



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2014 – 05:43 PM BST

PDB ID : 2B9M
Title : 30S ribosomal subunit, tRNAs, mRNA and release factor RF2 from a crystal structure of the whole ribosomal complex. This file contains the 30S ribosomal subunit, tRNAs, mRNA and release factor RF2 from a crystal structure of the whole ribosomal complex". The entire crystal structure contains one 70S ribosome, tRNAs, mRNA and release factor RF2 and is described in remark 400.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-10-12
Resolution : 6.76 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>

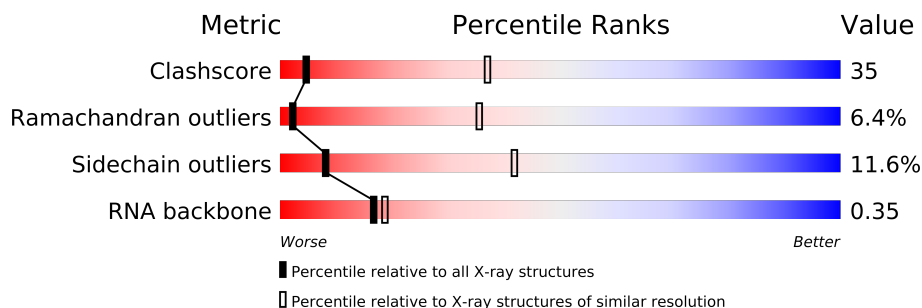
The following versions of software and data (see [references](#)) were used in the production of this report:

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 6.76 Å.



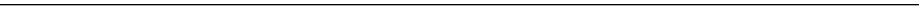


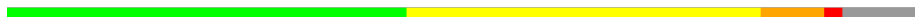


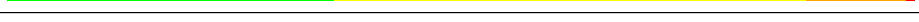



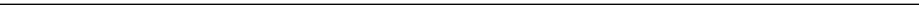

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 79885 | 1039 (10.00-3.52) |
| Ramachandran outliers | 78287 | 1291 (9.50-3.50) |
| Sidechain outliers | 78261 | 1265 (9.50-3.50) |
| RNA backbone | 1838 | 1045 (10.00-2.80) |


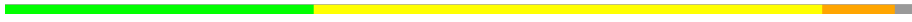


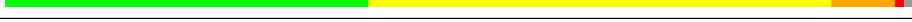

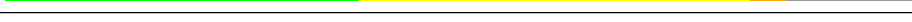

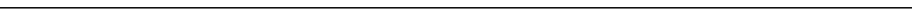

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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 | 1522 |  |
| 2 | V | 76 |  |
| 3 | W | 76 |  |
| 4 | X | 18 |  |
| 5 | B | 256 |  |
| 6 | C | 239 |  |
| 7 | D | 209 |  |
| 8 | E | 162 |  |
| 9 | F | 101 |  |
| 10 | G | 156 |  |
| 11 | H | 138 |  |
| 12 | I | 128 |  |
| 13 | J | 105 |  |
| 14 | K | 129 |  |
| 15 | L | 135 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 16 | M | 126 |  |
| 17 | N | 61 |  |
| 18 | O | 89 |  |
| 19 | P | 88 |  |
| 20 | Q | 105 |  |
| 21 | R | 88 |  |
| 22 | S | 93 |  |
| 23 | T | 106 |  |
| 24 | U | 27 |  |
| 25 | Y | 365 |  |

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 55543 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 ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1515 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32551 | 14490 | 6022 | 10525 | 1514 | | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-----------|
| A | 416 | G | - | INSERTION | GB 155076 |
| A | 905 | U | - | INSERTION | GB 155076 |
| A | 1395 | C | - | INSERTION | GB 155076 |

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2 | V | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1622 | 725 | 293 | 529 | 75 | | | |

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3 | W | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1638 | 736 | 294 | 533 | 75 | | | |

- Molecule 4 is a RNA chain called 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*AP*UP*A
P*CP*AP*AP*UP*AP*AP*U)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| 4 | X | 17 | Total | C | N | O | P | 0 | 0 | 11 |
| | | | 136 | 56 | 19 | 44 | 17 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | C | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1016 | 314 | 281 | 1 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | E | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1146 | 724 | 217 | 201 | 4 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | F | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | G | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | H | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 12 | I | 127 | Total | C | N | O | | | |
| | | | 1011 | 639 | 198 | 174 | 0 | 0 | 0 |

- Molecule 13 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | J | 98 | Total | C | N | O | S | | | |
| | | | 794 | 499 | 156 | 138 | 1 | 0 | 0 | 0 |

- Molecule 14 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | K | 119 | Total | C | N | O | S | | | |
| | | | 885 | 549 | 168 | 165 | 3 | 0 | 0 | 0 |

- Molecule 15 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | L | 124 | Total | C | N | O | S | | | |
| | | | 970 | 611 | 195 | 163 | 1 | 0 | 0 | 0 |

- Molecule 16 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | M | 125 | Total | C | N | O | S | | | |
| | | | 997 | 617 | 207 | 171 | 2 | 0 | 0 | 0 |

- Molecule 17 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 17 | N | 60 | Total | C | N | O | S | | | |
| | | | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |

- Molecule 18 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | O | 88 | Total | C | N | O | S | | | |
| | | | 734 | 459 | 147 | 126 | 2 | 0 | 0 | 0 |

- Molecule 19 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | P | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 700 | 443 | 139 | 117 | 1 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | Q | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 547 | 161 | 147 | 2 | | | |

- Molecule 21 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 21 | R | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 597 | 380 | 118 | 99 | | | | |

- Molecule 22 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | S | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 647 | 414 | 119 | 112 | 2 | | | |

- Molecule 23 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | T | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 469 | 162 | 129 | 2 | | | |

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

- Molecule 25 is a protein called Peptide chain release factor 2.

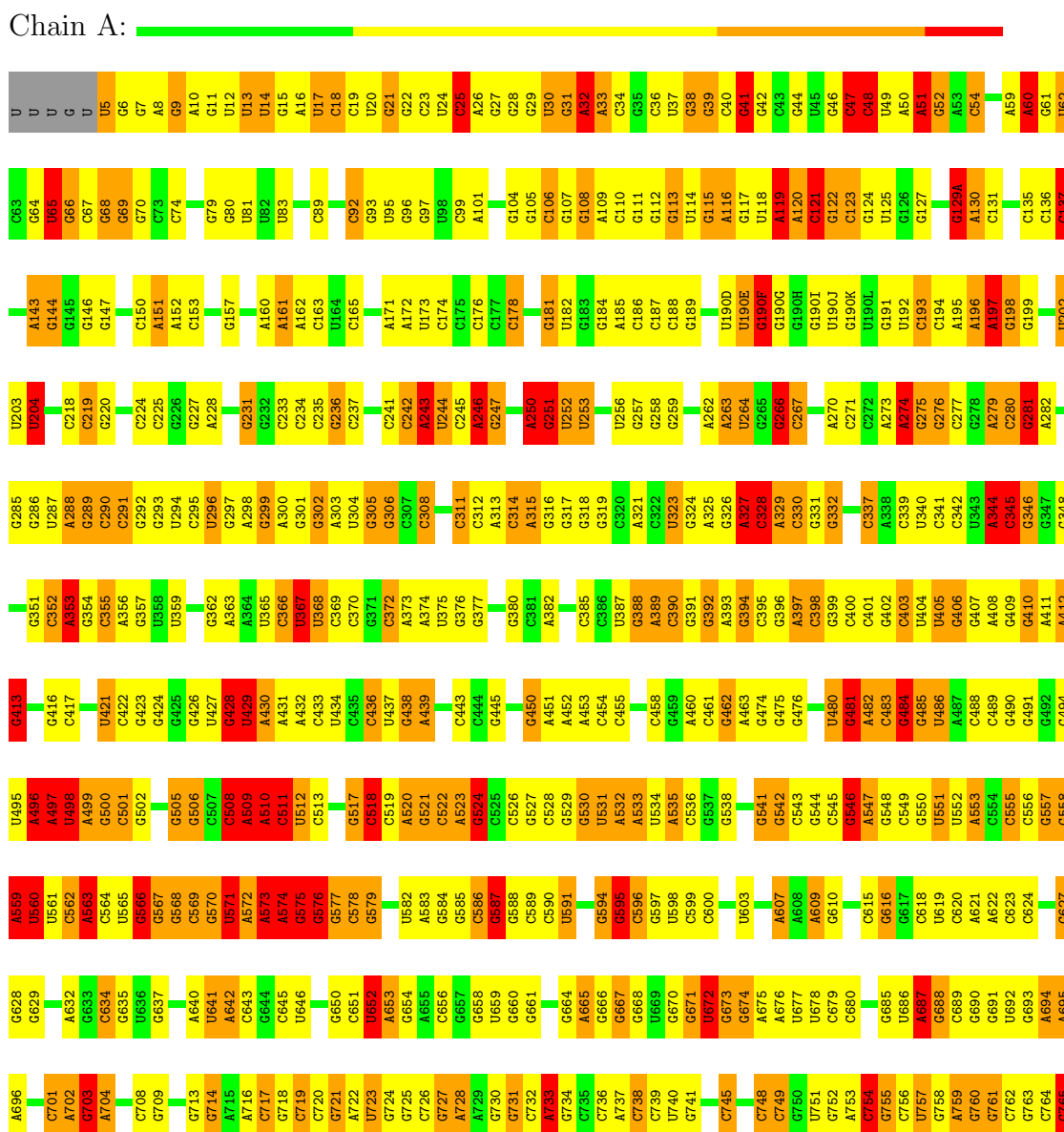
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 25 | Y | 365 | Total | C | 0 | 0 | 365 |
| | | | 365 | 365 | | | |

