:G:C5 | 1:A:792:A:N7 | 2.84 | 0.46 |
| 1:A:1129:C:O2' | 1:A:1130:A:N7 | 2.49 | 0.46 |
| 1:A:537:G:OP1 | 12:L:109:ARG:NH1 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:1131:G:O2' | 1:A:1132:C:O5' | 2.34 | 0.46 |
| 1:A:372:C:C4' | 1:A:373:A:OP1 | 2.64 | 0.46 |
| 1:A:1088:G:O2' | 1:A:1089:G:O5' | 2.34 | 0.46 |
| 1:A:1533:C:C3' | 1:A:1534:A:C5' | 2.85 | 0.46 |
| 1:A:1157:A:N3 | 1:A:1181:G:C4 | 2.83 | 0.46 |
| 2:B:72:LYS:C | 2:B:74:ALA:N | 2.69 | 0.46 |
| 1:A:1144:G:OP2 | 1:A:1144:G:C8 | 2.69 | 0.46 |
| 1:A:414:A:O2' | 1:A:415:A:O4' | 2.34 | 0.46 |
| 1:A:619:U:N3 | 4:D:130:ASN:CB | 2.79 | 0.46 |
| 1:A:1502:A:N6 | 1:A:1504:G:N2 | 2.64 | 0.46 |
| 2:B:166:ASP:OD1 | 2:B:167:HIS:N | 2.48 | 0.46 |
| 4:D:138:PRO:O | 4:D:139:ASN:CB | 2.64 | 0.46 |
| 1:A:1003:G:N2 | 1:A:1005:A:C5' | 2.79 | 0.46 |
| 5:E:152:VAL:O | 5:E:155:LYS:HE3 | 2.16 | 0.46 |
| 1:A:1501:C:C4 | 1:A:1504:G:C6 | 3.03 | 0.46 |
| 1:A:39:G:C5 | 1:A:40:C:C5 | 3.03 | 0.46 |
| 2:B:162:VAL:CG2 | 2:B:184:ALA:CB | 2.94 | 0.46 |
| 14:N:64:ARG:CB | 14:N:77:GLY:O | 2.64 | 0.46 |
| 17:Q:16:MET:CB | 17:Q:19:SER:HB3 | 2.23 | 0.46 |
| 1:A:1138:G:N2 | 1:A:1140:C:N4 | 2.64 | 0.46 |
| 1:A:517:G:C5' | 1:A:519:C:C2 | 2.99 | 0.46 |
| 2:B:185:ILE:CG1 | 2:B:185:ILE:O | 2.64 | 0.46 |
| 2:B:17:HIS:NE2 | 2:B:202:ASN:ND2 | 2.64 | 0.46 |
| 4:D:117:VAL:N | 4:D:122:ILE:CD1 | 2.79 | 0.46 |
| 1:A:292:G:N3 | 1:A:309:A:C2 | 2.84 | 0.46 |
| 1:A:113:G:C4 | 1:A:114:U:C5 | 3.03 | 0.46 |
| 5:E:153:ALA:C | 5:E:155:LYS:N | 2.66 | 0.46 |
| 1:A:1202:U:O4' | 14:N:68:ARG:CD | 2.63 | 0.46 |
| 4:D:16:THR:CG2 | 4:D:17:ASP:O | 2.64 | 0.46 |
| 5:E:82:HIS:NE2 | 8:H:95:MET:CE | 2.79 | 0.46 |
| 7:G:30:MET:CG | 7:G:31:VAL:N | 2.79 | 0.46 |
| 4:D:88:ASN:O | 4:D:92:LEU:N | 2.49 | 0.46 |
| 2:B:101:THR:N | 2:B:174:GLU:OE1 | 2.48 | 0.46 |
| 1:A:293:G:C4 | 1:A:294:U:C5 | 3.04 | 0.46 |
| 8:H:75:GLN:CA | 8:H:75:GLN:OE1 | 2.64 | 0.46 |
| 1:A:426:U:O2' | 1:A:427:U:C5' | 2.64 | 0.45 |
| 4:D:33:ILE:CG2 | 4:D:33:ILE:O | 2.63 | 0.45 |
| 1:A:1162:C:N3 | 1:A:1175:G:C2 | 2.84 | 0.45 |
| 1:A:66:A:N6 | 1:A:104:G:C4 | 2.84 | 0.45 |
| 1:A:827:U:C4 | 1:A:870:U:C2 | 3.03 | 0.45 |
| 1:A:67:C:O2' | 1:A:171:A:N3 | 2.49 | 0.45 |
| 19:S:4:LEU:CD2 | 19:S:9:PHE:N | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 7:G:110:ARG:CG | 7:G:111:GLY:N | 2.79 | 0.45 |
| 2:B:58:LYS:NZ | 2:B:62:ARG:CG | 2.79 | 0.45 |
| 5:E:11:GLN:CA | 5:E:11:GLN:NE2 | 2.79 | 0.45 |
| 1:A:1125:U:C5 | 1:A:1127:G:C5 | 3.03 | 0.45 |
| 4:D:54:LEU:CD2 | 4:D:55:ARG:N | 2.79 | 0.45 |
| 1:A:203:G:N2 | 1:A:215:C:C2 | 2.84 | 0.45 |
| 1:A:468:A:C2 | 1:A:469:C:C4 | 3.03 | 0.45 |
| 10:J:52:LEU:CD2 | 10:J:62:ARG:NE | 2.79 | 0.45 |
| 12:L:115:LYS:O | 12:L:116:TYR:CB | 2.64 | 0.45 |
| 4:D:172:VAL:CG2 | 4:D:173:ASP:N | 2.79 | 0.45 |
| 1:A:671:G:N2 | 1:A:736:C:C2 | 2.85 | 0.45 |
| 1:A:596:A:C8 | 1:A:596:A:C5' | 2.99 | 0.45 |
| 1:A:1014:A:C5' | 19:S:13:HIS:CD2 | 2.99 | 0.45 |
| 2:B:153:MET:O | 2:B:155:GLY:N | 2.49 | 0.45 |
| 1:A:814:A:P | 23:A:1634:HOH:O | 2.74 | 0.45 |
| 1:A:1202:U:O2' | 1:A:1203:C:O5' | 2.34 | 0.45 |
| 1:A:1256:A:C1' | 1:A:1258:G:C6 | 2.99 | 0.45 |
| 1:A:923:A:C6 | 1:A:924:C:C4 | 3.04 | 0.45 |
| 1:A:451:A:C2 | 1:A:480:U:C5 | 3.04 | 0.45 |
| 1:A:1079:G:C2 | 1:A:1080:A:C6 | 3.05 | 0.45 |
| 1:A:211:G:N1 | 1:A:212:G:N3 | 2.65 | 0.45 |
| 16:P:19:VAL:CG2 | 16:P:36:VAL:CG1 | 2.94 | 0.45 |
| 1:A:863:U:O2 | 1:A:867:G:C2 | 2.69 | 0.45 |
| 19:S:48:ILE:CD1 | 19:S:48:ILE:O | 2.65 | 0.45 |
| 19:S:47:THR:O | 19:S:48:ILE:C | 2.54 | 0.45 |
| 9:I:29:ILE:O | 9:I:30:ASN:C | 2.55 | 0.45 |
| 1:A:202:G:O2' | 1:A:468:A:C8 | 2.70 | 0.45 |
| 1:A:511:C:C2 | 1:A:512:U:C5 | 3.04 | 0.45 |
| 1:A:982:U:O2 | 1:A:983:A:N1 | 2.50 | 0.45 |
| 1:A:321:A:N7 | 1:A:328:C:O2' | 2.49 | 0.45 |
| 20:T:14:GLU:O | 20:T:15:LYS:C | 2.55 | 0.45 |
| 4:D:88:ASN:N | 4:D:88:ASN:OD1 | 2.49 | 0.45 |
| 1:A:622:A:C8 | 1:A:623:C:C6 | 3.04 | 0.45 |
| 1:A:484:G:O2' | 1:A:485:U:OP2 | 2.34 | 0.45 |
| 13:M:22:TYR:O | 13:M:22:TYR:CD2 | 2.70 | 0.45 |
| 1:A:1027:C:C6 | 1:A:1027:C:O5' | 2.70 | 0.45 |
| 17:Q:47:ASP:O | 17:Q:48:GLU:C | 2.55 | 0.45 |
| 1:A:1181:G:C2 | 1:A:1182:G:N2 | 2.84 | 0.45 |
| 1:A:978:A:C1' | 1:A:1322:C:C5 | 3.00 | 0.45 |
| 1:A:496:A:O2' | 1:A:497:G:C8 | 2.70 | 0.45 |
| 1:A:1511:G:C5 | 1:A:1512:U:C5 | 3.05 | 0.45 |
| 7:G:25:PHE:CE1 | 7:G:104:VAL:CG2 | 3.00 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 8:H:40:LYS:O | 8:H:42:GLU:N | 2.50 | 0.45 |
| 1:A:373:A:N1 | 1:A:391:G:O2' | 2.50 | 0.45 |
| 1:A:63:C:P | 1:A:384:G:N2 | 2.90 | 0.45 |
| 13:M:15:VAL:CA | 13:M:33:LEU:CD1 | 2.94 | 0.45 |
| 12:L:35:ARG:CB | 12:L:37:TYR:CE1 | 2.99 | 0.45 |
| 10:J:91:ASP:N | 10:J:91:ASP:OD1 | 2.49 | 0.45 |
| 17:Q:67:SER:O | 17:Q:68:LYS:C | 2.55 | 0.45 |
| 1:A:1202:U:C6 | 1:A:1203:C:C5 | 3.04 | 0.45 |
| 1:A:32:A:C2 | 1:A:33:A:C5 | 3.04 | 0.45 |
| 1:A:173:U:C2 | 1:A:197:A:N1 | 2.84 | 0.45 |
| 1:A:1064:G:O4' | 1:A:1066:C:C6 | 2.69 | 0.45 |
| 8:H:4:ASP:OD2 | 8:H:76:ARG:NH1 | 2.50 | 0.45 |
| 3:C:71:ARG:N | 3:C:72:PRO:CD | 2.80 | 0.45 |
| 16:P:74:LEU:O | 16:P:78:VAL:N | 2.50 | 0.45 |
| 1:A:522:C:OP2 | 12:L:65:TYR:OH | 2.35 | 0.45 |
| 1:A:1532:U:O2 | 1:A:1534:A:H8 | 1.99 | 0.45 |
| 17:Q:13:SER:HB3 | 17:Q:16:MET:HE1 | 1.98 | 0.45 |
| 17:Q:45:VAL:HA | 17:Q:72:TRP:O | 2.17 | 0.45 |
| 1:A:429:U:O3' | 4:D:8:LEU:CD2 | 2.65 | 0.45 |
| 1:A:444:G:O6 | 1:A:490:C:N4 | 2.50 | 0.45 |
| 1:A:1091:U:C2 | 1:A:1095:U:C4 | 3.05 | 0.45 |
| 1:A:1197:A:OP2 | 23:A:1656:HOH:O | 2.21 | 0.45 |
| 1:A:215:C:O2 | 1:A:465:A:N6 | 2.50 | 0.45 |
| 12:L:24:GLU:OE1 | 12:L:29:LYS:NZ | 2.50 | 0.45 |
| 7:G:119:LEU:O | 7:G:122:GLU:N | 2.50 | 0.45 |
| 1:A:689:C:OP1 | 11:K:45:THR:OG1 | 2.35 | 0.45 |
| 21:U:24:LYS:O | 21:U:26:GLY:N | 2.50 | 0.45 |
| 2:B:116:LEU:CD1 | 2:B:140:LEU:CD1 | 2.94 | 0.45 |
| 17:Q:48:GLU:OE1 | 17:Q:49:ASN:N | 2.41 | 0.45 |
| 17:Q:10:ARG:O | 17:Q:22:VAL:CG1 | 2.65 | 0.45 |
| 1:A:1154:G:N3 | 1:A:1155:A:C8 | 2.84 | 0.45 |
| 1:A:453:G:N1 | 1:A:454:G:C4 | 2.85 | 0.45 |
| 16:P:19:VAL:CG1 | 16:P:37:GLY:CA | 2.94 | 0.45 |
| 4:D:28:ASP:O | 4:D:29:THR:O | 2.35 | 0.45 |
| 1:A:583:A:C6 | 1:A:759:A:N7 | 2.84 | 0.45 |
| 1:A:877:G:N2 | 8:H:1:SER:N | 2.64 | 0.45 |
| 1:A:1331:G:C2' | 1:A:1332:A:OP2 | 2.64 | 0.45 |
| 10:J:36:VAL:CG2 | 10:J:76:ILE:CG1 | 2.95 | 0.45 |
| 1:A:727:G:N1 | 1:A:731:G:C6 | 2.84 | 0.45 |
| 2:B:27:LYS:N | 2:B:28:PRO:CD | 2.79 | 0.45 |
| 5:E:152:VAL:O | 5:E:155:LYS:CE | 2.65 | 0.45 |
| 1:A:204:G:N3 | 1:A:465:A:C4 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:965:U:O2 | 1:A:969:A:C2 | 2.70 | 0.45 |
| 1:A:961:U:O2 | 1:A:983:A:C4 | 2.70 | 0.45 |
| 1:A:858:G:O2' | 1:A:859:G:C5' | 2.65 | 0.45 |
| 1:A:737:C:C2 | 1:A:738:C:C5 | 3.04 | 0.45 |
| 7:G:53:SER:C | 7:G:55:LYS:N | 2.70 | 0.45 |
| 1:A:1507:A:C6 | 1:A:1530:G:C6 | 3.05 | 0.44 |
| 17:Q:18:LYS:CA | 17:Q:47:ASP:CB | 2.74 | 0.44 |
| 1:A:70:U:O2' | 1:A:71:A:C8 | 2.70 | 0.44 |
| 1:A:466:A:C6 | 1:A:468:A:N6 | 2.86 | 0.44 |
| 1:A:521:G:OP2 | 12:L:50:LYS:NZ | 2.50 | 0.44 |
| 1:A:1303:C:O2' | 1:A:1304:G:C8 | 2.69 | 0.44 |
| 17:Q:4:ILE:C | 17:Q:5:ARG:HG3 | 2.37 | 0.44 |
| 1:A:1315:U:O2' | 1:A:1360:A:O2' | 2.35 | 0.44 |
| 15:O:13:GLU:O | 15:O:83:ARG:NH2 | 2.49 | 0.44 |
| 19:S:55:GLN:CA | 19:S:55:GLN:NE2 | 2.80 | 0.44 |
| 10:J:20:GLN:NE2 | 10:J:20:GLN:CA | 2.79 | 0.44 |
| 12:L:45:ASN:N | 12:L:45:ASN:ND2 | 2.65 | 0.44 |
| 17:Q:16:MET:HB2 | 17:Q:19:SER:CB | 2.23 | 0.44 |
| 1:A:1159:U:OP1 | 2:B:131:LYS:NZ | 2.49 | 0.44 |
| 1:A:701:U:O2' | 1:A:702:A:P | 2.75 | 0.44 |
| 10:J:71:LEU:O | 10:J:72:ARG:CD | 2.66 | 0.44 |
| 1:A:251:G:N1 | 1:A:266:G:O6 | 2.50 | 0.44 |
| 17:Q:14:ASP:HB2 | 17:Q:54:ILE:HG22 | 1.99 | 0.44 |
| 1:A:1162:C:C2 | 1:A:1175:G:N2 | 2.85 | 0.44 |
| 1:A:1181:G:O2' | 1:A:1182:G:N9 | 2.51 | 0.44 |
| 1:A:408:A:C6 | 1:A:409:U:N3 | 2.85 | 0.44 |
| 12:L:113:ARG:O | 12:L:115:LYS:O | 2.36 | 0.44 |
| 2:B:42:LEU:CG | 2:B:43:GLU:N | 2.79 | 0.44 |
| 1:A:785:G:N2 | 1:A:798:U:C2 | 2.86 | 0.44 |
| 16:P:20:VAL:CG2 | 16:P:32:PHE:CB | 2.95 | 0.44 |
| 1:A:183:C:O2' | 1:A:184:G:C5' | 2.65 | 0.44 |
| 1:A:1282:C:O2' | 1:A:1283:U:C5' | 2.65 | 0.44 |
| 21:U:19:LYS:N | 21:U:19:LYS:CE | 2.81 | 0.44 |
| 1:A:500:G:C6 | 1:A:546:A:C2 | 3.05 | 0.44 |
| 11:K:51:PHE:CE1 | 11:K:60:PHE:CE2 | 3.05 | 0.44 |
| 1:A:627:G:C2 | 1:A:628:G:C4 | 3.05 | 0.44 |
| 9:I:103:VAL:CG2 | 9:I:104:THR:N | 2.81 | 0.44 |
| 1:A:261:U:OP2 | 20:T:70:LYS:NZ | 2.50 | 0.44 |
| 1:A:908:A:C2 | 1:A:909:A:C5 | 3.05 | 0.44 |
| 10:J:33:GLY:CA | 10:J:83:THR:CB | 2.96 | 0.44 |
| 18:R:28:LEU:C | 18:R:30:ASN:N | 2.70 | 0.44 |
| 1:A:860:A:N6 | 1:A:861:G:C2 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1447:A:C5' | 1:A:1448:C:OP2 | 2.66 | 0.44 |
| 1:A:70:U:O2' | 1:A:71:A:N7 | 2.51 | 0.44 |
| 1:A:1319:A:N7 | 1:A:1323:G:C5 | 2.85 | 0.44 |
| 1:A:1228:C:O2' | 1:A:1229:A:O4' | 2.36 | 0.44 |
| 1:A:1242:G:C6 | 1:A:1243:C:C5 | 3.05 | 0.44 |
| 1:A:946:A:C2 | 1:A:1236:A:N3 | 2.85 | 0.44 |