3 Residue-property plots

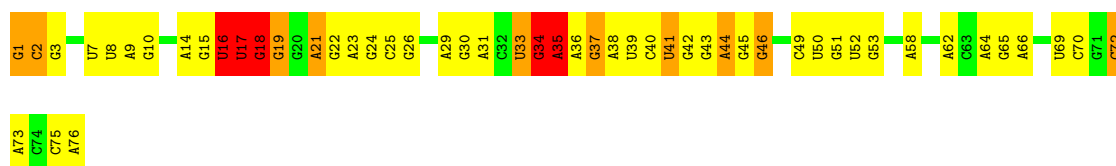
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

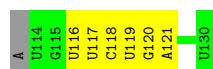






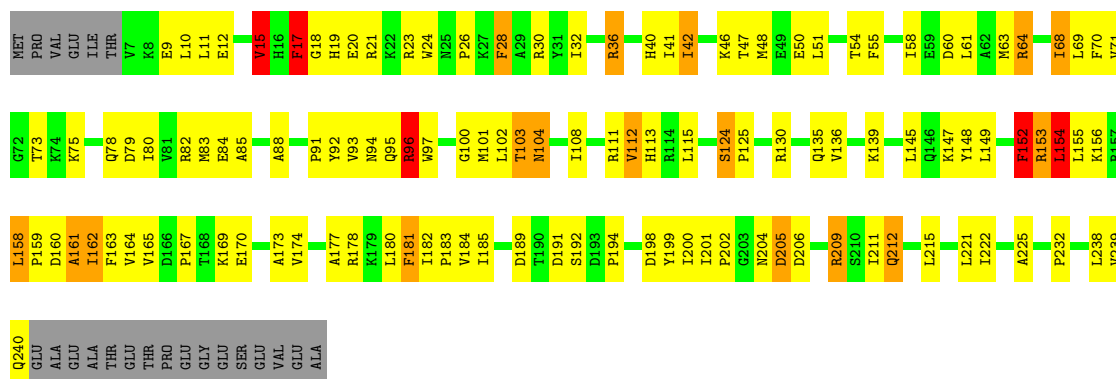
- Molecule 4: 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*AP*UP*AP*CP*AP*AP*UP*AP*A P*U)-3'

Chain X:



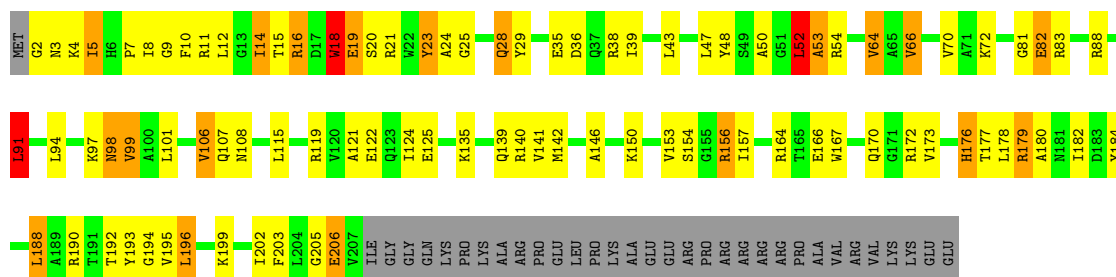
- Molecule 5: 30S ribosomal protein S2

Chain B:



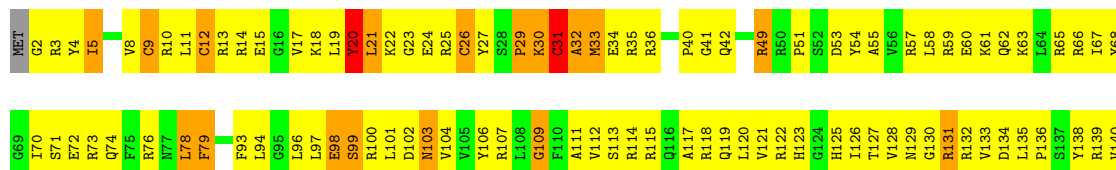
- Molecule 6: 30S ribosomal protein S3

Chain C:



- Molecule 7: 30S ribosomal protein S4

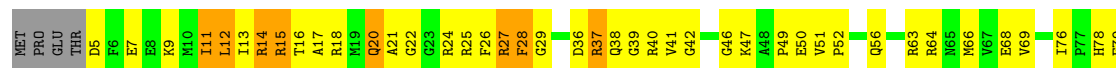
Chain D:





• Molecule 8: 30S ribosomal protein S5

Chain E:



• Molecule 9: 30S ribosomal protein S6

Chain F:



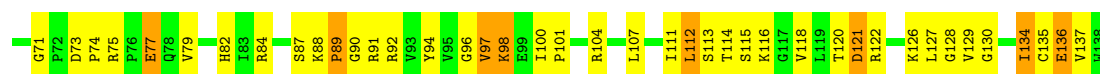
• Molecule 10: 30S ribosomal protein S7

Chain G:



• Molecule 11: 30S ribosomal protein S8

Chain H:



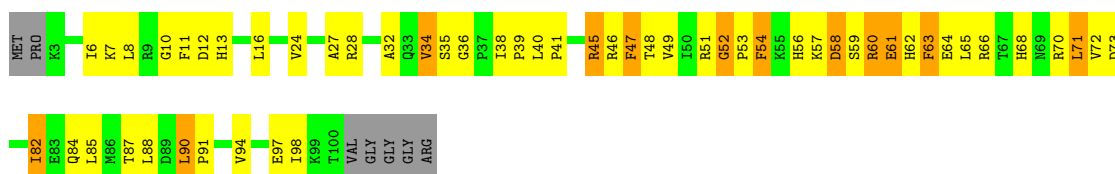
• Molecule 12: 30S ribosomal protein S9

Chain I:



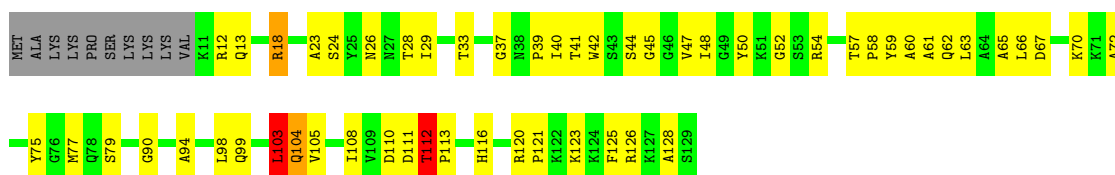
• Molecule 13: 30S ribosomal protein S10

Chain J:



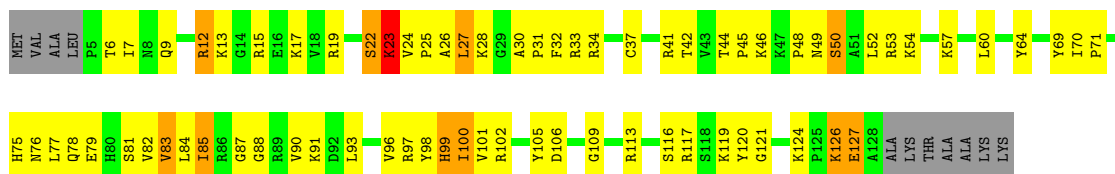
• Molecule 14: 30S ribosomal protein S11

Chain K:



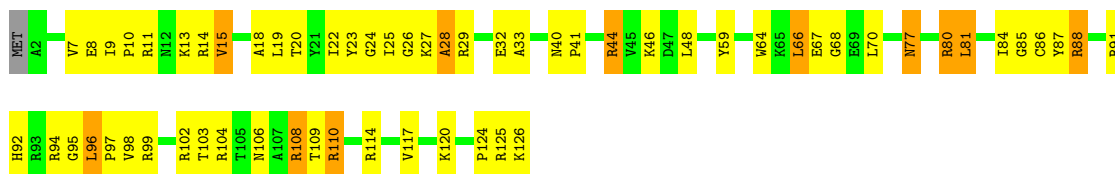
• Molecule 15: 30S ribosomal protein S12

Chain L:



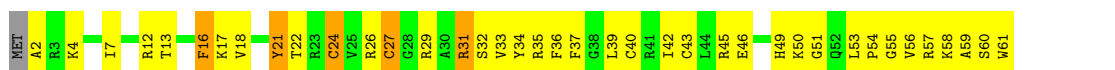
• Molecule 16: 30S ribosomal protein S13

Chain M:



• Molecule 17: 30S ribosomal protein S14

Chain N:



• Molecule 18: 30S ribosomal protein S15

Chain O:



• Molecule 19: 30S ribosomal protein S16

Chain P:



ALA
ARG
GLU
GLY
ALA

- Molecule 20: 30S ribosomal protein S17

Chain Q:

MET P2 K3 K4 V5 G8 V9 V10 V11 M15 T18 V19 T20 T21 V22 V23 E24 E25 H29 G33 K34 V35 I36 K37 K38 S39 K40 K41 Y42 L43 A44 H45 D46 P47 E48 G54 D55 V56 V57 E58 I59 I60 E61 S62 R63 P64 I65 S66 K67 R68 K69 R70 L74
R75 L76 V77 E78 S79 G80 R81 L84 V85 E86 K87 Y88 L89 I90 R91 Q92 Q93 N94 Y95 Q96 S97 S99 K100 R101 G102 G103 K104 A105

- Molecule 21: 30S ribosomal protein S18

Chain R:

MET SER THR LYS ASN ALA LYS PRO LYS LYS LYS ALA GLN ARG ARG P16 K21 E28 P29 D30 L31 R32 R33 Y34 R35 N36 V37 L40 L46 T47 G48 K49 R53 R54 R55 L58 S59 G60 K61 E62 L66 I70 R71 R72 A73 R74 I75 L76 G77 L78 P80
F81 T82 E83 K84 L85 V86 R87 K88

- Molecule 22: 30S ribosomal protein S19

Chain S:

MET P2 R3 S4 L5 K6 K7 G8 F10 D13 H14 L15 L16 E17 K18 K25 L30 T33 N34 S35 R36 R37 S38 T39 L40 E43 M44 Y45 G46 H47 Y52 N53 G54 K55 Q56 V60 Y61 T62 T63 E64 N65 M66 K70 L71 G72 E73 F74 T77 R78 T79
Y80 R81 GLY HIS GLY LYS GLU ALA THR LYS LYS LYS

- Molecule 23: 30S ribosomal protein S20

Chain T:

MET ALA GLN LYS PRO LYS R8 Q18 R23 N26 R27 A28 K29 K30 I33 K34 V41 Q45 K48 A49 E50 E60 S61 L62 I63 D64 K65 A66 A67 K68 G69 S70 T71 L72 H73 K74 N75 A76 A77 A78 R79 R80 K81 S82 R83 L84 M85 R86 K87 V88 R89
Q90 L91 L92 G96 A97 P98 L99 I100 G101 G102 G103 L104 S105 A106

- Molecule 24: 30S ribosomal protein Thx

Chain U:

MET G2 K3 G4 D5 R6 R10 G11 K12 R15 G16 T17 Y18 G19 K20 Y21 R22 P23 R24 K25 LYS LYS

- Molecule 25: Peptide chain release factor 2

Chain Y:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

| Property | Value | Source |
|--|---|-----------|
| Space group | P 43 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 520.21Å 520.21Å 365.90Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 43.35 – 6.76 | Depositor |
| % Data completeness (in resolution range) | 96.2 (43.35-6.76) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.19 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.11 (at 6.14Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.341 , 0.356 | Depositor |
| Wilson B-factor (Å ²) | 233.6 | Xtriage |
| Anisotropy | 0.105 | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$ | Xtriage |
| Outliers | 0 of 112763 reflections | Xtriage |
| Total number of atoms | 55543 | wwPDB-VP |
| Average B, all atoms (Å ²) | 354.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: YYG, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 1.34 | 66/36411 (0.2%) | 1.47 | 428/56769 (0.8%) |
| 2 | V | 1.58 | 5/1814 (0.3%) | 1.08 | 11/2827 (0.4%) |
| 3 | W | 1.77 | 16/1737 (0.9%) | 1.68 | 30/2690 (1.1%) |
| 4 | X | 0.18 | 0/139 | 0.66 | 0/213 |
| 5 | B | 0.61 | 2/1935 (0.1%) | 0.61 | 0/2609 |
| 6 | C | 0.43 | 1/1636 (0.1%) | 1.10 | 6/2205 (0.3%) |
| 7 | D | 0.79 | 5/1733 (0.3%) | 1.09 | 11/2318 (0.5%) |
| 8 | E | 0.92 | 1/1162 (0.1%) | 0.63 | 2/1564 (0.1%) |
| 9 | F | 0.35 | 0/856 | 0.54 | 0/1154 |
| 10 | G | 0.33 | 0/1276 | 0.76 | 3/1709 (0.2%) |
| 11 | H | 0.41 | 0/1136 | 0.66 | 0/1527 |
| 12 | I | 0.34 | 0/1029 | 0.54 | 0/1378 |
| 13 | J | 0.35 | 0/807 | 0.56 | 0/1085 |
| 14 | K | 0.64 | 1/900 (0.1%) | 0.56 | 0/1213 |
| 15 | L | 0.99 | 1/986 (0.1%) | 0.70 | 1/1320 (0.1%) |
| 16 | M | 0.35 | 0/1006 | 0.56 | 0/1341 |
| 17 | N | 0.49 | 0/501 | 0.64 | 1/664 (0.2%) |
| 18 | O | 0.32 | 0/745 | 0.54 | 0/992 |
| 19 | P | 0.40 | 0/716 | 0.59 | 1/963 (0.1%) |
| 20 | Q | 1.20 | 3/870 (0.3%) | 1.54 | 6/1159 (0.5%) |
| 21 | R | 0.40 | 0/603 | 0.70 | 0/799 |
| 22 | S | 0.34 | 0/661 | 0.53 | 0/890 |
| 23 | T | 0.31 | 0/764 | 0.57 | 1/1006 (0.1%) |
| 24 | U | 0.34 | 0/212 | 0.49 | 0/277 |
| All | All | 1.18 | 101/59635 (0.2%) | 1.30 | 501/88672 (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 |
|-----|-------|---------------------|---------------------|
| 3 | W | 1 | 5 |
| 6 | C | 0 | 1 |
| 14 | K | 0 | 1 |
| 20 | Q | 0 | 1 |
| All | All | 1 | 8 |