| 1:A:180:U:C3' | 1:A:180:U:C6 | 3.01 | 0.44 |
| 1:A:652:U:O4 | 1:A:752:G:O2' | 2.35 | 0.44 |
| 9:I:49:GLN:C | 9:I:51:LEU:N | 2.70 | 0.44 |
| 4:D:98:ASP:OD2 | 4:D:99:ASN:N | 2.50 | 0.44 |
| 4:D:166:LYS:CB | 4:D:166:LYS:NZ | 2.80 | 0.44 |
| 1:A:1293:C:C5 | 1:A:1294:G:N7 | 2.86 | 0.44 |
| 1:A:617:G:C2 | 1:A:618:C:C5 | 3.05 | 0.44 |
| 1:A:316:C:C2 | 1:A:317:U:C5 | 3.05 | 0.44 |
| 17:Q:55:GLY:CA | 17:Q:82:VAL:HG11 | 2.46 | 0.44 |
| 1:A:431:A:O2' | 1:A:432:A:C5' | 2.66 | 0.44 |
| 1:A:1142:G:O2' | 1:A:1143:G:O4' | 2.35 | 0.44 |
| 1:A:1231:G:C5 | 1:A:1232:U:C4 | 3.05 | 0.44 |
| 1:A:1399:C:O2 | 1:A:1401:G:C6 | 2.71 | 0.44 |
| 20:T:72:ALA:O | 20:T:73:ARG:C | 2.56 | 0.44 |
| 5:E:82:HIS:CE1 | 8:H:95:MET:CE | 3.01 | 0.44 |
| 1:A:484:G:C4' | 1:A:485:U:O5' | 2.65 | 0.44 |
| 1:A:53:A:C2' | 1:A:54:C:O5' | 2.65 | 0.44 |
| 1:A:661:G:C2 | 1:A:745:G:C2 | 3.05 | 0.44 |
| 1:A:579:A:O2' | 15:O:53:ARG:NH1 | 2.51 | 0.44 |
| 5:E:148:SER:O | 5:E:152:VAL:HA | 2.17 | 0.44 |
| 1:A:1130:A:C5' | 1:A:1130:A:C8 | 3.00 | 0.44 |
| 1:A:74:A:C6 | 1:A:97:G:C6 | 3.06 | 0.44 |
| 1:A:1133:G:N1 | 1:A:1142:G:C6 | 2.85 | 0.44 |
| 1:A:544:G:C5 | 1:A:545:C:C5 | 3.06 | 0.44 |
| 13:M:3:ILE:O | 13:M:3:ILE:CG1 | 2.65 | 0.44 |
| 3:C:10:ARG:O | 3:C:11:LEU:C | 2.56 | 0.44 |
| 16:P:21:VAL:O | 16:P:33:ILE:N | 2.50 | 0.44 |
| 1:A:1215:G:O2' | 1:A:1216:A:C5' | 2.66 | 0.44 |
| 8:H:112:ASP:OD1 | 8:H:112:ASP:N | 2.50 | 0.44 |
| 14:N:5:MET:SD | 14:N:8:ARG:NH1 | 2.91 | 0.44 |
| 17:Q:78:VAL:HG12 | 17:Q:79:GLU:HG3 | 2.00 | 0.44 |
| 1:A:198:G:C6 | 1:A:220:G:C4 | 3.05 | 0.44 |
| 14:N:42:ASN:ND2 | 14:N:46:LYS:NZ | 2.65 | 0.44 |
| 19:S:43:MET:O | 19:S:61:VAL:CG2 | 2.65 | 0.44 |
| 1:A:1072:G:C5 | 1:A:1073:U:C4 | 3.06 | 0.44 |
| 2:B:14:HIS:CG | 2:B:14:HIS:O | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 17:Q:62:GLU:HB2 | 17:Q:72:TRP:CE2 | 2.53 | 0.44 |
| 10:J:42:LEU:CB | 10:J:43:PRO:CD | 2.96 | 0.44 |
| 17:Q:32:ILE:HD12 | 17:Q:32:ILE:N | 2.33 | 0.44 |
| 1:A:1452:C:O4' | 1:A:1453:G:C2 | 2.71 | 0.44 |
| 17:Q:29:LYS:HG3 | 17:Q:36:PHE:CZ | 2.52 | 0.44 |
| 15:O:23:SER:O | 15:O:25:GLU:N | 2.51 | 0.44 |
| 4:D:160:LEU:N | 4:D:160:LEU:CD2 | 2.80 | 0.44 |
| 1:A:9:G:C6 | 1:A:26:A:N6 | 2.86 | 0.44 |
| 1:A:849:G:C6 | 1:A:850:U:N3 | 2.85 | 0.44 |
| 1:A:1237:C:O2' | 1:A:1300:G:N2 | 2.51 | 0.44 |
| 1:A:102:G:C4 | 1:A:103:U:C5 | 3.06 | 0.44 |
| 7:G:4:ARG:CA | 7:G:4:ARG:NE | 2.80 | 0.44 |
| 1:A:275:G:C4 | 1:A:276:G:C8 | 3.06 | 0.43 |
| 1:A:1299:A:C5 | 1:A:1301:U:C2 | 3.06 | 0.43 |
| 2:B:131:LYS:O | 2:B:135:MET:CB | 2.67 | 0.43 |
| 1:A:91:U:C2' | 1:A:92:U:O4' | 2.65 | 0.43 |
| 1:A:1200:C:OP1 | 1:A:1201:A:O2' | 2.36 | 0.43 |
| 1:A:497:G:N2 | 1:A:498:A:C6 | 2.86 | 0.43 |
| 10:J:49:PHE:CZ | 14:N:76:PHE:CZ | 3.06 | 0.43 |
| 7:G:14:ASP:OD1 | 7:G:17:PHE:CD1 | 2.71 | 0.43 |
| 2:B:150:ILE:O | 2:B:151:LYS:C | 2.56 | 0.43 |
| 1:A:1250:A:N3 | 1:A:1370:G:O2' | 2.51 | 0.43 |
| 7:G:88:VAL:CG2 | 7:G:89:GLU:N | 2.81 | 0.43 |
| 1:A:528:C:C6 | 1:A:528:C:C4' | 3.01 | 0.43 |
| 1:A:1160:G:C2 | 1:A:1161:C:C5 | 3.06 | 0.43 |
| 1:A:89:U:C2 | 1:A:90:C:C5 | 3.06 | 0.43 |
| 2:B:21:TYR:O | 2:B:22:TRP:CD1 | 2.71 | 0.43 |
| 1:A:450:G:C2' | 1:A:451:A:OP1 | 2.66 | 0.43 |
| 1:A:570:G:C4 | 1:A:571:U:C5 | 3.06 | 0.43 |
| 1:A:984:C:O2' | 1:A:985:C:O5' | 2.36 | 0.43 |
| 1:A:991:U:C5' | 1:A:992:U:OP1 | 2.66 | 0.43 |
| 3:C:35:ASP:O | 3:C:37:LYS:N | 2.50 | 0.43 |
| 1:A:1028:C:C4 | 1:A:1034:G:C6 | 3.06 | 0.43 |
| 6:F:18:VAL:N | 6:F:19:PRO:CD | 2.81 | 0.43 |
| 1:A:283:U:C4 | 1:A:284:C:C4 | 3.06 | 0.43 |
| 1:A:688:G:C5 | 1:A:700:G:C2 | 3.07 | 0.43 |
| 1:A:1118:U:O2 | 1:A:1179:A:C6 | 2.71 | 0.43 |
| 1:A:773:G:C6 | 1:A:774:G:N7 | 2.86 | 0.43 |
| 1:A:116:A:O2' | 1:A:117:G:O5' | 2.36 | 0.43 |
| 5:E:59:ILE:CD1 | 5:E:59:ILE:C | 2.86 | 0.43 |
| 17:Q:49:ASN:HD22 | 17:Q:49:ASN:C | 2.20 | 0.43 |
| 1:A:184:G:O2' | 1:A:185:U:P | 2.77 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1150:A:N6 | 1:A:1151:A:N6 | 2.66 | 0.43 |
| 10:J:41:PRO:O | 10:J:42:LEU:CB | 2.65 | 0.43 |
| 1:A:1162:C:C2 | 1:A:1175:G:C2 | 3.07 | 0.43 |
| 2:B:71:THR:O | 2:B:72:LYS:CG | 2.66 | 0.43 |
| 1:A:513:C:N3 | 1:A:539:A:C2 | 2.86 | 0.43 |
| 16:P:75:ILE:C | 16:P:77:GLU:N | 2.71 | 0.43 |
| 6:F:92:THR:O | 6:F:93:LYS:CG | 2.65 | 0.43 |
| 1:A:246:A:C4 | 1:A:282:A:N6 | 2.86 | 0.43 |
| 1:A:258:G:C2 | 1:A:259:G:C1' | 3.01 | 0.43 |
| 1:A:1108:G:C5 | 1:A:1109:C:C5 | 3.06 | 0.43 |
| 21:U:24:LYS:CG | 21:U:25:ALA:N | 2.81 | 0.43 |
| 1:A:1216:A:OP1 | 14:N:4:SER:CB | 2.66 | 0.43 |
| 1:A:775:G:C2 | 1:A:776:G:C4 | 3.06 | 0.43 |
| 1:A:592:G:C6 | 1:A:648:A:C6 | 3.07 | 0.43 |
| 1:A:932:C:O2 | 1:A:932:C:C2' | 2.67 | 0.43 |
| 7:G:61:PHE:C | 7:G:61:PHE:CD1 | 2.92 | 0.43 |
| 8:H:88:LYS:CG | 8:H:89:ASP:N | 2.81 | 0.43 |
| 17:Q:16:MET:CE | 17:Q:21:VAL:HG12 | 2.48 | 0.43 |
| 1:A:430:A:N3 | 1:A:431:A:C8 | 2.86 | 0.43 |
| 1:A:1154:G:C2 | 1:A:1155:A:C5 | 3.07 | 0.43 |
| 1:A:365:U:C5' | 1:A:366:A:OP1 | 2.67 | 0.43 |
| 1:A:70:U:N3 | 1:A:94:G:C5 | 2.86 | 0.43 |
| 1:A:565:U:C4 | 1:A:566:G:C5 | 3.05 | 0.43 |
| 1:A:495:A:N3 | 1:A:496:A:C6 | 2.87 | 0.43 |
| 1:A:25:C:C2' | 1:A:26:A:O5' | 2.66 | 0.43 |
| 4:D:7:LYS:NZ | 4:D:21:LYS:CG | 2.81 | 0.43 |
| 18:R:41:SER:O | 18:R:45:GLY:N | 2.52 | 0.43 |
| 12:L:55:ARG:NH1 | 12:L:61:GLU:OE1 | 2.50 | 0.43 |
| 11:K:26:PHE:CE1 | 11:K:88:PRO:CG | 3.01 | 0.43 |
| 1:A:1491:G:C5' | 1:A:1492:A:OP1 | 2.66 | 0.43 |
| 1:A:585:G:N2 | 1:A:879:C:C4' | 2.81 | 0.43 |
| 17:Q:48:GLU:CA | 17:Q:48:GLU:OE1 | 2.64 | 0.43 |
| 21:U:33:ARG:O | 21:U:34:ARG:C | 2.57 | 0.43 |
| 5:E:79:THR:CB | 5:E:121:ASN:ND2 | 2.81 | 0.43 |
| 1:A:1157:A:C1' | 1:A:1181:G:N2 | 2.81 | 0.43 |
| 10:J:80:THR:O | 10:J:81:GLU:C | 2.56 | 0.43 |
| 15:O:15:GLY:C | 15:O:17:ASP:N | 2.72 | 0.43 |
| 1:A:1124:G:C2' | 1:A:1145:A:N6 | 2.81 | 0.43 |
| 19:S:62:THR:O | 19:S:63:ASP:C | 2.56 | 0.43 |
| 9:I:78:ILE:O | 9:I:81:GLY:N | 2.51 | 0.43 |
| 7:G:110:ARG:NH1 | 7:G:122:GLU:CG | 2.81 | 0.43 |
| 1:A:1014:A:C4' | 19:S:13:HIS:CD2 | 3.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1072:G:N1 | 1:A:1104:G:C2 | 2.86 | 0.43 |
| 4:D:109:THR:CG2 | 4:D:112:GLU:CB | 2.97 | 0.43 |
| 1:A:928:G:O2' | 1:A:1533:C:OP1 | 2.37 | 0.43 |
| 17:Q:20:ILE:CA | 17:Q:47:ASP:OD1 | 2.66 | 0.43 |
| 1:A:99:C:C2' | 1:A:100:G:OP2 | 2.65 | 0.43 |
| 1:A:77:A:N6 | 1:A:90:C:C5 | 2.87 | 0.43 |
| 6:F:51:ILE:CD1 | 6:F:86:ARG:CG | 2.96 | 0.43 |
| 1:A:1138:G:C2 | 1:A:1140:C:C4 | 3.07 | 0.43 |
| 1:A:374:A:C6 | 1:A:375:U:C4 | 3.07 | 0.43 |
| 19:S:79:TYR:CD2 | 19:S:79:TYR:C | 2.88 | 0.43 |
| 1:A:949:A:O4' | 1:A:1364:U:C5 | 2.71 | 0.43 |
| 5:E:94:PHE:C | 5:E:94:PHE:CD1 | 2.92 | 0.43 |
| 1:A:1533:C:C2' | 1:A:1534:A:H5'' | 2.48 | 0.43 |
| 17:Q:12:VAL:CG1 | 17:Q:13:SER:N | 2.52 | 0.43 |
| 17:Q:18:LYS:O | 17:Q:47:ASP:OD2 | 2.36 | 0.43 |
| 17:Q:20:ILE:HD12 | 17:Q:20:ILE:HA | 1.63 | 0.43 |
| 17:Q:73:THR:HG22 | 17:Q:74:LEU:HD12 | 2.01 | 0.43 |
| 1:A:1283:U:O2' | 1:A:1284:C:C5' | 2.67 | 0.43 |
| 1:A:976:G:N1 | 1:A:1363:A:C2 | 2.87 | 0.43 |
| 1:A:1321:U:O3' | 19:S:77:ARG:NH2 | 2.51 | 0.43 |
| 1:A:335:C:O2' | 1:A:1433:A:N3 | 2.51 | 0.43 |
| 1:A:748:G:O6 | 1:A:749:A:N6 | 2.51 | 0.43 |
| 5:E:12:GLU:CB | 5:E:38:VAL:CG1 | 2.97 | 0.43 |
| 2:B:218:ALA:CA | 2:B:221:ARG:NH2 | 2.81 | 0.43 |
| 13:M:25:GLY:O | 13:M:27:THR:N | 2.52 | 0.43 |
| 13:M:84:CYS:O | 13:M:88:LEU:CD1 | 2.66 | 0.43 |
| 1:A:1246:A:C6 | 1:A:1292:G:C6 | 3.07 | 0.43 |
| 1:A:2:A:C6 | 1:A:3:A:N1 | 2.86 | 0.43 |
| 21:U:32:ARG:CG | 21:U:32:ARG:O | 2.65 | 0.43 |
| 1:A:184:G:O2' | 1:A:185:U:C5' | 2.67 | 0.43 |
| 1:A:184:G:N3 | 1:A:185:U:C6 | 2.87 | 0.43 |
| 11:K:125:LYS:O | 11:K:126:ARG:CB | 2.66 | 0.43 |
| 6:F:86:ARG:NH1 | 18:R:63:TYR:CB | 2.82 | 0.43 |
| 1:A:815:A:C2 | 1:A:1529:G:C4 | 3.06 | 0.43 |
| 1:A:373:A:N3 | 1:A:374:A:C8 | 2.86 | 0.43 |
| 20:T:4:LYS:O | 20:T:6:ALA:N | 2.52 | 0.43 |
| 15:O:24:THR:O | 15:O:25:GLU:C | 2.57 | 0.43 |
| 1:A:224:U:O2' | 1:A:225:C:C5' | 2.67 | 0.43 |
| 1:A:585:G:N2 | 1:A:879:C:O4' | 2.52 | 0.43 |
| 1:A:232:G:C2' | 1:A:233:C:C5' | 2.97 | 0.43 |
| 5:E:40:ASP:OD1 | 5:E:42:ASN:N | 2.52 | 0.43 |
| 1:A:1442:G:C6 | 1:A:1443:C:C4 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 4:D:84:ASN:ND2 | 4:D:84:ASN:C | 2.72 | 0.43 |
| 17:Q:55:GLY:HA3 | 17:Q:82:VAL:CG1 | 2.47 | 0.43 |
| 11:K:126:ARG:N | 21:U:33:ARG:NH1 | 2.67 | 0.43 |
| 1:A:79:G:N2 | 1:A:91:U:O4 | 2.52 | 0.43 |
| 1:A:205:A:N7 | 1:A:206:C:C4 | 2.87 | 0.43 |
| 1:A:414:A:C4 | 1:A:415:A:N7 | 2.87 | 0.43 |
| 1:A:451:A:C4' | 1:A:452:A:O5' | 2.67 | 0.43 |
| 10:J:80:THR:O | 10:J:84:VAL:N | 2.51 | 0.43 |
| 4:D:145:ARG:NH1 | 4:D:147:LYS:CE | 2.82 | 0.43 |
| 1:A:865:A:C4 | 1:A:866:C:C5 | 3.07 | 0.43 |
| 8:H:87:ARG:O | 8:H:121:GLY:CA | 2.67 | 0.43 |
| 5:E:29:ILE:CD1 | 5:E:30:PHE:N | 2.82 | 0.43 |
| 1:A:358:U:C2' | 1:A:359:G:O5' | 2.66 | 0.43 |
| 2:B:13:VAL:CG2 | 2:B:207:ARG:NH2 | 2.81 | 0.43 |
| 1:A:547:A:C4' | 1:A:548:G:O5' | 2.67 | 0.43 |
| 1:A:548:G:C2' | 1:A:549:C:C6 | 3.02 | 0.43 |
| 4:D:26:ALA:O | 4:D:27:ILE:C | 2.56 | 0.43 |