All (101) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | A | 1037 | C | O3'-P | -82.19 | 0.62 | 1.61 |
| 1 | A | 1255 | G | O3'-P | -72.80 | 0.73 | 1.61 |
| 1 | A | 1224 | G | O3'-P | 43.87 | 2.13 | 1.61 |
| 1 | A | 1046 | A | O3'-P | 43.16 | 2.12 | 1.61 |
| 1 | A | 1107 | C | O3'-P | 42.57 | 2.12 | 1.61 |
| 1 | A | 1361 | G | O3'-P | 40.49 | 2.09 | 1.61 |
| 1 | A | 937 | A | O3'-P | 40.34 | 2.09 | 1.61 |
| 1 | A | 115 | G | O3'-P | 40.27 | 2.09 | 1.61 |
| 1 | A | 703 | G | O3'-P | 38.46 | 2.07 | 1.61 |
| 2 | V | 73 | A | O3'-P | 36.97 | 2.05 | 1.61 |
| 1 | A | 394 | G | O3'-P | 36.59 | 2.05 | 1.61 |
| 1 | A | 576 | G | O3'-P | 35.42 | 2.03 | 1.61 |
| 3 | W | 21 | A | O3'-P | -34.91 | 1.19 | 1.61 |
| 1 | A | 38 | G | O3'-P | -33.16 | 1.21 | 1.61 |
| 2 | V | 65 | G | O3'-P | -32.22 | 1.22 | 1.61 |
| 1 | A | 820 | U | O3'-P | 31.95 | 1.99 | 1.61 |
| 1 | A | 546 | G | O3'-P | 31.92 | 1.99 | 1.61 |
| 2 | V | 7 | U | O3'-P | 31.20 | 1.98 | 1.61 |
| 1 | A | 1298 | C | O3'-P | 30.58 | 1.97 | 1.61 |
| 1 | A | 813 | U | O3'-P | -29.84 | 1.25 | 1.61 |
| 1 | A | 25 | C | O3'-P | 29.55 | 1.96 | 1.61 |
| 1 | A | 405 | U | O3'-P | 29.33 | 1.96 | 1.61 |
| 20 | Q | 22 | LEU | C-N | -28.10 | 0.69 | 1.34 |
| 1 | A | 143 | A | O3'-P | 28.04 | 1.94 | 1.61 |
| 15 | L | 23 | LYS | C-N | -27.79 | 0.70 | 1.34 |
| 8 | E | 144 | THR | C-N | 27.10 | 1.96 | 1.34 |
| 1 | A | 974 | A | O3'-P | 27.01 | 1.93 | 1.61 |
| 2 | V | 25 | C | O3'-P | 26.04 | 1.92 | 1.61 |
| 1 | A | 587 | G | O3'-P | 24.88 | 1.91 | 1.61 |
| 1 | A | 733 | A | O3'-P | 24.70 | 1.90 | 1.61 |
| 1 | A | 196 | A | O3'-P | 24.45 | 1.90 | 1.61 |
| 1 | A | 288 | A | O3'-P | 23.98 | 1.90 | 1.61 |
| 1 | A | 337 | C | O3'-P | 21.99 | 1.87 | 1.61 |
| 1 | A | 879 | C | O3'-P | 21.83 | 1.87 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | A | 1337 | G | O3'-P | -21.48 | 1.35 | 1.61 |
| 1 | A | 1004 | A | O3'-P | 21.41 | 1.86 | 1.61 |
| 1 | A | 765 | G | O3'-P | -20.96 | 1.36 | 1.61 |
| 1 | A | 1211 | U | O3'-P | -20.29 | 1.36 | 1.61 |
| 1 | A | 1377 | A | O3'-P | -19.75 | 1.37 | 1.61 |
| 2 | V | 45 | G | O3'-P | -19.71 | 1.37 | 1.61 |
| 1 | A | 1182 | G | O3'-P | -19.68 | 1.37 | 1.61 |
| 5 | B | 112 | VAL | C-N | 19.56 | 1.79 | 1.34 |
| 3 | W | 46 | G | C8-N7 | 19.39 | 1.42 | 1.30 |
| 1 | A | 672 | U | O3'-P | -18.99 | 1.38 | 1.61 |
| 1 | A | 858 | G | O3'-P | -18.99 | 1.38 | 1.61 |
| 3 | W | 16 | U | C5-C6 | 18.63 | 1.50 | 1.34 |
| 1 | A | 60 | A | O3'-P | 18.12 | 1.82 | 1.61 |
| 3 | W | 58 | A | C6-N6 | 17.74 | 1.48 | 1.33 |
| 1 | A | 884 | U | O3'-P | -17.59 | 1.40 | 1.61 |
| 3 | W | 17 | U | C5-C6 | 17.10 | 1.49 | 1.34 |
| 3 | W | 44 | A | O3'-P | -16.86 | 1.41 | 1.61 |
| 3 | W | 72 | C | O3'-P | -16.81 | 1.41 | 1.61 |
| 7 | D | 187 | ARG | C-N | 16.71 | 1.72 | 1.34 |
| 3 | W | 33 | U | O3'-P | -16.65 | 1.41 | 1.61 |
| 1 | A | 1117 | G | O3'-P | 16.51 | 1.80 | 1.61 |
| 7 | D | 98 | GLU | C-N | -16.38 | 0.96 | 1.34 |
| 1 | A | 311 | C | O3'-P | 15.63 | 1.79 | 1.61 |
| 14 | K | 112 | THR | C-N | -15.57 | 1.04 | 1.34 |
| 1 | A | 1101 | A | O3'-P | 15.50 | 1.79 | 1.61 |
| 1 | A | 754 | C | O3'-P | 14.64 | 1.78 | 1.61 |
| 20 | Q | 40 | LYS | C-N | -14.58 | 1.00 | 1.34 |
| 1 | A | 436 | C | O3'-P | 14.46 | 1.78 | 1.61 |
| 1 | A | 558 | G | O3'-P | 14.17 | 1.78 | 1.61 |
| 3 | W | 58 | A | C6-N1 | 13.86 | 1.45 | 1.35 |
| 1 | A | 108 | G | O3'-P | 13.54 | 1.77 | 1.61 |
| 1 | A | 869 | G | O3'-P | -11.11 | 1.47 | 1.61 |
| 3 | W | 16 | U | N1-C6 | 11.10 | 1.48 | 1.38 |
| 1 | A | 776 | G | O3'-P | -11.02 | 1.48 | 1.61 |
| 7 | D | 49 | ARG | C-N | 11.00 | 1.59 | 1.34 |
| 3 | W | 17 | U | N1-C6 | 10.87 | 1.47 | 1.38 |
| 1 | A | 286 | G | O3'-P | 10.79 | 1.74 | 1.61 |
| 3 | W | 46 | G | N9-C8 | 10.65 | 1.45 | 1.37 |
| 1 | A | 1085 | U | O3'-P | -10.63 | 1.48 | 1.61 |
| 1 | A | 717 | C | O3'-P | 10.55 | 1.73 | 1.61 |
| 1 | A | 566 | G | O3'-P | 10.21 | 1.73 | 1.61 |
| 20 | Q | 81 | ARG | C-N | 10.18 | 1.57 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3 | W | 17 | U | C4-C5 | 10.08 | 1.52 | 1.43 |
| 1 | A | 1534 | A | O3'-P | 9.85 | 1.73 | 1.61 |
| 1 | A | 1345 | U | O3'-P | 9.07 | 1.72 | 1.61 |
| 1 | A | 1024 | G | O3'-P | -9.05 | 1.50 | 1.61 |
| 1 | A | 1189 | C | O3'-P | 8.71 | 1.71 | 1.61 |
| 3 | W | 16 | U | C4-C5 | 8.37 | 1.51 | 1.43 |
| 3 | W | 35 | A | O3'-P | 8.14 | 1.71 | 1.61 |
| 1 | A | 243 | A | C3'-O3' | 8.10 | 1.53 | 1.42 |
| 6 | C | 106 | VAL | C-N | -7.95 | 1.15 | 1.34 |
| 1 | A | 960 | U | O3'-P | -7.74 | 1.51 | 1.61 |
| 1 | A | 497 | A | O3'-P | 7.72 | 1.70 | 1.61 |
| 5 | B | 148 | TYR | C-N | -7.24 | 1.17 | 1.34 |
| 1 | A | 1504 | G | O3'-P | 6.91 | 1.69 | 1.61 |
| 7 | D | 31 | CYS | CB-SG | 6.88 | 1.94 | 1.82 |
| 3 | W | 58 | A | C5-C6 | 6.67 | 1.47 | 1.41 |
| 1 | A | 1396 | A | O3'-P | -6.49 | 1.53 | 1.61 |
| 1 | A | 1278 | U | O3'-P | -5.96 | 1.53 | 1.61 |
| 1 | A | 1073 | U | O3'-P | -5.96 | 1.54 | 1.61 |
| 1 | A | 827 | U | O3'-P | -5.53 | 1.54 | 1.61 |
| 1 | A | 366 | C | C3'-O3' | 5.39 | 1.49 | 1.42 |
| 1 | A | 789 | U | C1'-N1 | 5.34 | 1.56 | 1.48 |
| 1 | A | 115 | G | C3'-O3' | 5.33 | 1.49 | 1.42 |
| 7 | D | 26 | CYS | CB-SG | 5.29 | 1.91 | 1.82 |
| 1 | A | 703 | G | C3'-O3' | 5.16 | 1.49 | 1.42 |
| 1 | A | 1101 | A | C3'-O3' | 5.05 | 1.49 | 1.42 |