| 1:A:1454:G:O2' | 1:A:1455:G:O4' | 2.36 | 0.43 |
| 1:A:581:G:N1 | 1:A:759:A:OP2 | 2.52 | 0.43 |
| 1:A:859:G:OP2 | 1:A:869:G:N1 | 2.51 | 0.43 |
| 1:A:1124:G:O2' | 10:J:40:ILE:CD1 | 2.67 | 0.43 |
| 1:A:420:U:C2' | 1:A:421:U:C5' | 2.96 | 0.43 |
| 9:I:5:TYR:CE1 | 9:I:88:GLU:OE2 | 2.72 | 0.43 |
| 4:D:60:VAL:CA | 4:D:63:ILE:CG2 | 2.97 | 0.43 |
| 15:O:18:ALA:O | 15:O:19:ASN:CB | 2.66 | 0.43 |
| 9:I:60:LEU:N | 9:I:60:LEU:CD2 | 2.82 | 0.43 |
| 1:A:1530:G:O2' | 1:A:1531:A:H5' | 2.18 | 0.42 |
| 17:Q:80:LYS:CB | 17:Q:80:LYS:NZ | 2.77 | 0.42 |
| 1:A:79:G:C6 | 1:A:80:A:C5 | 3.06 | 0.42 |
| 1:A:874:G:C6 | 1:A:875:U:C4 | 3.07 | 0.42 |
| 1:A:309:A:O2' | 1:A:607:A:N1 | 2.52 | 0.42 |
| 1:A:895:G:C5 | 1:A:896:C:C5 | 3.07 | 0.42 |
| 3:C:56:ILE:CG1 | 3:C:65:VAL:CG2 | 2.96 | 0.42 |
| 1:A:1004:A:C6 | 1:A:1005:A:C4 | 3.07 | 0.42 |
| 19:S:28:LYS:CB | 19:S:29:PRO:CD | 2.97 | 0.42 |
| 21:U:36:PHE:O | 21:U:37:TYR:CB | 2.66 | 0.42 |
| 1:A:352:C:C5' | 1:A:352:C:C6 | 3.02 | 0.42 |
| 4:D:22:SER:O | 4:D:23:GLY:C | 2.57 | 0.42 |
| 1:A:430:A:C2' | 1:A:431:A:C5' | 2.97 | 0.42 |
| 6:F:51:ILE:O | 6:F:51:ILE:CG2 | 2.67 | 0.42 |
| 12:L:42:LYS:O | 12:L:43:LYS:C | 2.57 | 0.42 |
| 1:A:1433:A:N7 | 1:A:1468:A:C6 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:462:G:N7 | 1:A:463:U:C5 | 2.87 | 0.42 |
| 20:T:5:SER:OG | 20:T:6:ALA:N | 2.50 | 0.42 |
| 1:A:1314:C:OP2 | 19:S:5:LYS:CD | 2.67 | 0.42 |
| 1:A:766:A:C2 | 1:A:814:A:C2 | 3.07 | 0.42 |
| 1:A:578:C:C5' | 23:A:1615:HOH:O | 2.67 | 0.42 |
| 20:T:54:GLN:N | 20:T:55:PRO:CD | 2.82 | 0.42 |
| 1:A:1397:C:O2' | 1:A:1398:A:OP1 | 2.37 | 0.42 |
| 1:A:203:G:C2 | 1:A:215:C:C4 | 3.07 | 0.42 |
| 1:A:1228:C:OP2 | 13:M:109:LYS:NZ | 2.52 | 0.42 |
| 1:A:1468:A:C3' | 1:A:1469:C:C5' | 2.97 | 0.42 |
| 11:K:60:PHE:C | 11:K:60:PHE:CD2 | 2.92 | 0.42 |
| 1:A:771:G:C5 | 1:A:772:U:C5 | 3.08 | 0.42 |
| 1:A:926:G:C6 | 1:A:1505:G:C6 | 3.08 | 0.42 |
| 4:D:151:GLN:O | 4:D:153:ARG:N | 2.52 | 0.42 |
| 1:A:941:G:C2' | 1:A:942:G:O5' | 2.68 | 0.42 |
| 18:R:33:THR:OG1 | 18:R:34:GLU:N | 2.52 | 0.42 |
| 10:J:88:MET:CE | 10:J:89:ARG:NH1 | 2.82 | 0.42 |
| 9:I:62:LEU:N | 9:I:62:LEU:CD2 | 2.83 | 0.42 |
| 9:I:12:LYS:CG | 9:I:12:LYS:O | 2.67 | 0.42 |
| 13:M:86:ARG:O | 13:M:90:HIS:CD2 | 2.73 | 0.42 |
| 1:A:251:G:C6 | 1:A:266:G:O6 | 2.71 | 0.42 |
| 1:A:428:G:N9 | 1:A:430:A:N7 | 2.67 | 0.42 |
| 1:A:198:G:C6 | 1:A:220:G:N3 | 2.87 | 0.42 |
| 1:A:819:A:C4' | 1:A:820:U:OP2 | 2.67 | 0.42 |
| 12:L:24:GLU:O | 12:L:25:ALA:C | 2.55 | 0.42 |
| 1:A:665:A:C2 | 1:A:732:C:C4 | 3.07 | 0.42 |
| 1:A:1046:A:C2' | 1:A:1047:G:C5' | 2.98 | 0.42 |
| 1:A:39:G:N3 | 1:A:40:C:C6 | 2.88 | 0.42 |
| 1:A:864:A:C2' | 1:A:865:A:C8 | 3.03 | 0.42 |
| 1:A:1421:G:C6 | 1:A:1422:G:N7 | 2.88 | 0.42 |
| 1:A:766:A:N3 | 1:A:814:A:C2 | 2.87 | 0.42 |
| 1:A:102:G:C2 | 1:A:103:U:C5 | 3.06 | 0.42 |
| 1:A:688:G:C4 | 1:A:700:G:N2 | 2.88 | 0.42 |
| 1:A:473:U:C2 | 1:A:474:G:N7 | 2.87 | 0.42 |
| 1:A:1136:C:C3' | 1:A:1136:C:O2 | 2.67 | 0.42 |
| 1:A:1045:C:OP2 | 1:A:1045:C:C6 | 2.72 | 0.42 |
| 1:A:1154:G:C2 | 1:A:1155:A:C8 | 3.07 | 0.42 |
| 1:A:76:G:C2' | 1:A:76:G:N3 | 2.82 | 0.42 |
| 2:B:20:ARG:O | 2:B:22:TRP:N | 2.52 | 0.42 |
| 1:A:110:C:O2' | 1:A:111:G:C5' | 2.68 | 0.42 |
| 1:A:993:G:N2 | 1:A:996:A:N6 | 2.67 | 0.42 |
| 12:L:72:ASN:O | 12:L:73:LEU:O | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 15:O:44:GLU:OE2 | 15:O:45:HIS:CE1 | 2.72 | 0.42 |
| 4:D:96:ARG:NH2 | 4:D:98:ASP:OD1 | 2.52 | 0.42 |
| 1:A:748:G:C6 | 1:A:749:A:C5 | 3.07 | 0.42 |
| 5:E:139:THR:O | 5:E:142:GLY:N | 2.52 | 0.42 |
| 1:A:1492:A:C2' | 1:A:1493:A:O5' | 2.67 | 0.42 |
| 2:B:172:ILE:O | 2:B:175:ALA:N | 2.53 | 0.42 |
| 14:N:1:ALA:O | 14:N:2:LYS:CB | 2.67 | 0.42 |
| 9:I:13:SER:OG | 9:I:13:SER:O | 2.38 | 0.42 |
| 1:A:397:A:C6 | 1:A:548:G:N7 | 2.88 | 0.42 |
| 1:A:468:A:C2' | 1:A:469:C:C5' | 2.98 | 0.42 |
| 1:A:120:A:C6 | 1:A:122:G:C6 | 3.07 | 0.42 |
| 19:S:46:LEU:N | 19:S:61:VAL:CG2 | 2.83 | 0.42 |
| 8:H:87:ARG:O | 8:H:88:LYS:CB | 2.66 | 0.42 |
| 1:A:1119:C:OP1 | 9:I:84:ARG:NH2 | 2.53 | 0.42 |
| 1:A:1525:G:OP1 | 11:K:121:ARG:NH2 | 2.52 | 0.42 |
| 1:A:595:A:C6 | 1:A:641:U:C5 | 3.08 | 0.42 |
| 1:A:1416:G:C2 | 1:A:1485:U:O2 | 2.73 | 0.42 |
| 5:E:81:GLN:CG | 5:E:149:PRO:CG | 2.98 | 0.42 |
| 8:H:65:PHE:O | 8:H:66:GLN:O | 2.37 | 0.42 |
| 1:A:185:U:O2' | 1:A:186:C:O4' | 2.38 | 0.42 |
| 1:A:1151:A:C5' | 10:J:42:LEU:O | 2.68 | 0.42 |
| 6:F:85:ILE:O | 6:F:86:ARG:C | 2.58 | 0.42 |
| 1:A:1141:C:C2 | 1:A:1142:G:N7 | 2.88 | 0.42 |
| 1:A:523:A:C2 | 1:A:527:G:C6 | 3.07 | 0.42 |
| 3:C:35:ASP:OD1 | 3:C:56:ILE:CG2 | 2.68 | 0.42 |
| 1:A:828:U:C6 | 1:A:828:U:C3' | 3.03 | 0.42 |
| 17:Q:46:HIS:HB3 | 17:Q:73:THR:HA | 2.02 | 0.42 |
| 1:A:1202:U:C5 | 1:A:1203:C:C4 | 3.07 | 0.42 |
| 1:A:204:G:N2 | 1:A:465:A:C8 | 2.88 | 0.42 |
| 1:A:820:U:C4' | 1:A:821:G:OP2 | 2.68 | 0.42 |
| 1:A:972:C:O2' | 1:A:973:G:P | 2.77 | 0.42 |
| 1:A:441:A:C5' | 1:A:442:G:OP2 | 2.66 | 0.42 |
| 1:A:1409:C:O2' | 1:A:1410:A:C5' | 2.68 | 0.42 |
| 1:A:191:G:C4 | 1:A:192:A:C8 | 3.08 | 0.42 |
| 18:R:50:TYR:O | 18:R:51:GLN:C | 2.58 | 0.42 |
| 5:E:13:LYS:NZ | 5:E:115:GLU:OE2 | 2.53 | 0.42 |
| 1:A:1216:A:C2 | 1:A:1217:C:C4 | 3.07 | 0.42 |
| 2:B:123:GLY:O | 2:B:125:PHE:CD2 | 2.72 | 0.42 |
| 1:A:845:A:C8 | 1:A:845:A:C3' | 3.03 | 0.42 |
| 2:B:71:THR:O | 2:B:72:LYS:O | 2.36 | 0.42 |
| 1:A:1084:G:C6 | 1:A:1085:U:C4 | 3.08 | 0.42 |
| 4:D:68:GLU:O | 4:D:69:ARG:C | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:B:49:PHE:O | 2:B:52:ALA:N | 2.53 | 0.42 |
| 4:D:131:ILE:C | 4:D:133:SER:N | 2.73 | 0.42 |
| 1:A:625:U:O2' | 1:A:626:G:C5' | 2.68 | 0.42 |
| 1:A:626:G:C4 | 1:A:627:G:C8 | 3.08 | 0.42 |
| 1:A:1049:U:C1' | 1:A:1201:A:N7 | 2.83 | 0.42 |
| 1:A:1031:C:C2' | 1:A:1032:G:OP2 | 2.68 | 0.42 |
| 15:O:9:LYS:O | 15:O:13:GLU:CG | 2.68 | 0.42 |
| 18:R:36:GLY:O | 18:R:62:ARG:NH2 | 2.52 | 0.42 |
| 1:A:28:A:C2 | 1:A:29:U:C2 | 3.08 | 0.42 |
| 14:N:15:LEU:O | 14:N:17:ASP:N | 2.53 | 0.42 |
| 17:Q:47:ASP:C | 17:Q:51:GLU:OE2 | 2.59 | 0.42 |
| 1:A:487:A:C2' | 1:A:488:C:C5' | 2.98 | 0.42 |
| 1:A:97:G:O2' | 1:A:98:A:C5' | 2.68 | 0.42 |
| 1:A:198:G:C4 | 1:A:199:A:C8 | 3.07 | 0.42 |
| 1:A:982:U:C2 | 1:A:983:A:C6 | 3.07 | 0.42 |
| 1:A:1225:A:C2' | 1:A:1226:C:C6 | 3.03 | 0.42 |
| 7:G:74:VAL:CG2 | 7:G:85:GLN:NE2 | 2.83 | 0.42 |
| 1:A:1511:G:C6 | 1:A:1512:U:C4 | 3.08 | 0.42 |
| 1:A:970:C:C5' | 1:A:971:G:OP1 | 2.67 | 0.42 |
| 1:A:617:G:N1 | 1:A:618:C:C5 | 2.88 | 0.42 |
| 19:S:40:PHE:CB | 19:S:42:ASN:ND2 | 2.83 | 0.42 |
| 2:B:40:ILE:CG1 | 2:B:41:ASN:N | 2.83 | 0.42 |
| 2:B:40:ILE:O | 2:B:41:ASN:CB | 2.68 | 0.42 |
| 15:O:55:LEU:CD1 | 15:O:55:LEU:C | 2.87 | 0.42 |
| 1:A:1532:U:O5' | 1:A:1532:U:H6 | 2.03 | 0.41 |
| 1:A:1381:U:O2' | 1:A:1382:C:O5' | 2.38 | 0.41 |
| 1:A:373:A:C2 | 1:A:374:A:C8 | 3.08 | 0.41 |
| 20:T:82:ILE:O | 20:T:86:ALA:CB | 2.68 | 0.41 |
| 3:C:57:GLU:O | 3:C:59:PRO:CD | 2.68 | 0.41 |
| 10:J:91:ASP:C | 10:J:92:LEU:CD2 | 2.88 | 0.41 |
| 1:A:457:G:C6 | 1:A:458:U:C4 | 3.08 | 0.41 |
| 17:Q:74:LEU:C | 17:Q:74:LEU:HD13 | 2.40 | 0.41 |
| 1:A:872:A:C8 | 1:A:874:G:C8 | 3.08 | 0.41 |
| 1:A:624:C:C4 | 1:A:625:U:C4 | 3.07 | 0.41 |
| 1:A:55:A:C5 | 1:A:56:U:C6 | 3.08 | 0.41 |
| 1:A:82:G:N2 | 1:A:84:U:O4 | 2.53 | 0.41 |
| 1:A:1386:G:N3 | 1:A:1387:G:C8 | 2.88 | 0.41 |
| 1:A:1077:G:C6 | 1:A:1081:A:C6 | 3.08 | 0.41 |
| 1:A:233:C:C2 | 1:A:234:C:C5 | 3.08 | 0.41 |
| 9:I:41:GLU:O | 9:I:43:ALA:N | 2.53 | 0.41 |
| 8:H:103:VAL:N | 8:H:110:MET:O | 2.52 | 0.41 |
| 5:E:155:LYS:NZ | 5:E:156:ARG:HG3 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:267:C:C6 | 1:A:268:U:C5 | 3.09 | 0.41 |
| 17:Q:11:VAL:O | 17:Q:12:VAL:HB | 2.20 | 0.41 |
| 17:Q:60:ILE:HG22 | 17:Q:72:TRP:HE3 | 1.80 | 0.41 |
| 1:A:1451:U:O5' | 1:A:1452:C:C5 | 2.74 | 0.41 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 3.08 | 0.41 |
| 1:A:1336:C:O2' | 1:A:1337:G:P | 2.78 | 0.41 |
| 1:A:957:U:C2 | 1:A:959:A:OP2 | 2.74 | 0.41 |
| 1:A:550:G:C6 | 1:A:551:U:C4 | 3.07 | 0.41 |
| 2:B:89:PHE:CE1 | 2:B:153:MET:CG | 3.03 | 0.41 |
| 6:F:36:ILE:CG2 | 6:F:64:VAL:CG2 | 2.98 | 0.41 |
| 6:F:99:ALA:O | 6:F:100:SER:CB | 2.66 | 0.41 |
| 6:F:97:THR:CG2 | 6:F:98:GLU:N | 2.83 | 0.41 |
| 17:Q:78:VAL:C | 17:Q:79:GLU:HG3 | 2.41 | 0.41 |
| 1:A:1258:G:O2' | 1:A:1259:C:P | 2.77 | 0.41 |
| 1:A:1061:G:C5 | 1:A:1197:A:C2 | 3.09 | 0.41 |
| 1:A:922:G:N2 | 1:A:1396:A:C5 | 2.88 | 0.41 |
| 2:B:71:THR:CG2 | 2:B:72:LYS:N | 2.83 | 0.41 |
| 1:A:199:A:C2 | 1:A:200:G:C4 | 3.08 | 0.41 |
| 4:D:114:ARG:O | 4:D:115:GLN:C | 2.59 | 0.41 |
| 1:A:243:A:C6 | 1:A:246:A:N7 | 2.89 | 0.41 |
| 1:A:1399:C:C4 | 1:A:1502:A:C2 | 3.08 | 0.41 |
| 8:H:112:ASP:O | 8:H:113:ARG:C | 2.58 | 0.41 |
| 10:J:87:LEU:CD1 | 10:J:88:MET:N | 2.83 | 0.41 |
| 1:A:1171:A:C2 | 1:A:1172:C:C2 | 3.09 | 0.41 |
| 11:K:96:ILE:O | 11:K:97:ARG:C | 2.59 | 0.41 |
| 14:N:55:SER:O | 14:N:59:GLN:NE2 | 2.54 | 0.41 |
| 11:K:106:ILE:O | 11:K:106:ILE:CD1 | 2.68 | 0.41 |
| 1:A:1258:G:O2' | 1:A:1259:C:O5' | 2.38 | 0.41 |
| 6:F:8:PHE:CE2 | 6:F:60:VAL:CG1 | 3.03 | 0.41 |
| 4:D:134:TYR:C | 4:D:134:TYR:CD2 | 2.93 | 0.41 |
| 1:A:815:A:O2' | 1:A:816:A:OP1 | 2.38 | 0.41 |
| 1:A:512:U:O2' | 1:A:513:C:O4' | 2.39 | 0.41 |
| 12:L:24:GLU:CD | 12:L:29:LYS:NZ | 2.74 | 0.41 |
| 1:A:1117:A:N1 | 1:A:1184:G:C6 | 2.88 | 0.41 |
| 1:A:1087:G:C2 | 1:A:1088:G:C5 | 3.09 | 0.41 |
| 4:D:159:GLU:C | 4:D:161:ALA:N | 2.73 | 0.41 |
| 12:L:32:VAL:O | 12:L:33:CYS:SG | 2.78 | 0.41 |
| 1:A:1312:G:N2 | 1:A:1313:U:C2 | 2.88 | 0.41 |
| 1:A:646:G:C2' | 1:A:647:C:C5' | 2.99 | 0.41 |
| 7:G:7:GLY:O | 7:G:8:GLN:CB | 2.68 | 0.41 |
| 1:A:1418:A:C2 | 1:A:1483:A:C2 | 3.09 | 0.41 |
| 14:N:47:LEU:CD2 | 14:N:47:LEU:O | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:1160:G:C2 | 1:A:1161:C:C6 | 3.08 | 0.41 |
| 1:A:74:A:C2 | 1:A:75:G:C5 | 3.09 | 0.41 |
| 1:A:439:U:O4' | 4:D:118:SER:O | 2.39 | 0.41 |
| 1:A:978:A:C2 | 1:A:1318:A:C4 | 3.08 | 0.41 |
| 1:A:520:A:N7 | 1:A:521:G:C8 | 2.88 | 0.41 |
| 1:A:371:A:C2 | 1:A:372:C:C5 | 3.09 | 0.41 |
| 15:O:87:ARG:O | 15:O:88:ARG:C | 2.59 | 0.41 |
| 16:P:77:GLU:C | 16:P:79:ASN:N | 2.73 | 0.41 |
| 1:A:1012:A:C6 | 1:A:1013:G:C6 | 3.08 | 0.41 |
| 1:A:935:A:N3 | 1:A:936:C:C6 | 2.88 | 0.41 |
| 1:A:858:G:N7 | 1:A:869:G:N7 | 2.69 | 0.41 |
| 1:A:39:G:C4 | 1:A:40:C:C6 | 3.08 | 0.41 |
| 5:E:115:GLU:O | 5:E:118:GLY:N | 2.53 | 0.41 |
| 1:A:52:C:O2' | 1:A:53:A:C5' | 2.68 | 0.41 |
| 21:U:35:GLU:O | 21:U:36:PHE:CB | 2.69 | 0.41 |
| 5:E:64:GLU:O | 5:E:67:ARG:N | 2.54 | 0.41 |
| 1:A:1219:A:C6 | 1:A:1220:G:C6 | 3.08 | 0.41 |
| 1:A:75:G:N1 | 1:A:96:U:C4 | 2.88 | 0.41 |
| 1:A:924:C:O2' | 1:A:925:G:C5' | 2.69 | 0.41 |
| 1:A:1316:G:C5' | 1:A:1317:C:OP2 | 2.68 | 0.41 |
| 17:Q:30:HIS:ND1 | 17:Q:31:PRO:HD2 | 2.34 | 0.41 |
| 16:P:37:GLY:CA | 16:P:51:ARG:NH1 | 2.84 | 0.41 |
| 1:A:587:G:C2 | 1:A:755:G:C5 | 3.08 | 0.41 |
| 1:A:224:U:N3 | 1:A:225:C:C5 | 2.89 | 0.41 |
| 1:A:579:A:C4 | 1:A:580:C:C5 | 3.09 | 0.41 |
| 4:D:83:GLY:O | 4:D:84:ASN:C | 2.58 | 0.41 |
| 9:I:79:ARG:O | 9:I:83:THR:CG2 | 2.69 | 0.41 |
| 1:A:1165:U:C5 | 1:A:1166:G:N7 | 2.88 | 0.41 |
| 3:C:153:SER:CB | 3:C:164:THR:CG2 | 2.98 | 0.41 |
| 1:A:548:G:O2' | 1:A:549:C:O5' | 2.39 | 0.41 |
| 1:A:1160:G:N2 | 1:A:1161:C:N1 | 2.69 | 0.41 |
| 1:A:914:A:C4 | 1:A:915:A:N7 | 2.89 | 0.41 |
| 6:F:50:PRO:O | 6:F:51:ILE:C | 2.59 | 0.41 |
| 1:A:1284:C:C5 | 1:A:1285:A:N7 | 2.89 | 0.41 |
| 1:A:519:C:O2' | 1:A:520:A:C5' | 2.69 | 0.41 |
| 1:A:1399:C:C2 | 1:A:1401:G:C5 | 3.09 | 0.41 |
| 1:A:596:A:C2 | 1:A:597:G:C8 | 3.09 | 0.41 |
| 2:B:40:ILE:CD1 | 2:B:201:GLY:CA | 2.98 | 0.41 |
| 1:A:1425:U:O2 | 1:A:1476:A:C2 | 2.74 | 0.41 |
| 10:J:35:GLN:CG | 10:J:77:VAL:CB | 2.98 | 0.41 |
| 17:Q:64:ARG:HD3 | 17:Q:64:ARG:H | 1.85 | 0.41 |
| 3:C:143:LEU:N | 3:C:143:LEU:CD1 | 2.83 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 17:Q:74:LEU:C | 17:Q:74:LEU:CD1 | 2.89 | 0.41 |
| 13:M:10:ASP:O | 13:M:11:HIS:CB | 2.68 | 0.41 |
| 1:A:1255:G:N1 | 1:A:1279:G:C8 | 2.89 | 0.41 |
| 1:A:205:A:C8 | 1:A:206:C:C5 | 3.09 | 0.41 |
| 1:A:1319:A:C6 | 1:A:1323:G:C4 | 3.08 | 0.41 |
| 1:A:544:G:C6 | 1:A:545:C:C4 | 3.09 | 0.41 |
| 1:A:1358:U:OP2 | 1:A:1359:C:N4 | 2.54 | 0.41 |
| 1:A:536:C:O2' | 1:A:537:G:C5' | 2.69 | 0.41 |
| 1:A:687:A:N7 | 1:A:701:U:C5 | 2.88 | 0.41 |
| 1:A:1055:A:C5 | 1:A:1206:G:C2 | 3.08 | 0.41 |
| 1:A:57:G:C6 | 1:A:58:C:N3 | 2.89 | 0.41 |
| 1:A:949:A:C2' | 1:A:950:U:C5' | 2.98 | 0.41 |
| 4:D:116:LEU:C | 4:D:122:ILE:CD1 | 2.90 | 0.41 |
| 10:J:17:LEU:CD2 | 10:J:17:LEU:C | 2.89 | 0.41 |
| 1:A:246:A:C4' | 1:A:247:G:OP1 | 2.69 | 0.41 |
| 1:A:453:G:C6 | 1:A:454:G:C6 | 3.09 | 0.41 |
| 6:F:55:HIS:ND1 | 6:F:55:HIS:N | 2.69 | 0.41 |
| 9:I:56:MET:O | 9:I:58:GLU:N | 2.54 | 0.41 |
| 1:A:368:U:O2' | 1:A:369:G:P | 2.78 | 0.41 |
| 1:A:369:G:C5 | 1:A:393:A:C2 | 3.09 | 0.41 |
| 1:A:384:G:C5 | 1:A:385:C:C4 | 3.09 | 0.41 |
| 1:A:258:G:N2 | 1:A:259:G:C1' | 2.83 | 0.41 |
| 14:N:79:SER:O | 14:N:80:ARG:C | 2.59 | 0.41 |
| 14:N:42:ASN:C | 14:N:44:VAL:N | 2.74 | 0.41 |
| 1:A:290:C:C2' | 1:A:291:U:C5' | 2.98 | 0.41 |
| 2:B:81:ASP:OD1 | 2:B:82:ALA:N | 2.53 | 0.41 |
| 7:G:80:GLY:C | 7:G:82:SER:N | 2.74 | 0.41 |
| 1:A:849:G:N1 | 1:A:850:U:C2 | 2.89 | 0.41 |
| 3:C:59:PRO:O | 3:C:60:ALA:O | 2.38 | 0.41 |
| 1:A:551:U:C6 | 1:A:551:U:C3' | 3.03 | 0.41 |
| 19:S:4:LEU:O | 19:S:5:LYS:CB | 2.69 | 0.41 |
| 19:S:55:GLN:NE2 | 19:S:56:HIS:N | 2.69 | 0.41 |
| 16:P:20:VAL:CG2 | 16:P:21:VAL:N | 2.83 | 0.41 |
| 6:F:97:THR:O | 6:F:98:GLU:CG | 2.69 | 0.41 |
| 1:A:1290:G:OP1 | 7:G:34:LYS:NZ | 2.53 | 0.41 |
| 1:A:1103:C:C3' | 1:A:1103:C:C6 | 3.04 | 0.41 |
| 17:Q:22:VAL:CG2 | 17:Q:45:VAL:HG21 | 2.51 | 0.41 |
| 1:A:1256:A:N9 | 1:A:1258:G:C6 | 2.89 | 0.41 |
| 1:A:1322:C:O2' | 1:A:1323:G:P | 2.79 | 0.41 |
| 4:D:31:CYS:SG | 4:D:32:LYS:N | 2.94 | 0.41 |
| 1:A:1078:U:C5 | 1:A:1079:G:N7 | 2.89 | 0.41 |
| 1:A:1078:U:C6 | 1:A:1078:U:C3' | 3.04 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:527:G:O2' | 1:A:535:A:N1 | 2.54 | 0.41 |
| 1:A:506:G:C5 | 1:A:507:C:C4 | 3.09 | 0.41 |
| 2:B:58:LYS:C | 2:B:58:LYS:CD | 2.89 | 0.41 |
| 8:H:40:LYS:O | 8:H:43:GLY:N | 2.54 | 0.41 |
| 1:A:879:C:C3' | 1:A:879:C:C6 | 3.04 | 0.41 |
| 1:A:1343:G:C5 | 1:A:1344:C:C4 | 3.09 | 0.41 |
| 1:A:890:G:O2' | 1:A:906:A:N6 | 2.54 | 0.41 |
| 1:A:1460:C:C2' | 1:A:1461:G:O5' | 2.69 | 0.41 |
| 1:A:1473:G:C2' | 1:A:1474:U:C5' | 2.99 | 0.41 |
| 5:E:96:GLN:N | 5:E:123:LEU:O | 2.54 | 0.41 |
| 17:Q:16:MET:O | 17:Q:17:GLU:C | 2.59 | 0.40 |
| 1:A:254:G:OP1 | 17:Q:68:LYS:O | 2.38 | 0.40 |
| 17:Q:27:PHE:C | 17:Q:28:VAL:CG1 | 2.89 | 0.40 |
| 1:A:1283:U:O2' | 1:A:1284:C:O5' | 2.39 | 0.40 |
| 2:B:52:ALA:O | 2:B:56:LEU:CB | 2.69 | 0.40 |
| 1:A:1049:U:O2' | 1:A:1050:G:P | 2.79 | 0.40 |
| 1:A:1079:G:N1 | 1:A:1080:A:C6 | 2.89 | 0.40 |
| 1:A:960:U:O2' | 1:A:961:U:OP2 | 2.39 | 0.40 |
| 4:D:121:ALA:C | 4:D:122:ILE:CD1 | 2.89 | 0.40 |
| 15:O:81:ILE:O | 15:O:82:GLU:C | 2.58 | 0.40 |
| 4:D:167:PRO:CB | 4:D:170:LEU:CD1 | 2.99 | 0.40 |
| 1:A:1312:G:C2 | 1:A:1313:U:C2 | 3.08 | 0.40 |
| 1:A:774:G:C4 | 1:A:775:G:C8 | 3.10 | 0.40 |
| 4:D:59:LYS:O | 4:D:62:ARG:N | 2.54 | 0.40 |
| 1:A:250:A:O4' | 1:A:252:U:C6 | 2.75 | 0.40 |
| 2:B:168:GLU:O | 2:B:169:HIS:C | 2.59 | 0.40 |
| 4:D:102:TYR:C | 4:D:102:TYR:CD2 | 2.95 | 0.40 |
| 6:F:49:TYR:CD2 | 6:F:49:TYR:C | 2.94 | 0.40 |
| 17:Q:12:VAL:HG12 | 17:Q:21:VAL:O | 2.20 | 0.40 |
| 1:A:428:G:C4 | 1:A:430:A:N7 | 2.89 | 0.40 |
| 1:A:1256:A:N3 | 1:A:1258:G:O6 | 2.54 | 0.40 |
| 1:A:1084:G:C4 | 1:A:1085:U:C4 | 3.09 | 0.40 |
| 1:A:937:A:C2 | 1:A:1379:G:O6 | 2.75 | 0.40 |
| 9:I:6:TYR:O | 9:I:85:ALA:CA | 2.69 | 0.40 |
| 1:A:148:G:C2' | 1:A:149:A:O5' | 2.69 | 0.40 |
| 13:M:2:ARG:C | 13:M:3:ILE:CG2 | 2.89 | 0.40 |
| 16:P:75:ILE:O | 16:P:77:GLU:N | 2.54 | 0.40 |
| 1:A:1032:G:C2 | 1:A:1033:G:C1' | 3.04 | 0.40 |
| 1:A:257:G:C2 | 1:A:258:G:C5 | 3.09 | 0.40 |
| 1:A:1101:A:C4' | 1:A:1102:A:O5' | 2.70 | 0.40 |
| 1:A:929:G:C6 | 1:A:930:C:C4 | 3.09 | 0.40 |
| 15:O:73:ASP:O | 15:O:74:VAL:C | 2.60 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|----------------|-----------------|-------------|----------|
| 15:O:74:VAL:O | 15:O:75:ALA:C | 2.59 | 0.40 |
| 1:A:188:C:O2 | 1:A:188:C:C2' | 2.70 | 0.40 |
| 1:A:266:G:OP2 | 1:A:267:C:C5 | 2.74 | 0.40 |
| 1:A:429:U:C3' | 4:D:8:LEU:CD2 | 2.99 | 0.40 |
| 6:F:51:ILE:O | 6:F:52:ASN:CB | 2.70 | 0.40 |
| 1:A:32:A:O2' | 1:A:33:A:O4' | 2.40 | 0.40 |
| 1:A:1316:G:C5 | 1:A:1318:A:OP2 | 2.74 | 0.40 |
| 1:A:1069:C:C4 | 1:A:1070:U:C5 | 3.10 | 0.40 |
| 1:A:1115:U:C2 | 1:A:1116:U:C5 | 3.09 | 0.40 |
| 5:E:112:ALA:O | 5:E:115:GLU:N | 2.54 | 0.40 |
| 1:A:1422:G:C2 | 1:A:1423:G:C8 | 3.09 | 0.40 |
| 1:A:766:A:C4 | 1:A:814:A:C2 | 3.09 | 0.40 |
| 1:A:1331:G:O2' | 1:A:1332:A:P | 2.79 | 0.40 |
| 1:A:1441:A:N7 | 1:A:1442:G:N7 | 2.69 | 0.40 |
| 1:A:600:A:C2 | 1:A:639:G:C4 | 3.09 | 0.40 |
| 1:A:1247:U:O2' | 1:A:1248:A:C5' | 2.69 | 0.40 |
| 1:A:21:G:N2 | 1:A:22:G:C6 | 2.89 | 0.40 |
| 3:C:49:ALA:O | 3:C:50:SER:C | 2.59 | 0.40 |
| 8:H:17:GLN:O | 8:H:18:ALA:C | 2.59 | 0.40 |
| 1:A:402:G:C5 | 1:A:403:C:C5 | 3.10 | 0.40 |
| 5:E:76:ASN:ND2 | 5:E:76:ASN:C | 2.74 | 0.40 |
| 2:B:57:ASN:C | 2:B:57:ASN:ND2 | 2.75 | 0.40 |
| 13:M:89:ARG:CB | 13:M:96:VAL:CG2 | 2.99 | 0.40 |
| 1:A:251:G:C2 | 1:A:266:G:C5 | 3.08 | 0.40 |
| 1:A:1298:U:C4' | 1:A:1299:A:O5' | 2.69 | 0.40 |
| 1:A:1284:C:C2' | 1:A:1285:A:C8 | 3.04 | 0.40 |
| 1:A:214:C:C6 | 1:A:215:C:C5 | 3.09 | 0.40 |
| 1:A:438:U:C6 | 1:A:494:G:O6 | 2.75 | 0.40 |
| 1:A:978:A:OP1 | 1:A:980:C:N4 | 2.54 | 0.40 |
| 1:A:500:G:C2' | 1:A:501:C:C6 | 3.04 | 0.40 |
| 9:I:31:GLN:O | 9:I:32:ARG:CB | 2.70 | 0.40 |
| 1:A:417:G:C6 | 1:A:418:C:N4 | 2.90 | 0.40 |
| 1:A:1069:C:C2' | 1:A:1070:U:C5' | 2.99 | 0.40 |
| 1:A:582:C:C4 | 1:A:583:A:N7 | 2.90 | 0.40 |
| 1:A:131:A:C2 | 1:A:132:C:C4 | 3.09 | 0.40 |
| 2:B:140:LEU:O | 2:B:142:LYS:N | 2.54 | 0.40 |
| 1:A:1331:G:O2' | 1:A:1332:A:O5' | 2.39 | 0.40 |
| 1:A:585:G:N2 | 1:A:878:A:O2' | 2.55 | 0.40 |