All (501) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 3 | W | 33 | U | P-O3'-C3' | 27.30 | 152.45 | 119.70 |
| 3 | W | 35 | A | P-O3'-C3' | 27.16 | 152.29 | 119.70 |
| 20 | Q | 22 | LEU | O-C-N | 27.15 | 166.15 | 122.70 |
| 1 | A | 1073 | U | P-O3'-C3' | -25.83 | 88.70 | 119.70 |
| 2 | V | 73 | A | P-O3'-C3' | -24.87 | 89.86 | 119.70 |
| 6 | C | 106 | VAL | O-C-N | 24.40 | 161.75 | 122.70 |
| 1 | A | 913 | A | P-O3'-C3' | 24.20 | 148.74 | 119.70 |
| 1 | A | 1224 | G | P-O3'-C3' | 23.87 | 148.35 | 119.70 |
| 1 | A | 1255 | G | P-O3'-C3' | -23.66 | 91.31 | 119.70 |
| 3 | W | 17 | U | C5-C6-N1 | -23.17 | 111.11 | 122.70 |
| 1 | A | 1085 | U | P-O3'-C3' | 22.94 | 147.22 | 119.70 |
| 6 | C | 106 | VAL | CA-C-N | -22.70 | 67.26 | 117.20 |
| 1 | A | 178 | C | P-O3'-C3' | 22.57 | 146.78 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 20 | Q | 22 | LEU | CA-C-N | -22.07 | 68.65 | 117.20 |
| 6 | C | 18 | TRP | O-C-N | -22.02 | 87.47 | 122.70 |
| 7 | D | 98 | GLU | O-C-N | 21.91 | 157.76 | 122.70 |
| 1 | A | 1337 | G | P-O3'-C3' | 21.87 | 145.94 | 119.70 |
| 1 | A | 288 | A | O3'-P-O5' | -21.28 | 63.56 | 104.00 |
| 1 | A | 1255 | G | OP2-P-O3' | 21.19 | 151.81 | 105.20 |
| 3 | W | 16 | U | C5-C6-N1 | -20.92 | 112.24 | 122.70 |
| 1 | A | 944 | G | P-O3'-C3' | -19.47 | 96.34 | 119.70 |
| 1 | A | 1396 | A | P-O3'-C3' | -19.28 | 96.57 | 119.70 |
| 6 | C | 106 | VAL | C-N-CA | -18.86 | 74.54 | 121.70 |
| 20 | Q | 22 | LEU | C-N-CA | -18.58 | 75.25 | 121.70 |
| 3 | W | 21 | A | P-O3'-C3' | 18.46 | 141.85 | 119.70 |
| 1 | A | 1278 | U | OP2-P-O3' | 18.40 | 145.68 | 105.20 |
| 1 | A | 1278 | U | O3'-P-O5' | -17.76 | 70.25 | 104.00 |
| 20 | Q | 40 | LYS | CA-C-N | -17.43 | 78.85 | 117.20 |
| 2 | V | 73 | A | O3'-P-O5' | 17.10 | 136.49 | 104.00 |
| 1 | A | 1345 | U | P-O3'-C3' | 16.97 | 140.07 | 119.70 |
| 3 | W | 72 | C | OP2-P-O3' | 16.80 | 142.15 | 105.20 |
| 2 | V | 73 | A | OP2-P-O3' | -16.69 | 68.47 | 105.20 |
| 10 | G | 12 | LEU | O-C-N | -16.63 | 96.09 | 122.70 |
| 7 | D | 98 | GLU | CA-C-N | -16.39 | 81.14 | 117.20 |
| 1 | A | 1278 | U | P-O3'-C3' | 15.80 | 138.67 | 119.70 |
| 1 | A | 1255 | G | OP1-P-O3' | -15.62 | 70.84 | 105.20 |
| 2 | V | 25 | C | P-O3'-C3' | -15.49 | 101.12 | 119.70 |
| 7 | D | 187 | ARG | O-C-N | 15.48 | 147.46 | 122.70 |
| 1 | A | 1107 | C | P-O3'-C3' | -15.30 | 101.34 | 119.70 |
| 20 | Q | 40 | LYS | C-N-CA | -15.22 | 83.65 | 121.70 |
| 1 | A | 311 | C | O3'-P-O5' | -14.97 | 75.55 | 104.00 |
| 1 | A | 436 | C | O3'-P-O5' | -14.90 | 75.68 | 104.00 |
| 1 | A | 1073 | U | OP2-P-O3' | 14.71 | 137.56 | 105.20 |
| 3 | W | 35 | A | OP1-P-O3' | 14.50 | 137.09 | 105.20 |
| 1 | A | 944 | G | OP2-P-O3' | 14.12 | 136.26 | 105.20 |
| 1 | A | 1396 | A | O3'-P-O5' | -14.01 | 77.39 | 104.00 |
| 20 | Q | 40 | LYS | O-C-N | 13.92 | 144.98 | 122.70 |
| 2 | V | 65 | G | P-O3'-C3' | 13.52 | 135.93 | 119.70 |
| 1 | A | 243 | A | P-O3'-C3' | 13.45 | 135.84 | 119.70 |
| 3 | W | 58 | A | N1-C6-N6 | 13.24 | 126.55 | 118.60 |
| 1 | A | 38 | G | OP1-P-O3' | 13.05 | 133.91 | 105.20 |
| 7 | D | 98 | GLU | C-N-CA | -13.02 | 89.15 | 121.70 |
| 1 | A | 115 | G | OP2-P-O3' | 12.95 | 133.68 | 105.20 |
| 1 | A | 311 | C | OP2-P-O3' | 12.81 | 133.39 | 105.20 |
| 1 | A | 497 | A | OP2-P-O3' | -12.76 | 77.12 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 7 | D | 49 | ARG | O-C-N | 12.72 | 143.06 | 122.70 |
| 3 | W | 33 | U | OP1-P-O3' | 12.71 | 133.17 | 105.20 |
| 1 | A | 1224 | G | OP2-P-O3' | 12.62 | 132.96 | 105.20 |
| 1 | A | 879 | C | P-O3'-C3' | -12.59 | 104.59 | 119.70 |
| 1 | A | 178 | C | OP2-P-O3' | -12.46 | 77.79 | 105.20 |
| 1 | A | 351 | G | P-O3'-C3' | 12.42 | 134.61 | 119.70 |
| 1 | A | 558 | G | OP1-P-O3' | -12.32 | 78.09 | 105.20 |
| 1 | A | 1073 | U | OP1-P-O3' | -12.31 | 78.12 | 105.20 |
| 1 | A | 1024 | G | O3'-P-O5' | 12.28 | 127.32 | 104.00 |
| 3 | W | 58 | A | C4-C5-C6 | 12.21 | 123.11 | 117.00 |
| 1 | A | 703 | G | P-O3'-C3' | 12.03 | 134.14 | 119.70 |
| 3 | W | 17 | U | C4-C5-C6 | -11.98 | 112.51 | 119.70 |
| 2 | V | 45 | G | O3'-P-O5' | 11.96 | 126.72 | 104.00 |
| 7 | D | 187 | ARG | CA-C-N | -11.93 | 90.96 | 117.20 |
| 1 | A | 1337 | G | O3'-P-O5' | 11.89 | 126.60 | 104.00 |
| 10 | G | 12 | LEU | CA-C-N | 11.61 | 142.74 | 117.20 |
| 3 | W | 21 | A | OP1-P-O3' | 11.59 | 130.69 | 105.20 |
| 3 | W | 46 | G | N7-C8-N9 | -11.54 | 107.33 | 113.10 |
| 1 | A | 566 | G | O3'-P-O5' | 11.42 | 125.69 | 104.00 |
| 7 | D | 49 | ARG | CA-C-N | -11.33 | 92.27 | 117.20 |
| 1 | A | 1189 | C | OP2-P-O3' | 11.16 | 129.76 | 105.20 |
| 3 | W | 1 | G | P-O3'-C3' | 11.14 | 133.07 | 119.70 |
| 1 | A | 804 | U | P-O3'-C3' | -10.99 | 106.51 | 119.70 |
| 1 | A | 1107 | C | O3'-P-O5' | 10.82 | 124.56 | 104.00 |
| 1 | A | 1224 | G | OP1-P-O3' | -10.79 | 81.46 | 105.20 |
| 1 | A | 575 | G | P-O3'-C3' | 10.79 | 132.64 | 119.70 |
| 1 | A | 913 | A | OP1-P-O3' | 10.61 | 128.54 | 105.20 |
| 3 | W | 33 | U | O3'-P-O5' | -10.58 | 83.90 | 104.00 |
| 1 | A | 1189 | C | P-O3'-C3' | -10.46 | 107.15 | 119.70 |
| 3 | W | 58 | A | C5-C6-N1 | -10.46 | 112.47 | 117.70 |
| 1 | A | 1201 | A | P-O3'-C3' | 10.42 | 132.20 | 119.70 |
| 1 | A | 121 | C | P-O3'-C3' | 10.37 | 132.15 | 119.70 |
| 1 | A | 818 | G | O4'-C1'-N9 | 10.23 | 116.38 | 108.20 |
| 1 | A | 1377 | A | OP2-P-O3' | 10.18 | 127.60 | 105.20 |
| 10 | G | 12 | LEU | C-N-CA | 10.06 | 146.86 | 121.70 |
| 1 | A | 178 | C | OP1-P-O3' | 10.03 | 127.28 | 105.20 |
| 1 | A | 509 | A | P-O3'-C3' | 10.04 | 131.74 | 119.70 |
| 1 | A | 813 | U | P-O3'-C3' | 10.03 | 131.73 | 119.70 |
| 1 | A | 1064 | G | C1'-O4'-C4' | -9.98 | 101.92 | 109.90 |
| 1 | A | 405 | U | O3'-P-O5' | -9.98 | 85.05 | 104.00 |
| 3 | W | 16 | U | C4-C5-C6 | -9.96 | 113.73 | 119.70 |
| 7 | D | 26 | CYS | CA-CB-SG | 9.92 | 131.86 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1117 | G | P-O3'-C3' | 9.92 | 131.60 | 119.70 |
| 1 | A | 884 | U | OP1-P-O3' | 9.91 | 127.00 | 105.20 |
| 1 | A | 558 | G | OP2-P-O3' | 9.90 | 126.98 | 105.20 |