| 1:A:1461:G:C5 | 1:A:1462:C:C5 | 3.10 | 0.40 |
| 10:J:73:LEU:O | 10:J:74:VAL:CB | 2.69 | 0.40 |
| 1:A:640:A:O2' | 8:H:107:LYS:NZ | 2.54 | 0.40 |
| 20:T:9:ARG:NH1 | 20:T:12:GLN:NE2 | 2.70 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|----------------|-----------------|-------------|----------|
| 1:A:1256:A:C6 | 1:A:1278:G:C2 | 3.09 | 0.40 |
| 1:A:1169:A:O2' | 1:A:1170:A:O4' | 2.40 | 0.40 |
| 1:A:464:U:C6 | 1:A:466:A:OP2 | 2.74 | 0.40 |
| 21:U:8:ASN:O | 21:U:11:PHE:CE2 | 2.75 | 0.40 |
| 1:A:1141:C:C2 | 1:A:1142:G:C8 | 3.10 | 0.40 |
| 1:A:198:G:N1 | 1:A:220:G:C4 | 2.89 | 0.40 |
| 1:A:1241:G:N2 | 1:A:1242:G:C5 | 2.90 | 0.40 |
| 10:J:82:LYS:O | 10:J:86:ALA:N | 2.54 | 0.40 |
| 12:L:56:LEU:C | 12:L:58:ASN:N | 2.73 | 0.40 |
| 1:A:1117:A:O3' | 9:I:105:ARG:NE | 2.55 | 0.40 |
| 1:A:384:G:C6 | 1:A:385:C:N3 | 2.89 | 0.40 |
| 1:A:242:G:C2 | 1:A:245:U:C4 | 3.09 | 0.40 |
| 1:A:1442:G:C4 | 1:A:1443:C:C5 | 3.08 | 0.40 |
| 1:A:157:U:O2 | 1:A:165:G:C2 | 2.74 | 0.40 |
| 1:A:832:G:C2 | 1:A:833:G:C8 | 3.10 | 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 | 216/218 (99%) | 133 (62%) | 51 (24%) | 32 (15%) | 0 | 2 |
| 3 | C | 204/206 (99%) | 144 (71%) | 36 (18%) | 24 (12%) | 1 | 4 |
| 4 | D | 203/205 (99%) | 127 (63%) | 43 (21%) | 33 (16%) | 0 | 0 |
| 5 | E | 148/150 (99%) | 97 (66%) | 28 (19%) | 23 (16%) | 0 | 1 |
| 6 | F | 98/100 (98%) | 71 (72%) | 15 (15%) | 12 (12%) | 1 | 4 |
| 7 | G | 149/151 (99%) | 100 (67%) | 37 (25%) | 12 (8%) | 1 | 10 |
| 8 | H | 127/129 (98%) | 101 (80%) | 15 (12%) | 11 (9%) | 1 | 9 |
| 9 | I | 125/127 (98%) | 81 (65%) | 28 (22%) | 16 (13%) | 0 | 3 |
| 10 | J | 96/98 (98%) | 69 (72%) | 10 (10%) | 17 (18%) | 0 | 0 |
| 11 | K | 115/117 (98%) | 80 (70%) | 20 (17%) | 15 (13%) | 0 | 3 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 12 | L | 121/123 (98%) | 88 (73%) | 21 (17%) | 12 (10%) | 1 | 6 |
| 13 | M | 112/114 (98%) | 83 (74%) | 19 (17%) | 10 (9%) | 1 | 8 |
| 14 | N | 92/100 (92%) | 60 (65%) | 18 (20%) | 14 (15%) | 0 | 1 |
| 15 | O | 86/88 (98%) | 59 (69%) | 19 (22%) | 8 (9%) | 1 | 7 |
| 16 | P | 80/82 (98%) | 59 (74%) | 12 (15%) | 9 (11%) | 1 | 4 |
| 17 | Q | 78/80 (98%) | 48 (62%) | 24 (31%) | 6 (8%) | 1 | 11 |
| 18 | R | 53/55 (96%) | 40 (76%) | 10 (19%) | 3 (6%) | 3 | 18 |
| 19 | S | 77/79 (98%) | 51 (66%) | 15 (20%) | 11 (14%) | 0 | 2 |
| 20 | T | 83/85 (98%) | 57 (69%) | 21 (25%) | 5 (6%) | 2 | 17 |
| 21 | U | 49/51 (96%) | 25 (51%) | 12 (24%) | 12 (24%) | 0 | 0 |
| All | All | 2312/2358 (98%) | 1573 (68%) | 454 (20%) | 285 (12%) | 1 | 3 |

All (285) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 21 | TYR |
| 2 | B | 33 | ALA |
| 2 | B | 37 | VAL |
| 2 | B | 72 | LYS |
| 2 | B | 75 | ALA |
| 2 | B | 119 | GLN |
| 2 | B | 150 | ILE |
| 3 | C | 16 | PRO |
| 3 | C | 17 | TRP |
| 3 | C | 60 | ALA |
| 3 | C | 126 | ARG |
| 3 | C | 165 | GLU |
| 3 | C | 192 | TYR |
| 3 | C | 205 | GLU |
| 4 | D | 24 | VAL |
| 4 | D | 25 | ARG |
| 4 | D | 26 | ALA |
| 4 | D | 28 | ASP |
| 4 | D | 29 | THR |
| 4 | D | 32 | LYS |
| 4 | D | 33 | ILE |
| 4 | D | 34 | GLU |
| 4 | D | 36 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 147 | LYS |
| 4 | D | 152 | SER |
| 4 | D | 159 | GLU |
| 4 | D | 172 | VAL |
| 4 | D | 173 | ASP |
| 4 | D | 191 | SER |
| 4 | D | 192 | ALA |
| 5 | E | 97 | PRO |
| 5 | E | 110 | MET |
| 5 | E | 137 | ARG |
| 5 | E | 153 | ALA |
| 6 | F | 91 | ARG |
| 7 | G | 93 | VAL |
| 8 | H | 48 | PHE |
| 8 | H | 49 | LYS |
| 8 | H | 66 | GLN |
| 8 | H | 88 | LYS |
| 9 | I | 8 | THR |
| 9 | I | 40 | ARG |
| 9 | I | 43 | ALA |
| 9 | I | 71 | ILE |
| 9 | I | 119 | LYS |
| 9 | I | 128 | LYS |
| 10 | J | 57 | VAL |
| 10 | J | 101 | SER |
| 11 | K | 46 | ALA |
| 11 | K | 126 | ARG |
| 12 | L | 23 | LEU |
| 12 | L | 43 | LYS |
| 12 | L | 73 | LEU |
| 12 | L | 75 | GLU |
| 12 | L | 88 | ASP |
| 13 | M | 2 | ARG |
| 13 | M | 46 | GLU |
| 14 | N | 27 | LYS |
| 14 | N | 33 | VAL |
| 14 | N | 51 | PRO |
| 14 | N | 52 | ARG |
| 15 | O | 17 | ASP |
| 15 | O | 24 | THR |
| 15 | O | 72 | LYS |
| 16 | P | 11 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 80 | LYS |
| 17 | Q | 12 | VAL |
| 17 | Q | 50 | ASN |
| 17 | Q | 52 | CYS |
| 17 | Q | 75 | VAL |
| 18 | R | 47 | ARG |
| 19 | S | 27 | LYS |
| 20 | T | 3 | ILE |
| 20 | T | 67 | HIS |
| 21 | U | 11 | PHE |
| 21 | U | 12 | ASP |
| 21 | U | 23 | GLU |
| 2 | B | 17 | HIS |
| 2 | B | 18 | GLN |
| 2 | B | 20 | ARG |
| 2 | B | 40 | ILE |
| 2 | B | 44 | LYS |
| 2 | B | 63 | LYS |
| 2 | B | 96 | LEU |
| 2 | B | 125 | PHE |
| 2 | B | 133 | ALA |
| 2 | B | 169 | HIS |
| 2 | B | 209 | VAL |
| 2 | B | 210 | THR |
| 2 | B | 219 | THR |
| 3 | C | 148 | ILE |
| 4 | D | 23 | GLY |
| 4 | D | 35 | GLN |
| 4 | D | 124 | VAL |
| 4 | D | 132 | ALA |
| 4 | D | 167 | PRO |
| 4 | D | 174 | ALA |
| 4 | D | 195 | ASN |
| 4 | D | 196 | GLU |
| 4 | D | 197 | HIS |
| 5 | E | 11 | GLN |
| 5 | E | 50 | GLY |
| 5 | E | 75 | LEU |
| 5 | E | 103 | GLY |
| 5 | E | 108 | GLY |
| 5 | E | 112 | ALA |
| 5 | E | 113 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 121 | ASN |
| 5 | E | 157 | GLY |
| 6 | F | 54 | LEU |
| 6 | F | 69 | GLU |
| 6 | F | 86 | ARG |
| 7 | G | 8 | GLN |
| 7 | G | 79 | VAL |
| 7 | G | 84 | TYR |
| 8 | H | 2 | MET |
| 8 | H | 74 | ILE |
| 9 | I | 30 | ASN |
| 10 | J | 34 | ALA |
| 10 | J | 61 | ALA |
| 10 | J | 74 | VAL |
| 10 | J | 92 | LEU |
| 11 | K | 88 | PRO |
| 11 | K | 102 | ALA |
| 12 | L | 33 | CYS |
| 12 | L | 117 | GLY |
| 12 | L | 122 | LYS |
| 13 | M | 6 | ILE |
| 13 | M | 104 | ASN |
| 13 | M | 113 | LYS |
| 14 | N | 22 | LYS |
| 14 | N | 41 | TRP |
| 14 | N | 43 | ALA |
| 14 | N | 80 | ARG |
| 15 | O | 74 | VAL |
| 15 | O | 85 | GLY |
| 16 | P | 24 | SER |
| 17 | Q | 67 | SER |
| 19 | S | 79 | TYR |
| 20 | T | 5 | SER |
| 21 | U | 8 | ASN |
| 21 | U | 35 | GLU |
| 21 | U | 37 | TYR |
| 2 | B | 22 | TRP |
| 2 | B | 41 | ASN |
| 2 | B | 71 | THR |
| 2 | B | 73 | ARG |
| 2 | B | 148 | GLY |
| 3 | C | 11 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 50 | SER |
| 3 | C | 62 | SER |
| 3 | C | 145 | ALA |
| 4 | D | 22 | SER |
| 4 | D | 31 | CYS |
| 4 | D | 148 | ALA |
| 4 | D | 165 | GLU |
| 4 | D | 189 | ASP |
| 5 | E | 23 | THR |
| 5 | E | 25 | LYS |
| 5 | E | 44 | ARG |
| 5 | E | 98 | ALA |
| 5 | E | 156 | ARG |
| 6 | F | 53 | LYS |
| 6 | F | 92 | THR |
| 6 | F | 94 | HIS |
| 7 | G | 129 | ASN |
| 7 | G | 130 | LYS |
| 7 | G | 147 | ASN |
| 9 | I | 38 | PHE |
| 9 | I | 56 | MET |
| 9 | I | 88 | GLU |
| 9 | I | 90 | ASP |
| 9 | I | 120 | ALA |
| 10 | J | 81 | GLU |
| 11 | K | 40 | ALA |
| 11 | K | 51 | PHE |
| 13 | M | 3 | ILE |
| 13 | M | 4 | ALA |
| 14 | N | 14 | ALA |
| 14 | N | 16 | ALA |
| 14 | N | 61 | ASN |
| 14 | N | 91 | GLU |
| 15 | O | 2 | LEU |
| 15 | O | 16 | ARG |
| 16 | P | 76 | LYS |
| 18 | R | 33 | THR |
| 19 | S | 4 | LEU |
| 19 | S | 5 | LYS |
| 19 | S | 26 | ASP |
| 19 | S | 42 | ASN |
| 21 | U | 25 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 141 | GLU |
| 3 | C | 65 | VAL |
| 3 | C | 106 | ARG |
| 3 | C | 139 | ASN |
| 4 | D | 6 | PRO |
| 4 | D | 166 | LYS |
| 5 | E | 74 | ALA |
| 5 | E | 77 | ASN |
| 6 | F | 39 | LEU |
| 6 | F | 51 | ILE |
| 6 | F | 56 | LYS |
| 6 | F | 63 | ASN |
| 7 | G | 112 | ASP |
| 8 | H | 47 | ASP |
| 8 | H | 77 | VAL |
| 9 | I | 12 | LYS |
| 10 | J | 35 | GLN |
| 10 | J | 36 | VAL |
| 10 | J | 41 | PRO |
| 10 | J | 62 | ARG |
| 10 | J | 75 | ASP |
| 11 | K | 13 | LYS |
| 11 | K | 16 | SER |
| 11 | K | 97 | ARG |
| 11 | K | 124 | LYS |
| 12 | L | 57 | THR |
| 13 | M | 26 | LYS |
| 13 | M | 84 | CYS |
| 14 | N | 2 | LYS |
| 16 | P | 42 | ILE |
| 19 | S | 3 | SER |
| 19 | S | 48 | ILE |
| 19 | S | 63 | ASP |
| 20 | T | 17 | ARG |
| 20 | T | 72 | ALA |
| 21 | U | 36 | PHE |
| 2 | B | 42 | LEU |
| 2 | B | 154 | GLY |
| 2 | B | 157 | PRO |
| 3 | C | 14 | VAL |
| 3 | C | 21 | TRP |
| 3 | C | 35 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 36 | PHE |
| 3 | C | 107 | LYS |
| 3 | C | 186 | SER |
| 6 | F | 99 | ALA |
| 8 | H | 41 | GLU |
| 8 | H | 95 | MET |
| 9 | I | 31 | GLN |
| 9 | I | 32 | ARG |
| 10 | J | 42 | LEU |
| 11 | K | 14 | GLN |
| 12 | L | 24 | GLU |
| 12 | L | 77 | SER |
| 13 | M | 9 | PRO |
| 15 | O | 45 | HIS |
| 16 | P | 79 | ASN |
| 19 | S | 8 | PRO |
| 21 | U | 24 | LYS |
| 21 | U | 26 | GLY |
| 2 | B | 211 | LEU |
| 3 | C | 191 | THR |
| 5 | E | 148 | SER |
| 7 | G | 52 | ARG |
| 8 | H | 26 | MET |
| 9 | I | 66 | VAL |
| 10 | J | 93 | ALA |
| 11 | K | 77 | GLY |
| 16 | P | 9 | HIS |
| 16 | P | 13 | LYS |
| 18 | R | 54 | LEU |
| 21 | U | 9 | GLU |
| 2 | B | 70 | GLY |
| 10 | J | 33 | GLY |
| 16 | P | 78 | VAL |
| 17 | Q | 11 | VAL |
| 2 | B | 200 | PRO |
| 3 | C | 93 | ILE |
| 4 | D | 44 | LYS |
| 5 | E | 104 | ILE |
| 5 | E | 149 | PRO |
| 7 | G | 6 | ILE |
| 10 | J | 39 | PRO |