| 1 | A | 328 | C | P-O3'-C3' | 9.89 | 131.57 | 119.70 |
| 1 | A | 1085 | U | O3'-P-O5' | 9.88 | 122.77 | 104.00 |
| 1 | A | 793 | U | C1'-O4'-C4' | -9.88 | 102.00 | 109.90 |
| 1 | A | 1504 | G | O3'-P-O5' | -9.87 | 85.26 | 104.00 |
| 1 | A | 405 | U | OP1-P-O3' | 9.82 | 126.81 | 105.20 |
| 1 | A | 1504 | G | P-O3'-C3' | 9.76 | 131.41 | 119.70 |
| 3 | W | 35 | A | OP2-P-O3' | -9.64 | 83.99 | 105.20 |
| 3 | W | 34 | G | O3'-P-O5' | 9.62 | 122.27 | 104.00 |
| 1 | A | 1298 | C | OP2-P-O3' | -9.54 | 84.20 | 105.20 |
| 3 | W | 72 | C | O3'-P-O5' | -9.53 | 85.89 | 104.00 |
| 3 | W | 44 | A | OP2-P-O3' | 9.51 | 126.13 | 105.20 |
| 1 | A | 1345 | U | OP2-P-O3' | 9.48 | 126.05 | 105.20 |
| 1 | A | 1361 | G | P-O3'-C3' | 9.44 | 131.03 | 119.70 |
| 1 | A | 366 | C | P-O3'-C3' | 9.41 | 131.00 | 119.70 |
| 7 | D | 187 | ARG | C-N-CA | -9.40 | 98.20 | 121.70 |
| 1 | A | 1298 | C | P-O3'-C3' | -9.40 | 108.42 | 119.70 |
| 1 | A | 1298 | C | O3'-P-O5' | 9.39 | 121.83 | 104.00 |
| 1 | A | 266 | G | P-O3'-C3' | 9.37 | 130.94 | 119.70 |
| 1 | A | 687 | A | P-O3'-C3' | 9.37 | 130.94 | 119.70 |
| 1 | A | 405 | U | P-O3'-C3' | -9.36 | 108.47 | 119.70 |
| 1 | A | 944 | G | OP1-P-O3' | -9.35 | 84.62 | 105.20 |
| 1 | A | 1504 | G | OP2-P-O3' | 9.32 | 125.71 | 105.20 |
| 3 | W | 34 | G | OP2-P-O3' | -9.30 | 84.74 | 105.20 |
| 1 | A | 372 | C | P-O3'-C3' | 9.29 | 130.85 | 119.70 |
| 1 | A | 60 | A | O3'-P-O5' | 9.29 | 121.65 | 104.00 |
| 1 | A | 754 | C | P-O3'-C3' | 9.28 | 130.83 | 119.70 |
| 1 | A | 812 | C | P-O3'-C3' | 9.27 | 130.83 | 119.70 |
| 1 | A | 1505 | G | P-O3'-C3' | 9.27 | 130.82 | 119.70 |
| 1 | A | 1065 | U | P-O3'-C3' | 9.20 | 130.74 | 119.70 |
| 1 | A | 1085 | U | OP1-P-O3' | -9.12 | 85.13 | 105.20 |
| 1 | A | 1024 | G | P-O3'-C3' | -9.09 | 108.79 | 119.70 |
| 1 | A | 1396 | A | OP2-P-O3' | 9.07 | 125.16 | 105.20 |
| 1 | A | 817 | C | P-O3'-C3' | 9.06 | 130.58 | 119.70 |
| 1 | A | 394 | G | P-O3'-C3' | -9.04 | 108.85 | 119.70 |
| 1 | A | 914 | A | C1'-O4'-C4' | -8.99 | 102.71 | 109.90 |
| 1 | A | 914 | A | O4'-C1'-N9 | 8.99 | 115.39 | 108.20 |
| 1 | A | 1037 | C | O3'-P-O5' | 8.92 | 120.95 | 104.00 |
| 1 | A | 884 | U | O3'-P-O5' | -8.81 | 87.26 | 104.00 |
| 2 | V | 45 | G | OP1-P-O3' | -8.81 | 85.83 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 563 | A | C1'-O4'-C4' | -8.75 | 102.90 | 109.90 |
| 1 | A | 820 | U | OP2-P-O3' | 8.74 | 124.43 | 105.20 |
| 2 | V | 65 | G | OP1-P-O3' | 8.72 | 124.38 | 105.20 |
| 7 | D | 49 | ARG | C-N-CA | -8.72 | 99.91 | 121.70 |
| 1 | A | 1502 | A | C1'-O4'-C4' | -8.70 | 102.94 | 109.90 |
| 1 | A | 1337 | G | OP2-P-O3' | -8.69 | 86.08 | 105.20 |
| 1 | A | 884 | U | P-O3'-C3' | -8.63 | 109.34 | 119.70 |
| 1 | A | 197 | A | P-O3'-C3' | 8.61 | 130.04 | 119.70 |
| 1 | A | 518 | C | P-O3'-C3' | 8.61 | 130.03 | 119.70 |
| 1 | A | 765 | G | O3'-P-O5' | -8.57 | 87.72 | 104.00 |
| 1 | A | 436 | C | P-O3'-C3' | -8.54 | 109.45 | 119.70 |
| 1 | A | 1347 | G | P-O3'-C3' | 8.54 | 129.95 | 119.70 |
| 1 | A | 765 | G | OP1-P-O3' | 8.50 | 123.90 | 105.20 |
| 1 | A | 1345 | U | O3'-P-O5' | -8.49 | 87.86 | 104.00 |
| 1 | A | 717 | C | OP2-P-O3' | -8.47 | 86.56 | 105.20 |
| 3 | W | 18 | G | C5'-C4'-O4' | -8.42 | 98.99 | 109.10 |
| 1 | A | 1226 | C | P-O3'-C3' | 8.38 | 129.75 | 119.70 |
| 1 | A | 569 | C | P-O3'-C3' | -8.37 | 109.65 | 119.70 |
| 1 | A | 576 | G | P-O3'-C3' | 8.37 | 129.74 | 119.70 |
| 1 | A | 687 | A | OP2-P-O3' | 8.37 | 123.61 | 105.20 |
| 1 | A | 47 | C | P-O3'-C3' | 8.31 | 129.67 | 119.70 |
| 1 | A | 877 | C | C3'-C2'-C1' | -8.27 | 94.88 | 101.50 |
| 1 | A | 889 | A | P-O3'-C3' | 8.27 | 129.62 | 119.70 |
| 1 | A | 1377 | A | OP1-P-O3' | -8.26 | 87.03 | 105.20 |
| 1 | A | 560 | U | P-O3'-C3' | 8.26 | 129.61 | 119.70 |
| 1 | A | 1101 | A | O3'-P-O5' | 8.24 | 119.66 | 104.00 |
| 1 | A | 1380 | U | P-O3'-C3' | 8.15 | 129.48 | 119.70 |
| 3 | W | 72 | C | OP1-P-O3' | -8.15 | 87.28 | 105.20 |
| 1 | A | 992 | U | P-O3'-C3' | 8.12 | 129.45 | 119.70 |
| 1 | A | 559 | A | P-O3'-C3' | 8.10 | 129.42 | 119.70 |
| 1 | A | 1257 | U | P-O3'-C3' | 8.10 | 129.41 | 119.70 |
| 1 | A | 497 | A | OP1-P-O3' | 8.08 | 122.98 | 105.20 |
| 1 | A | 717 | C | OP1-P-O3' | 8.04 | 122.89 | 105.20 |
| 1 | A | 1004 | A | P-O3'-C3' | 8.03 | 129.34 | 119.70 |
| 1 | A | 1189 | C | O3'-P-O5' | -8.03 | 88.74 | 104.00 |
| 6 | C | 18 | TRP | CA-C-N | 8.03 | 134.87 | 117.20 |
| 1 | A | 143 | A | P-O3'-C3' | -8.02 | 110.07 | 119.70 |
| 1 | A | 1346 | A | P-O3'-C3' | 7.99 | 129.29 | 119.70 |
| 1 | A | 484 | G | P-O3'-C3' | 7.98 | 129.28 | 119.70 |
| 1 | A | 38 | G | O3'-P-O5' | -7.96 | 88.87 | 104.00 |
| 1 | A | 246 | A | P-O3'-C3' | 7.94 | 129.23 | 119.70 |
| 1 | A | 274 | A | P-O3'-C3' | 7.92 | 129.20 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1 | A | 1182 | G | OP2-P-O3' | 7.91 | 122.60 | 105.20 |
| 3 | W | 58 | A | C6-C5-N7 | -7.91 | 126.77 | 132.30 |
| 1 | A | 535 | A | P-O3'-C3' | 7.90 | 129.18 | 119.70 |
| 2 | V | 25 | C | OP1-P-O3' | -7.90 | 87.83 | 105.20 |
| 1 | A | 499 | A | P-O3'-C3' | 7.88 | 129.16 | 119.70 |
| 1 | A | 365 | U | OP1-P-O3' | 7.87 | 122.52 | 105.20 |
| 1 | A | 1281 | U | P-O3'-C3' | 7.86 | 129.13 | 119.70 |
| 3 | W | 44 | A | O3'-P-O5' | -7.85 | 89.08 | 104.00 |
| 1 | A | 429 | U | C1'-O4'-C4' | -7.83 | 103.64 | 109.90 |
| 1 | A | 129(A) | G | P-O3'-C3' | 7.74 | 128.99 | 119.70 |
| 1 | A | 251 | G | P-O3'-C3' | 7.73 | 128.98 | 119.70 |
| 3 | W | 72 | C | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 1 | A | 190(F) | G | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 1 | A | 965 | A | P-O3'-C3' | 7.69 | 128.93 | 119.70 |
| 1 | A | 701 | C | P-O3'-C3' | 7.64 | 128.86 | 119.70 |
| 1 | A | 927 | G | C3'-C2'-C1' | -7.63 | 95.40 | 101.50 |
| 1 | A | 727 | G | C3'-C2'-C1' | -7.62 | 95.41 | 101.50 |
| 1 | A | 1049 | U | P-O3'-C3' | 7.56 | 128.77 | 119.70 |
| 1 | A | 311 | C | P-O3'-C3' | -7.54 | 110.65 | 119.70 |
| 1 | A | 281 | G | P-O3'-C3' | 7.53 | 128.74 | 119.70 |
| 1 | A | 566 | G | P-O3'-C3' | -7.52 | 110.67 | 119.70 |
| 1 | A | 863 | U | C1'-O4'-C4' | -7.52 | 103.89 | 109.90 |
| 1 | A | 869 | G | P-O3'-C3' | 7.52 | 128.72 | 119.70 |
| 1 | A | 558 | G | P-O3'-C3' | 7.49 | 128.69 | 119.70 |
| 1 | A | 819 | A | O4'-C1'-N9 | -7.46 | 102.24 | 108.20 |
| 1 | A | 327 | A | P-O3'-C3' | 7.43 | 128.62 | 119.70 |
| 1 | A | 288 | A | OP1-P-O3' | 7.40 | 121.48 | 105.20 |
| 1 | A | 1190 | G | P-O3'-C3' | 7.37 | 128.54 | 119.70 |
| 1 | A | 394 | G | O3'-P-O5' | 7.37 | 117.99 | 104.00 |
| 1 | A | 497 | A | O3'-P-O5' | 7.31 | 117.89 | 104.00 |
| 1 | A | 288 | A | P-O3'-C3' | -7.30 | 110.94 | 119.70 |
| 1 | A | 993 | G | P-O3'-C3' | 7.30 | 128.46 | 119.70 |
| 1 | A | 258 | G | C1'-O4'-C4' | -7.24 | 104.11 | 109.90 |
| 1 | A | 501 | C | O4'-C1'-N1 | 7.22 | 113.97 | 108.20 |
| 1 | A | 1301 | U | C1'-O4'-C4' | -7.21 | 104.13 | 109.90 |
| 1 | A | 1145 | C | P-O3'-C3' | 7.21 | 128.35 | 119.70 |
| 1 | A | 51 | A | P-O3'-C3' | 7.20 | 128.34 | 119.70 |
| 1 | A | 569 | C | OP2-P-O3' | 7.17 | 120.98 | 105.20 |
| 1 | A | 1101 | A | OP1-P-O3' | -7.17 | 89.43 | 105.20 |
| 1 | A | 5 | U | P-O3'-C3' | 7.13 | 128.25 | 119.70 |
| 1 | A | 851 | G | C4'-C3'-C2' | -7.13 | 95.47 | 102.60 |
| 1 | A | 429 | U | P-O3'-C3' | 7.09 | 128.21 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 143 | A | O3'-P-O5' | -7.07 | 90.57 | 104.00 |
| 1 | A | 202 | U | P-O3'-C3' | 7.02 | 128.12 | 119.70 |
| 1 | A | 975 | A | P-O3'-C3' | 6.99 | 128.09 | 119.70 |
| 1 | A | 428 | G | P-O3'-C3' | 6.98 | 128.08 | 119.70 |
| 1 | A | 733 | A | P-O3'-C3' | 6.97 | 128.07 | 119.70 |
| 1 | A | 1498 | U | P-O3'-C3' | 6.97 | 128.07 | 119.70 |
| 1 | A | 1522 | U | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 1 | A | 436 | C | OP2-P-O3' | 6.95 | 120.48 | 105.20 |
| 1 | A | 914 | A | C4'-C3'-C2' | -6.94 | 95.66 | 102.60 |
| 1 | A | 818 | G | C1'-O4'-C4' | -6.89 | 104.38 | 109.90 |
| 1 | A | 1117 | G | OP1-P-O3' | 6.88 | 120.35 | 105.20 |
| 1 | A | 569 | C | O3'-P-O5' | -6.87 | 90.94 | 104.00 |
| 1 | A | 1224 | G | C1'-O4'-C4' | -6.87 | 104.40 | 109.90 |
| 1 | A | 591 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 1 | A | 877 | C | C4'-C3'-C2' | -6.84 | 95.76 | 102.60 |
| 1 | A | 1528 | U | P-O3'-C3' | 6.83 | 127.90 | 119.70 |
| 1 | A | 1532 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 1 | A | 770 | C | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 1 | A | 1502 | A | O4'-C1'-N9 | 6.80 | 113.64 | 108.20 |
| 1 | A | 701 | C | C1'-O4'-C4' | -6.80 | 104.46 | 109.90 |
| 1 | A | 891 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 1 | A | 318 | G | O4'-C1'-N9 | 6.78 | 113.63 | 108.20 |
| 1 | A | 115 | G | O3'-P-O5' | -6.77 | 91.13 | 104.00 |
| 1 | A | 869 | G | OP1-P-O3' | -6.77 | 90.31 | 105.20 |
| 1 | A | 776 | G | P-O3'-C3' | 6.72 | 127.76 | 119.70 |
| 1 | A | 9 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 1 | A | 879 | C | OP2-P-O3' | 6.68 | 119.91 | 105.20 |
| 1 | A | 578 | C | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 1 | A | 365 | U | OP2-P-O3' | -6.66 | 90.55 | 105.20 |
| 1 | A | 181 | G | P-O3'-C3' | 6.62 | 127.64 | 119.70 |
| 1 | A | 1101 | A | P-O3'-C3' | -6.61 | 111.76 | 119.70 |
| 1 | A | 960 | U | OP1-P-O3' | -6.60 | 90.67 | 105.20 |
| 1 | A | 394 | G | OP1-P-O3' | -6.59 | 90.69 | 105.20 |
| 1 | A | 1084 | G | P-O3'-C3' | 6.57 | 127.59 | 119.70 |
| 1 | A | 506 | G | O4'-C1'-N9 | 6.54 | 113.44 | 108.20 |
| 1 | A | 356 | A | C4'-C3'-C2' | -6.49 | 96.11 | 102.60 |
| 1 | A | 337 | C | O3'-P-O5' | -6.49 | 91.67 | 104.00 |
| 1 | A | 884 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 1 | A | 28 | G | C3'-C2'-C1' | -6.46 | 96.33 | 101.50 |
| 1 | A | 873 | A | P-O3'-C3' | 6.43 | 127.42 | 119.70 |
| 1 | A | 879 | C | OP1-P-O3' | -6.43 | 91.06 | 105.20 |
| 1 | A | 1398 | A | C3'-C2'-C1' | -6.42 | 96.37 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1400 | C | C3'-C2'-C1' | 6.41 | 106.63 | 101.50 |
| 1 | A | 501 | C | C3'-C2'-C1' | -6.41 | 96.37 | 101.50 |
| 1 | A | 859 | A | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 1 | A | 1532 | U | C3'-C2'-C1' | -6.40 | 96.38 | 101.50 |
| 1 | A | 890 | G | C1'-O4'-C4' | -6.39 | 104.79 | 109.90 |
| 1 | A | 1024 | G | OP2-P-O3' | -6.38 | 91.15 | 105.20 |
| 1 | A | 1452 | C | C2-N1-C1' | 6.38 | 125.82 | 118.80 |
| 1 | A | 1255 | G | O3'-P-O5' | -6.37 | 91.90 | 104.00 |
| 1 | A | 1453 | G | C1'-O4'-C4' | -6.34 | 104.83 | 109.90 |
| 1 | A | 939 | G | C1'-O4'-C4' | -6.33 | 104.84 | 109.90 |
| 15 | L | 23 | LYS | O-C-N | -6.30 | 112.62 | 122.70 |
| 1 | A | 30 | U | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 1 | A | 913 | A | OP2-P-O3' | -6.28 | 91.38 | 105.20 |
| 1 | A | 652 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 1 | A | 917 | G | C4'-C3'-C2' | -6.27 | 96.33 | 102.60 |
| 1 | A | 32 | A | C1'-O4'-C4' | -6.27 | 104.89 | 109.90 |
| 1 | A | 1300 | G | P-O3'-C3' | 6.25 | 127.20 | 119.70 |
| 1 | A | 1481 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 1 | A | 723 | U | C2-N1-C1' | 6.23 | 125.18 | 117.70 |
| 1 | A | 396 | G | C1'-O4'-C4' | -6.22 | 104.92 | 109.90 |
| 1 | A | 543 | C | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 1 | A | 634 | C | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 1 | A | 1285 | A | P-O3'-C3' | 6.22 | 127.16 | 119.70 |
| 1 | A | 1004 | A | C1'-O4'-C4' | -6.21 | 104.93 | 109.90 |
| 1 | A | 27 | G | P-O3'-C3' | 6.21 | 127.15 | 119.70 |
| 1 | A | 1108 | G | C4'-C3'-C2' | -6.21 | 96.39 | 102.60 |
| 1 | A | 250 | A | P-O3'-C3' | 6.20 | 127.14 | 119.70 |
| 1 | A | 353 | A | O4'-C1'-N9 | 6.19 | 113.15 | 108.20 |
| 1 | A | 573 | A | P-O3'-C3' | 6.18 | 127.11 | 119.70 |
| 1 | A | 1397 | C | N1-C2-O2 | 6.17 | 122.60 | 118.90 |
| 1 | A | 290 | C | C5-C6-N1 | 6.17 | 124.09 | 121.00 |
| 1 | A | 915 | A | C3'-C2'-C1' | -6.17 | 96.56 | 101.50 |
| 1 | A | 92 | C | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 1 | A | 859 | A | C1'-O4'-C4' | -6.14 | 104.99 | 109.90 |
| 1 | A | 1413 | A | C3'-C2'-C1' | -6.14 | 96.59 | 101.50 |
| 1 | A | 908 | A | C3'-C2'-C1' | -6.13 | 96.60 | 101.50 |