| 11 | K | 73 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | S | 44 | ILE |
| 7 | G | 5 | VAL |
| 7 | G | 7 | GLY |
| 12 | L | 41 | PRO |
| 10 | J | 100 | ILE |
| 11 | K | 38 | GLY |
| 11 | K | 89 | GLY |
| 14 | N | 44 | VAL |
| 3 | C | 59 | PRO |
| 21 | U | 52 | 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 | 180/180 (100%) | 142 (79%) | 38 (21%) | 1 | 7 |
| 3 | C | 170/170 (100%) | 136 (80%) | 34 (20%) | 2 | 8 |
| 4 | D | 172/172 (100%) | 138 (80%) | 34 (20%) | 2 | 8 |
| 5 | E | 113/113 (100%) | 77 (68%) | 36 (32%) | 0 | 1 |
| 6 | F | 87/87 (100%) | 71 (82%) | 16 (18%) | 2 | 9 |
| 7 | G | 124/124 (100%) | 111 (90%) | 13 (10%) | 10 | 35 |
| 8 | H | 104/104 (100%) | 83 (80%) | 21 (20%) | 2 | 8 |
| 9 | I | 105/105 (100%) | 82 (78%) | 23 (22%) | 1 | 6 |
| 10 | J | 86/86 (100%) | 70 (81%) | 16 (19%) | 2 | 9 |
| 11 | K | 90/90 (100%) | 73 (81%) | 17 (19%) | 2 | 9 |
| 12 | L | 103/103 (100%) | 76 (74%) | 27 (26%) | 1 | 2 |
| 13 | M | 92/92 (100%) | 84 (91%) | 8 (9%) | 15 | 49 |
| 14 | N | 79/83 (95%) | 71 (90%) | 8 (10%) | 11 | 38 |
| 15 | O | 76/76 (100%) | 59 (78%) | 17 (22%) | 1 | 6 |
| 16 | P | 65/65 (100%) | 54 (83%) | 11 (17%) | 3 | 11 |
| 17 | Q | 74/74 (100%) | 60 (81%) | 14 (19%) | 2 | 9 |
| 18 | R | 48/48 (100%) | 44 (92%) | 4 (8%) | 16 | 53 |

Continued on next page...

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|-------------|----|
| 19 | S | 70/70 (100%) | 63 (90%) | 7 (10%) | 11 | 38 |
| 20 | T | 65/65 (100%) | 48 (74%) | 17 (26%) | 1 | 2 |
| 21 | U | 44/44 (100%) | 36 (82%) | 8 (18%) | 2 | 10 |
| All | All | 1947/1951 (100%) | 1578 (81%) | 369 (19%) | 2 | 9 |

All (369) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 10 | LYS |
| 2 | B | 13 | VAL |
| 2 | B | 15 | PHE |
| 2 | B | 19 | THR |
| 2 | B | 20 | ARG |
| 2 | B | 22 | TRP |
| 2 | B | 26 | MET |
| 2 | B | 36 | LYS |
| 2 | B | 38 | HIS |
| 2 | B | 48 | MET |
| 2 | B | 57 | ASN |
| 2 | B | 67 | LEU |
| 2 | B | 73 | ARG |
| 2 | B | 81 | ASP |
| 2 | B | 87 | ASP |
| 2 | B | 88 | GLN |
| 2 | B | 90 | PHE |
| 2 | B | 94 | ARG |
| 2 | B | 100 | LEU |
| 2 | B | 102 | ASN |
| 2 | B | 108 | GLN |
| 2 | B | 112 | ARG |
| 2 | B | 119 | GLN |
| 2 | B | 122 | ASP |
| 2 | B | 124 | THR |
| 2 | B | 128 | LEU |
| 2 | B | 130 | LYS |
| 2 | B | 136 | ARG |
| 2 | B | 138 | ARG |
| 2 | B | 143 | LEU |
| 2 | B | 156 | LEU |
| 2 | B | 158 | ASP |
| 2 | B | 170 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 193 | ASP |
| 2 | B | 206 | ILE |
| 2 | B | 211 | LEU |
| 2 | B | 219 | THR |
| 2 | B | 221 | ARG |
| 3 | C | 2 | GLN |
| 3 | C | 13 | ILE |
| 3 | C | 15 | LYS |
| 3 | C | 17 | TRP |
| 3 | C | 22 | PHE |
| 3 | C | 24 | ASN |
| 3 | C | 25 | THR |
| 3 | C | 26 | LYS |
| 3 | C | 27 | GLU |
| 3 | C | 32 | LEU |
| 3 | C | 35 | ASP |
| 3 | C | 36 | PHE |
| 3 | C | 42 | LEU |
| 3 | C | 50 | SER |
| 3 | C | 54 | ILE |
| 3 | C | 58 | ARG |
| 3 | C | 69 | THR |
| 3 | C | 79 | LYS |
| 3 | C | 89 | VAL |
| 3 | C | 99 | GLN |
| 3 | C | 102 | ILE |
| 3 | C | 106 | ARG |
| 3 | C | 133 | MET |
| 3 | C | 139 | ASN |
| 3 | C | 143 | LEU |
| 3 | C | 148 | ILE |
| 3 | C | 150 | VAL |
| 3 | C | 165 | GLU |
| 3 | C | 166 | TRP |
| 3 | C | 177 | LEU |
| 3 | C | 184 | ASN |
| 3 | C | 186 | SER |
| 3 | C | 189 | HIS |
| 3 | C | 199 | VAL |
| 4 | D | 19 | PHE |
| 4 | D | 21 | LYS |
| 4 | D | 25 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 30 | LYS |
| 4 | D | 31 | CYS |
| 4 | D | 47 | LEU |
| 4 | D | 52 | VAL |
| 4 | D | 54 | LEU |
| 4 | D | 55 | ARG |
| 4 | D | 57 | LYS |
| 4 | D | 63 | ILE |
| 4 | D | 69 | ARG |
| 4 | D | 84 | ASN |
| 4 | D | 88 | ASN |
| 4 | D | 89 | LEU |
| 4 | D | 92 | LEU |
| 4 | D | 101 | VAL |
| 4 | D | 102 | TYR |
| 4 | D | 115 | GLN |
| 4 | D | 122 | ILE |
| 4 | D | 127 | ARG |
| 4 | D | 131 | ILE |
| 4 | D | 145 | ARG |
| 4 | D | 147 | LYS |
| 4 | D | 153 | ARG |
| 4 | D | 160 | LEU |
| 4 | D | 162 | GLU |
| 4 | D | 163 | GLN |
| 4 | D | 165 | GLU |
| 4 | D | 166 | LYS |
| 4 | D | 170 | LEU |
| 4 | D | 193 | ASP |
| 4 | D | 199 | ILE |
| 4 | D | 205 | LYS |
| 5 | E | 9 | GLU |
| 5 | E | 10 | LEU |
| 5 | E | 11 | GLN |
| 5 | E | 14 | LEU |
| 5 | E | 18 | ASN |
| 5 | E | 24 | VAL |
| 5 | E | 25 | LYS |
| 5 | E | 29 | ILE |
| 5 | E | 31 | SER |
| 5 | E | 37 | VAL |
| 5 | E | 42 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 47 | PHE |
| 5 | E | 53 | ARG |
| 5 | E | 59 | ILE |
| 5 | E | 68 | ARG |
| 5 | E | 75 | LEU |
| 5 | E | 76 | ASN |
| 5 | E | 79 | THR |
| 5 | E | 81 | GLN |
| 5 | E | 92 | ARG |
| 5 | E | 93 | VAL |
| 5 | E | 95 | MET |
| 5 | E | 96 | GLN |
| 5 | E | 113 | VAL |
| 5 | E | 116 | VAL |
| 5 | E | 119 | VAL |
| 5 | E | 121 | ASN |
| 5 | E | 123 | LEU |
| 5 | E | 135 | VAL |
| 5 | E | 136 | VAL |
| 5 | E | 139 | THR |
| 5 | E | 140 | ILE |
| 5 | E | 141 | ASP |
| 5 | E | 152 | VAL |
| 5 | E | 155 | LYS |
| 5 | E | 156 | ARG |
| 6 | F | 7 | VAL |
| 6 | F | 14 | GLN |
| 6 | F | 15 | SER |
| 6 | F | 17 | GLN |
| 6 | F | 24 | ARG |
| 6 | F | 36 | ILE |
| 6 | F | 54 | LEU |
| 6 | F | 55 | HIS |
| 6 | F | 64 | VAL |
| 6 | F | 68 | GLN |
| 6 | F | 69 | GLU |
| 6 | F | 77 | THR |
| 6 | F | 84 | VAL |
| 6 | F | 86 | ARG |
| 6 | F | 89 | VAL |
| 6 | F | 93 | LYS |
| 7 | G | 3 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 4 | ARG |
| 7 | G | 8 | GLN |
| 7 | G | 12 | LEU |
| 7 | G | 22 | LEU |
| 7 | G | 26 | VAL |
| 7 | G | 37 | THR |
| 7 | G | 47 | GLU |
| 7 | G | 72 | VAL |
| 7 | G | 93 | VAL |
| 7 | G | 121 | ASN |
| 7 | G | 123 | LEU |
| 7 | G | 143 | MET |
| 8 | H | 12 | ARG |
| 8 | H | 21 | LYS |
| 8 | H | 24 | VAL |
| 8 | H | 41 | GLU |
| 8 | H | 48 | PHE |
| 8 | H | 50 | VAL |
| 8 | H | 54 | THR |
| 8 | H | 58 | LEU |
| 8 | H | 66 | GLN |
| 8 | H | 72 | GLU |
| 8 | H | 76 | ARG |
| 8 | H | 82 | LEU |
| 8 | H | 86 | LYS |
| 8 | H | 89 | ASP |
| 8 | H | 90 | GLU |
| 8 | H | 98 | LEU |
| 8 | H | 103 | VAL |
| 8 | H | 106 | SER |
| 8 | H | 110 | MET |
| 8 | H | 120 | LEU |
| 8 | H | 124 | ILE |
| 9 | I | 13 | SER |
| 9 | I | 21 | LYS |
| 9 | I | 27 | ILE |
| 9 | I | 29 | ILE |
| 9 | I | 37 | TYR |
| 9 | I | 44 | ARG |
| 9 | I | 47 | VAL |
| 9 | I | 48 | ARG |
| 9 | I | 56 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 60 | LEU |
| 9 | I | 62 | LEU |
| 9 | I | 64 | ILE |
| 9 | I | 67 | LYS |
| 9 | I | 84 | ARG |
| 9 | I | 86 | LEU |
| 9 | I | 87 | MET |
| 9 | I | 93 | LEU |
| 9 | I | 105 | ARG |
| 9 | I | 106 | ASP |
| 9 | I | 110 | VAL |
| 9 | I | 115 | VAL |
| 9 | I | 126 | PHE |
| 9 | I | 128 | LYS |
| 10 | J | 6 | ILE |
| 10 | J | 7 | ARG |
| 10 | J | 8 | ILE |
| 10 | J | 17 | LEU |
| 10 | J | 19 | ASP |
| 10 | J | 22 | THR |
| 10 | J | 35 | GLN |
| 10 | J | 48 | ARG |
| 10 | J | 59 | LYS |
| 10 | J | 63 | ASP |
| 10 | J | 70 | HIS |
| 10 | J | 73 | LEU |
| 10 | J | 84 | VAL |
| 10 | J | 87 | LEU |
| 10 | J | 89 | ARG |
| 10 | J | 98 | VAL |
| 11 | K | 15 | VAL |
| 11 | K | 17 | ASP |
| 11 | K | 30 | ILE |
| 11 | K | 45 | THR |
| 11 | K | 51 | PHE |
| 11 | K | 55 | ARG |
| 11 | K | 57 | SER |
| 11 | K | 64 | VAL |
| 11 | K | 78 | ILE |
| 11 | K | 82 | GLU |
| 11 | K | 96 | ILE |
| 11 | K | 100 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | K | 106 | ILE |
| 11 | K | 124 | LYS |
| 11 | K | 125 | LYS |
| 11 | K | 127 | ARG |
| 11 | K | 128 | VAL |
| 12 | L | 6 | LEU |
| 12 | L | 9 | LYS |
| 12 | L | 13 | ARG |
| 12 | L | 17 | LYS |
| 12 | L | 18 | SER |
| 12 | L | 26 | CYS |
| 12 | L | 32 | VAL |
| 12 | L | 33 | CYS |
| 12 | L | 35 | ARG |
| 12 | L | 40 | THR |
| 12 | L | 43 | LYS |
| 12 | L | 45 | ASN |
| 12 | L | 49 | ARG |
| 12 | L | 51 | VAL |
| 12 | L | 57 | THR |
| 12 | L | 63 | THR |
| 12 | L | 64 | SER |
| 12 | L | 66 | ILE |
| 12 | L | 72 | ASN |
| 12 | L | 73 | LEU |
| 12 | L | 82 | ARG |
| 12 | L | 87 | LYS |
| 12 | L | 88 | ASP |
| 12 | L | 89 | LEU |
| 12 | L | 96 | THR |
| 12 | L | 101 | LEU |
| 12 | L | 109 | ARG |
| 13 | M | 3 | ILE |
| 13 | M | 6 | ILE |
| 13 | M | 7 | ASN |
| 13 | M | 18 | LEU |
| 13 | M | 47 | LEU |
| 13 | M | 71 | GLU |
| 13 | M | 100 | ARG |
| 13 | M | 103 | THR |
| 14 | N | 17 | ASP |
| 14 | N | 27 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | N | 58 | ARG |
| 14 | N | 59 | GLN |
| 14 | N | 83 | VAL |
| 14 | N | 84 | ARG |
| 14 | N | 88 | MET |
| 14 | N | 96 | LYS |
| 15 | O | 5 | GLU |
| 15 | O | 7 | THR |
| 15 | O | 10 | ILE |
| 15 | O | 16 | ARG |
| 15 | O | 21 | THR |
| 15 | O | 30 | LEU |
| 15 | O | 38 | LEU |
| 15 | O | 39 | GLN |
| 15 | O | 47 | LYS |
| 15 | O | 56 | LEU |
| 15 | O | 57 | ARG |
| 15 | O | 60 | SER |
| 15 | O | 63 | ARG |
| 15 | O | 65 | LEU |
| 15 | O | 78 | THR |
| 15 | O | 82 | GLU |
| 15 | O | 86 | LEU |
| 16 | P | 1 | MET |
| 16 | P | 3 | THR |
| 16 | P | 6 | LEU |
| 16 | P | 19 | VAL |
| 16 | P | 28 | ARG |
| 16 | P | 29 | ASN |
| 16 | P | 46 | LYS |
| 16 | P | 55 | ASP |
| 16 | P | 63 | GLN |
| 16 | P | 68 | SER |
| 16 | P | 77 | GLU |
| 17 | Q | 3 | LYS |
| 17 | Q | 8 | GLN |
| 17 | Q | 16 | MET |
| 17 | Q | 20 | ILE |
| 17 | Q | 21 | VAL |
| 17 | Q | 37 | ILE |
| 17 | Q | 48 | GLU |
| 17 | Q | 49 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Q | 51 | GLU |
| 17 | Q | 54 | ILE |
| 17 | Q | 64 | ARG |
| 17 | Q | 74 | LEU |
| 17 | Q | 75 | VAL |
| 17 | Q | 80 | LYS |
| 18 | R | 28 | LEU |
| 18 | R | 33 | THR |
| 18 | R | 60 | ARG |
| 18 | R | 70 | THR |
| 19 | S | 20 | LYS |
| 19 | S | 42 | ASN |
| 19 | S | 54 | ARG |
| 19 | S | 55 | GLN |
| 19 | S | 60 | PHE |
| 19 | S | 64 | GLU |
| 19 | S | 79 | TYR |
| 20 | T | 2 | ASN |
| 20 | T | 4 | LYS |
| 20 | T | 7 | LYS |
| 20 | T | 11 | ILE |
| 20 | T | 17 | ARG |
| 20 | T | 26 | MET |
| 20 | T | 27 | MET |
| 20 | T | 33 | LYS |
| 20 | T | 35 | TYR |
| 20 | T | 38 | ILE |
| 20 | T | 42 | ASP |
| 20 | T | 48 | LYS |
| 20 | T | 53 | MET |
| 20 | T | 65 | LEU |
| 20 | T | 75 | LYS |
| 20 | T | 77 | ASN |
| 20 | T | 84 | LYS |
| 21 | U | 4 | LYS |
| 21 | U | 5 | VAL |
| 21 | U | 15 | LEU |
| 21 | U | 18 | PHE |
| 21 | U | 27 | VAL |
| 21 | U | 31 | VAL |
| 21 | U | 39 | LYS |
| 21 | U | 42 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Q | 8 | GLN |
| 17 | Q | 44 | HIS |
| 17 | Q | 46 | HIS |
| 17 | Q | 49 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1532/1533 (99%) | 518 (33%) | 236 (15%) |

All (518) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | U |
| 1 | A | 6 | G |
| 1 | A | 7 | A |
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 13 | U |
| 1 | A | 14 | U |
| 1 | A | 22 | G |
| 1 | A | 31 | G |
| 1 | A | 32 | A |
| 1 | A | 33 | A |
| 1 | A | 39 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 50 | A |
| 1 | A | 51 | A |
| 1 | A | 55 | A |
| 1 | A | 61 | G |
| 1 | A | 63 | C |
| 1 | A | 65 | A |
| 1 | A | 66 | A |
| 1 | A | 67 | C |
| 1 | A | 70 | U |
| 1 | A | 71 | A |
| 1 | A | 72 | A |
| 1 | A | 73 | C |
| 1 | A | 74 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 75 | G |
| 1 | A | 76 | G |
| 1 | A | 77 | A |
| 1 | A | 79 | G |
| 1 | A | 82 | G |
| 1 | A | 83 | C |
| 1 | A | 85 | U |
| 1 | A | 86 | G |
| 1 | A | 87 | C |
| 1 | A | 88 | U |
| 1 | A | 89 | U |
| 1 | A | 90 | C |
| 1 | A | 91 | U |
| 1 | A | 92 | U |
| 1 | A | 93 | U |
| 1 | A | 94 | G |
| 1 | A | 95 | C |
| 1 | A | 97 | G |
| 1 | A | 98 | A |
| 1 | A | 109 | A |
| 1 | A | 110 | C |
| 1 | A | 111 | G |
| 1 | A | 116 | A |
| 1 | A | 117 | G |
| 1 | A | 120 | A |
| 1 | A | 121 | U |
| 1 | A | 122 | G |
| 1 | A | 127 | G |
| 1 | A | 129 | A |
| 1 | A | 130 | A |
| 1 | A | 131 | A |
| 1 | A | 132 | C |
| 1 | A | 140 | U |
| 1 | A | 141 | G |
| 1 | A | 142 | G |
| 1 | A | 143 | A |
| 1 | A | 151 | A |
| 1 | A | 159 | G |
| 1 | A | 163 | C |
| 1 | A | 164 | G |
| 1 | A | 166 | U |
| 1 | A | 174 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 175 | C |
| 1 | A | 181 | A |
| 1 | A | 182 | A |
| 1 | A | 183 | C |
| 1 | A | 185 | U |
| 1 | A | 186 | C |
| 1 | A | 197 | A |
| 1 | A | 198 | G |
| 1 | A | 199 | A |
| 1 | A | 200 | G |
| 1 | A | 202 | G |
| 1 | A | 205 | A |
| 1 | A | 208 | U |
| 1 | A | 209 | U |
| 1 | A | 210 | C |
| 1 | A | 211 | G |
| 1 | A | 212 | G |
| 1 | A | 214 | C |
| 1 | A | 243 | A |
| 1 | A | 244 | U |
| 1 | A | 245 | U |
| 1 | A | 247 | G |
| 1 | A | 250 | A |
| 1 | A | 251 | G |
| 1 | A | 252 | U |
| 1 | A | 253 | A |
| 1 | A | 258 | G |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 268 | U |
| 1 | A | 274 | A |
| 1 | A | 275 | G |
| 1 | A | 276 | G |
| 1 | A | 279 | A |
| 1 | A | 280 | C |
| 1 | A | 285 | C |
| 1 | A | 289 | G |
| 1 | A | 305 | G |
| 1 | A | 306 | A |
| 1 | A | 307 | C |
| 1 | A | 315 | A |
| 1 | A | 316 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 330 | C |
| 1 | A | 331 | G |
| 1 | A | 332 | G |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 346 | G |
| 1 | A | 347 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 365 | U |
| 1 | A | 366 | A |
| 1 | A | 367 | U |
| 1 | A | 368 | U |
| 1 | A | 369 | G |
| 1 | A | 373 | A |
| 1 | A | 374 | A |
| 1 | A | 382 | A |
| 1 | A | 384 | G |
| 1 | A | 385 | C |
| 1 | A | 388 | G |
| 1 | A | 389 | A |
| 1 | A | 390 | U |
| 1 | A | 392 | C |
| 1 | A | 398 | U |
| 1 | A | 401 | C |
| 1 | A | 406 | G |
| 1 | A | 411 | A |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 414 | A |
| 1 | A | 415 | A |
| 1 | A | 421 | U |
| 1 | A | 422 | C |
| 1 | A | 423 | G |
| 1 | A | 424 | G |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 430 | A |
| 1 | A | 431 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 439 | U |
| 1 | A | 440 | C |
| 1 | A | 451 | A |
| 1 | A | 452 | A |
| 1 | A | 453 | G |
| 1 | A | 456 | A |
| 1 | A | 458 | U |
| 1 | A | 459 | A |
| 1 | A | 461 | A |
| 1 | A | 462 | G |
| 1 | A | 463 | U |
| 1 | A | 464 | U |
| 1 | A | 466 | A |
| 1 | A | 467 | U |
| 1 | A | 468 | A |
| 1 | A | 469 | C |
| 1 | A | 470 | C |
| 1 | A | 476 | U |
| 1 | A | 478 | A |
| 1 | A | 481 | G |
| 1 | A | 482 | A |
| 1 | A | 484 | G |
| 1 | A | 485 | U |
| 1 | A | 486 | U |
| 1 | A | 487 | A |
| 1 | A | 488 | C |
| 1 | A | 489 | C |
| 1 | A | 490 | C |
| 1 | A | 496 | A |
| 1 | A | 497 | G |
| 1 | A | 498 | A |
| 1 | A | 499 | A |
| 1 | A | 500 | G |
| 1 | A | 501 | C |
| 1 | A | 508 | U |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 512 | U |
| 1 | A | 513 | C |
| 1 | A | 514 | C |
| 1 | A | 517 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 518 | C |
| 1 | A | 519 | C |
| 1 | A | 520 | A |
| 1 | A | 522 | C |
| 1 | A | 527 | G |
| 1 | A | 532 | A |
| 1 | A | 534 | U |
| 1 | A | 535 | A |
| 1 | A | 536 | C |
| 1 | A | 537 | G |
| 1 | A | 546 | A |
| 1 | A | 548 | G |
| 1 | A | 549 | C |
| 1 | A | 550 | G |
| 1 | A | 552 | U |
| 1 | A | 556 | C |
| 1 | A | 557 | G |
| 1 | A | 559 | A |
| 1 | A | 560 | A |
| 1 | A | 562 | U |
| 1 | A | 563 | A |
| 1 | A | 564 | C |
| 1 | A | 566 | G |
| 1 | A | 567 | G |
| 1 | A | 570 | G |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 575 | G |
| 1 | A | 576 | C |
| 1 | A | 577 | G |
| 1 | A | 588 | G |
| 1 | A | 595 | A |
| 1 | A | 596 | A |
| 1 | A | 597 | G |
| 1 | A | 615 | G |
| 1 | A | 620 | C |
| 1 | A | 642 | A |
| 1 | A | 643 | C |
| 1 | A | 652 | U |
| 1 | A | 653 | U |
| 1 | A | 654 | G |
| 1 | A | 655 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 663 | A |
| 1 | A | 665 | A |
| 1 | A | 682 | G |
| 1 | A | 688 | G |
| 1 | A | 689 | C |
| 1 | A | 695 | A |
| 1 | A | 701 | U |
| 1 | A | 702 | A |
| 1 | A | 703 | G |
| 1 | A | 704 | A |
| 1 | A | 705 | G |
| 1 | A | 717 | U |
| 1 | A | 718 | A |
| 1 | A | 719 | C |
| 1 | A | 721 | G |
| 1 | A | 722 | G |
| 1 | A | 723 | U |
| 1 | A | 731 | G |
| 1 | A | 748 | G |
| 1 | A | 752 | G |
| 1 | A | 753 | A |
| 1 | A | 754 | C |
| 1 | A | 755 | G |
| 1 | A | 777 | A |
| 1 | A | 782 | A |
| 1 | A | 792 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 795 | C |
| 1 | A | 809 | G |
| 1 | A | 813 | U |
| 1 | A | 814 | A |
| 1 | A | 815 | A |
| 1 | A | 816 | A |
| 1 | A | 817 | C |
| 1 | A | 818 | G |
| 1 | A | 828 | U |
| 1 | A | 829 | G |
| 1 | A | 832 | G |
| 1 | A | 841 | C |
| 1 | A | 843 | U |
| 1 | A | 845 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 846 | G |
| 1 | A | 849 | G |
| 1 | A | 859 | G |
| 1 | A | 871 | U |
| 1 | A | 874 | G |
| 1 | A | 875 | U |
| 1 | A | 885 | G |
| 1 | A | 889 | A |
| 1 | A | 890 | G |
| 1 | A | 910 | C |
| 1 | A | 913 | A |
| 1 | A | 914 | A |
| 1 | A | 915 | A |
| 1 | A | 920 | U |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 932 | C |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 936 | C |
| 1 | A | 942 | G |
| 1 | A | 960 | U |
| 1 | A | 961 | U |
| 1 | A | 962 | C |
| 1 | A | 966 | G |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 972 | C |
| 1 | A | 973 | G |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 978 | A |
| 1 | A | 979 | C |
| 1 | A | 982 | U |
| 1 | A | 983 | A |
| 1 | A | 984 | C |
| 1 | A | 985 | C |
| 1 | A | 989 | U |
| 1 | A | 992 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 993 | G |
| 1 | A | 994 | A |
| 1 | A | 995 | C |
| 1 | A | 1003 | G |
| 1 | A | 1004 | A |
| 1 | A | 1008 | U |
| 1 | A | 1018 | G |
| 1 | A | 1022 | A |
| 1 | A | 1026 | G |
| 1 | A | 1028 | C |
| 1 | A | 1030 | U |
| 1 | A | 1031 | C |
| 1 | A | 1032 | G |
| 1 | A | 1033 | G |
| 1 | A | 1034 | G |
| 1 | A | 1037 | C |
| 1 | A | 1050 | G |
| 1 | A | 1051 | C |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1068 | G |
| 1 | A | 1069 | C |
| 1 | A | 1070 | U |
| 1 | A | 1078 | U |
| 1 | A | 1079 | G |
| 1 | A | 1085 | U |
| 1 | A | 1086 | U |
| 1 | A | 1088 | G |
| 1 | A | 1089 | G |
| 1 | A | 1090 | U |
| 1 | A | 1091 | U |
| 1 | A | 1092 | A |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1096 | C |
| 1 | A | 1101 | A |
| 1 | A | 1102 | A |
| 1 | A | 1103 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1104 | G |
| 1 | A | 1113 | C |
| 1 | A | 1124 | G |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1127 | G |
| 1 | A | 1128 | C |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1133 | G |
| 1 | A | 1135 | U |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1140 | C |
| 1 | A | 1141 | C |
| 1 | A | 1142 | G |
| 1 | A | 1143 | G |
| 1 | A | 1144 | G |
| 1 | A | 1145 | A |
| 1 | A | 1151 | A |
| 1 | A | 1152 | A |
| 1 | A | 1153 | G |
| 1 | A | 1154 | G |
| 1 | A | 1158 | C |
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1161 | C |
| 1 | A | 1162 | C |
| 1 | A | 1163 | A |
| 1 | A | 1167 | A |
| 1 | A | 1168 | U |
| 1 | A | 1169 | A |
| 1 | A | 1170 | A |
| 1 | A | 1178 | G |
| 1 | A | 1181 | G |
| 1 | A | 1182 | G |
| 1 | A | 1183 | U |
| 1 | A | 1184 | G |
| 1 | A | 1185 | G |
| 1 | A | 1190 | G |
| 1 | A | 1191 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1192 | C |
| 1 | A | 1196 | A |
| 1 | A | 1197 | A |
| 1 | A | 1198 | G |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | U |
| 1 | A | 1203 | C |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1215 | G |
| 1 | A | 1216 | A |
| 1 | A | 1224 | U |
| 1 | A | 1225 | A |
| 1 | A | 1226 | C |
| 1 | A | 1227 | A |
| 1 | A | 1228 | C |
| 1 | A | 1229 | A |
| 1 | A | 1238 | A |
| 1 | A | 1239 | A |
| 1 | A | 1240 | U |
| 1 | A | 1241 | G |
| 1 | A | 1242 | G |
| 1 | A | 1256 | A |
| 1 | A | 1259 | C |
| 1 | A | 1260 | G |
| 1 | A | 1275 | A |
| 1 | A | 1278 | G |
| 1 | A | 1279 | G |
| 1 | A | 1280 | A |
| 1 | A | 1282 | C |
| 1 | A | 1283 | U |
| 1 | A | 1284 | C |
| 1 | A | 1285 | A |
| 1 | A | 1286 | U |
| 1 | A | 1287 | A |
| 1 | A | 1293 | C |
| 1 | A | 1299 | A |
| 1 | A | 1301 | U |
| 1 | A | 1303 | C |
| 1 | A | 1304 | G |
| 1 | A | 1305 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1315 | U |
| 1 | A | 1316 | G |
| 1 | A | 1317 | C |
| 1 | A | 1318 | A |
| 1 | A | 1319 | A |
| 1 | A | 1320 | C |
| 1 | A | 1321 | U |
| 1 | A | 1322 | C |
| 1 | A | 1323 | G |
| 1 | A | 1324 | A |
| 1 | A | 1325 | C |
| 1 | A | 1332 | A |
| 1 | A | 1333 | A |
| 1 | A | 1337 | G |
| 1 | A | 1338 | G |
| 1 | A | 1346 | A |
| 1 | A | 1348 | U |
| 1 | A | 1349 | A |
| 1 | A | 1353 | G |
| 1 | A | 1362 | A |
| 1 | A | 1364 | U |
| 1 | A | 1365 | G |
| 1 | A | 1370 | G |
| 1 | A | 1379 | G |
| 1 | A | 1380 | U |
| 1 | A | 1381 | U |
| 1 | A | 1382 | C |
| 1 | A | 1394 | A |
| 1 | A | 1395 | C |
| 1 | A | 1396 | A |
| 1 | A | 1397 | C |
| 1 | A | 1398 | A |
| 1 | A | 1399 | C |
| 1 | A | 1400 | C |
| 1 | A | 1402 | C |
| 1 | A | 1411 | C |
| 1 | A | 1414 | U |
| 1 | A | 1432 | G |
| 1 | A | 1433 | A |
| 1 | A | 1441 | A |
| 1 | A | 1446 | A |
| 1 | A | 1448 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1449 | C |
| 1 | A | 1451 | U |
| 1 | A | 1452 | C |
| 1 | A | 1453 | G |
| 1 | A | 1454 | G |
| 1 | A | 1455 | G |
| 1 | A | 1469 | C |
| 1 | A | 1470 | U |
| 1 | A | 1491 | G |
| 1 | A | 1492 | A |
| 1 | A | 1494 | G |
| 1 | A | 1497 | G |
| 1 | A | 1498 | U |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |
| 1 | A | 1503 | A |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1507 | A |
| 1 | A | 1508 | A |
| 1 | A | 1509 | C |
| 1 | A | 1517 | G |
| 1 | A | 1522 | U |
| 1 | A | 1526 | G |
| 1 | A | 1528 | U |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1531 | A |
| 1 | A | 1532 | U |

All (236) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 7 | A |
| 1 | A | 13 | U |
| 1 | A | 14 | U |
| 1 | A | 30 | U |
| 1 | A | 32 | A |
| 1 | A | 47 | C |
| 1 | A | 52 | C |
| 1 | A | 60 | A |
| 1 | A | 61 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 64 | G |
| 1 | A | 66 | A |
| 1 | A | 71 | A |
| 1 | A | 72 | A |
| 1 | A | 74 | A |
| 1 | A | 87 | C |
| 1 | A | 91 | U |
| 1 | A | 93 | U |
| 1 | A | 94 | G |
| 1 | A | 95 | C |
| 1 | A | 97 | G |
| 1 | A | 109 | A |
| 1 | A | 110 | C |
| 1 | A | 115 | G |
| 1 | A | 119 | A |
| 1 | A | 121 | U |
| 1 | A | 122 | G |
| 1 | A | 129 | A |
| 1 | A | 131 | A |
| 1 | A | 141 | G |
| 1 | A | 173 | U |
| 1 | A | 174 | A |
| 1 | A | 180 | U |
| 1 | A | 185 | U |
| 1 | A | 197 | A |
| 1 | A | 198 | G |
| 1 | A | 199 | A |
| 1 | A | 243 | A |
| 1 | A | 246 | A |
| 1 | A | 247 | G |
| 1 | A | 250 | A |
| 1 | A | 251 | G |
| 1 | A | 252 | U |
| 1 | A | 257 | G |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 274 | A |
| 1 | A | 275 | G |
| 1 | A | 279 | A |
| 1 | A | 305 | G |
| 1 | A | 306 | A |
| 1 | A | 327 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 330 | C |
| 1 | A | 331 | G |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 346 | G |
| 1 | A | 351 | G |
| 1 | A | 352 | C |
| 1 | A | 366 | A |
| 1 | A | 368 | U |
| 1 | A | 372 | C |
| 1 | A | 373 | A |
| 1 | A | 388 | G |
| 1 | A | 389 | A |
| 1 | A | 411 | A |
| 1 | A | 414 | A |
| 1 | A | 421 | U |
| 1 | A | 424 | G |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 430 | A |
| 1 | A | 438 | U |
| 1 | A | 439 | U |
| 1 | A | 451 | A |
| 1 | A | 452 | A |
| 1 | A | 462 | G |
| 1 | A | 463 | U |
| 1 | A | 466 | A |
| 1 | A | 468 | A |
| 1 | A | 469 | C |
| 1 | A | 484 | G |
| 1 | A | 486 | U |
| 1 | A | 487 | A |
| 1 | A | 488 | C |
| 1 | A | 495 | A |
| 1 | A | 496 | A |
| 1 | A | 497 | G |
| 1 | A | 499 | A |
| 1 | A | 500 | G |
| 1 | A | 501 | C |
| 1 | A | 508 | U |
| 1 | A | 509 | A |
| 1 | A | 511 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 512 | U |
| 1 | A | 517 | G |
| 1 | A | 519 | C |
| 1 | A | 531 | U |
| 1 | A | 534 | U |
| 1 | A | 535 | A |
| 1 | A | 536 | C |
| 1 | A | 537 | G |
| 1 | A | 547 | A |
| 1 | A | 548 | G |
| 1 | A | 559 | A |
| 1 | A | 563 | A |
| 1 | A | 566 | G |
| 1 | A | 575 | G |
| 1 | A | 577 | G |
| 1 | A | 595 | A |
| 1 | A | 596 | A |
| 1 | A | 642 | A |
| 1 | A | 652 | U |
| 1 | A | 654 | G |
| 1 | A | 686 | U |
| 1 | A | 688 | G |
| 1 | A | 701 | U |
| 1 | A | 704 | A |
| 1 | A | 717 | U |
| 1 | A | 718 | A |
| 1 | A | 721 | G |
| 1 | A | 722 | G |
| 1 | A | 752 | G |
| 1 | A | 754 | C |
| 1 | A | 755 | G |
| 1 | A | 792 | A |
| 1 | A | 794 | A |
| 1 | A | 812 | G |
| 1 | A | 813 | U |
| 1 | A | 815 | A |
| 1 | A | 816 | A |
| 1 | A | 817 | C |
| 1 | A | 870 | U |
| 1 | A | 874 | G |
| 1 | A | 884 | U |
| 1 | A | 889 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 913 | A |
| 1 | A | 914 | A |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 960 | U |
| 1 | A | 961 | U |
| 1 | A | 965 | U |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 972 | C |
| 1 | A | 974 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 978 | A |
| 1 | A | 982 | U |
| 1 | A | 984 | C |
| 1 | A | 991 | U |
| 1 | A | 994 | A |
| 1 | A | 1031 | C |
| 1 | A | 1049 | U |
| 1 | A | 1050 | G |
| 1 | A | 1053 | G |
| 1 | A | 1064 | G |
| 1 | A | 1066 | C |
| 1 | A | 1068 | G |
| 1 | A | 1085 | U |
| 1 | A | 1087 | G |
| 1 | A | 1088 | G |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1101 | A |
| 1 | A | 1102 | A |
| 1 | A | 1126 | U |
| 1 | A | 1127 | G |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1136 | C |
| 1 | A | 1142 | G |
| 1 | A | 1152 | A |
| 1 | A | 1153 | G |
| 1 | A | 1157 | A |
| 1 | A | 1162 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1168 | U |
| 1 | A | 1169 | A |
| 1 | A | 1181 | G |
| 1 | A | 1184 | G |
| 1 | A | 1190 | G |
| 1 | A | 1191 | A |
| 1 | A | 1196 | A |
| 1 | A | 1197 | A |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | U |
| 1 | A | 1203 | C |
| 1 | A | 1215 | G |
| 1 | A | 1224 | U |
| 1 | A | 1228 | C |
| 1 | A | 1239 | A |
| 1 | A | 1241 | G |
| 1 | A | 1258 | G |
| 1 | A | 1259 | C |
| 1 | A | 1278 | G |
| 1 | A | 1282 | C |
| 1 | A | 1283 | U |
| 1 | A | 1284 | C |
| 1 | A | 1298 | U |
| 1 | A | 1303 | C |
| 1 | A | 1304 | G |
| 1 | A | 1319 | A |
| 1 | A | 1320 | C |
| 1 | A | 1322 | C |
| 1 | A | 1323 | G |
| 1 | A | 1331 | G |
| 1 | A | 1332 | A |
| 1 | A | 1336 | C |
| 1 | A | 1337 | G |
| 1 | A | 1345 | U |
| 1 | A | 1348 | U |
| 1 | A | 1349 | A |
| 1 | A | 1365 | G |
| 1 | A | 1380 | U |
| 1 | A | 1381 | U |
| 1 | A | 1382 | C |
| 1 | A | 1394 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1395 | C |
| 1 | A | 1396 | A |
| 1 | A | 1398 | A |
| 1 | A | 1399 | C |
| 1 | A | 1432 | G |
| 1 | A | 1447 | A |
| 1 | A | 1448 | C |
| 1 | A | 1451 | U |
| 1 | A | 1453 | G |
| 1 | A | 1454 | G |
| 1 | A | 1498 | U |
| 1 | A | 1502 | A |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1507 | A |
| 1 | A | 1528 | U |
| 1 | A | 1531 | A |

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 ⓘ

Of 43 ligands modelled in this entry, 43 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.