| 1 | A | 871 | U | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 3 | W | 21 | A | O3'-P-O5' | -6.11 | 92.39 | 104.00 |
| 1 | A | 315 | A | OP1-P-O3' | 6.10 | 118.62 | 105.20 |
| 1 | A | 806 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 1 | A | 603 | U | C3'-C2'-C1' | -6.09 | 96.63 | 101.50 |
| 1 | A | 1278 | U | OP1-P-O3' | -6.09 | 91.81 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 733 | A | O3'-P-O5' | 6.08 | 115.56 | 104.00 |
| 1 | A | 302 | G | C8-N9-C4 | -6.08 | 103.97 | 106.40 |
| 1 | A | 849 | C | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 1 | A | 372 | C | C1'-O4'-C4' | -6.07 | 105.05 | 109.90 |
| 1 | A | 344 | A | P-O3'-C3' | 6.06 | 126.98 | 119.70 |
| 1 | A | 904 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 8 | E | 12 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 1 | A | 339 | C | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 1 | A | 510 | A | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 1 | A | 1297 | C | P-O3'-C3' | 6.03 | 126.93 | 119.70 |
| 1 | A | 917 | G | C3'-C2'-C1' | -6.02 | 96.68 | 101.50 |
| 1 | A | 727 | G | O4'-C4'-C3' | -6.02 | 97.98 | 104.00 |
| 1 | A | 748 | C | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 1 | A | 553 | A | O4'-C1'-N9 | 6.01 | 113.01 | 108.20 |
| 2 | V | 25 | C | OP2-P-O3' | 5.96 | 118.30 | 105.20 |
| 1 | A | 870 | U | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 1 | A | 728 | A | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 1 | A | 1453 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 1 | A | 65 | U | C3'-C2'-C1' | 5.92 | 106.24 | 101.50 |
| 3 | W | 15 | G | N9-C1'-C2' | -5.92 | 105.49 | 112.00 |
| 1 | A | 296 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 1 | A | 115 | G | OP1-P-O3' | -5.91 | 92.21 | 105.20 |
| 1 | A | 1125 | U | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 1 | A | 127 | G | C3'-C2'-C1' | -5.90 | 96.78 | 101.50 |
| 1 | A | 1094 | G | C1'-O4'-C4' | -5.86 | 105.21 | 109.90 |
| 1 | A | 740 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 1 | A | 882 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 1 | A | 542 | G | C4'-C3'-C2' | -5.81 | 96.79 | 102.60 |
| 1 | A | 607 | A | C4'-C3'-C2' | -5.80 | 96.80 | 102.60 |
| 1 | A | 1418 | A | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 1 | A | 888 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 1 | A | 367 | U | P-O3'-C3' | 5.78 | 126.63 | 119.70 |
| 1 | A | 1193 | G | C3'-C2'-C1' | -5.76 | 96.89 | 101.50 |
| 1 | A | 1452 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 1 | A | 413 | G | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |
| 1 | A | 1297 | C | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 1 | A | 18 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 1 | A | 524 | G | P-O3'-C3' | 5.74 | 126.58 | 119.70 |
| 1 | A | 902 | G | P-O3'-C3' | 5.71 | 126.55 | 119.70 |
| 1 | A | 776 | G | O3'-P-O5' | 5.70 | 114.83 | 104.00 |
| 1 | A | 976 | G | C1'-O4'-C4' | -5.70 | 105.34 | 109.90 |
| 1 | A | 1192 | C | C3'-C2'-C1' | -5.69 | 96.95 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 732 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 1 | A | 801 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 1 | A | 738 | C | C3'-C2'-C1' | -5.68 | 96.95 | 101.50 |
| 1 | A | 403 | C | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 1 | A | 586 | C | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 1 | A | 960 | U | O3'-P-O5' | 5.67 | 114.77 | 104.00 |
| 1 | A | 498 | U | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 1 | A | 508 | C | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 1 | A | 776 | G | OP2-P-O3' | -5.66 | 92.75 | 105.20 |
| 1 | A | 1399 | C | C1'-O4'-C4' | -5.65 | 105.38 | 109.90 |
| 1 | A | 481 | G | C3'-C2'-C1' | 5.64 | 106.01 | 101.50 |
| 1 | A | 1451 | A | C3'-C2'-C1' | -5.64 | 96.99 | 101.50 |
| 1 | A | 438 | G | C3'-C2'-C1' | 5.64 | 106.01 | 101.50 |
| 17 | N | 27 | CYS | CA-CB-SG | 5.64 | 124.14 | 114.00 |
| 1 | A | 1182 | G | OP1-P-O3' | -5.62 | 92.83 | 105.20 |
| 1 | A | 290 | C | C3'-C2'-C1' | -5.61 | 97.01 | 101.50 |
| 1 | A | 359 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 1 | A | 342 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 1 | A | 522 | C | C4'-C3'-C2' | -5.60 | 97.00 | 102.60 |
| 1 | A | 1301 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 1 | A | 234 | C | C3'-C2'-C1' | -5.60 | 97.02 | 101.50 |
| 1 | A | 616 | G | C3'-C2'-C1' | -5.60 | 97.02 | 101.50 |
| 1 | A | 1400 | C | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 1 | A | 485 | G | C1'-O4'-C4' | -5.59 | 105.43 | 109.90 |
| 1 | A | 571 | U | C2-N1-C1' | 5.59 | 124.41 | 117.70 |
| 1 | A | 1380 | U | C1'-O4'-C4' | -5.59 | 105.43 | 109.90 |
| 1 | A | 288 | A | OP2-P-O3' | 5.58 | 117.48 | 105.20 |
| 1 | A | 893 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 1 | A | 1084 | G | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 1 | A | 233 | C | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 1 | A | 1397 | C | C2-N1-C1' | 5.55 | 124.90 | 118.80 |
| 2 | V | 7 | U | OP1-P-O3' | 5.55 | 117.40 | 105.20 |
| 23 | T | 84 | LEU | CA-CB-CG | 5.54 | 128.05 | 115.30 |
| 1 | A | 709 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 1 | A | 1510 | U | C3'-C2'-C1' | -5.54 | 97.07 | 101.50 |
| 1 | A | 412 | A | C1'-O4'-C4' | -5.53 | 105.48 | 109.90 |
| 1 | A | 656 | C | C3'-C2'-C1' | -5.51 | 97.09 | 101.50 |
| 1 | A | 836 | G | C4'-C3'-C2' | -5.49 | 97.11 | 102.60 |
| 1 | A | 1064 | G | O4'-C1'-N9 | 5.49 | 112.60 | 108.20 |
| 1 | A | 276 | G | C3'-C2'-C1' | -5.49 | 97.11 | 101.50 |
| 1 | A | 969 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 1 | A | 574 | A | C8-N9-C4 | -5.47 | 103.61 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 496 | A | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 1 | A | 804 | U | OP1-P-O3' | -5.47 | 93.18 | 105.20 |
| 1 | A | 231 | G | C5'-C4'-O4' | 5.45 | 115.64 | 109.10 |
| 3 | W | 46 | G | C5-N7-C8 | 5.45 | 107.02 | 104.30 |
| 1 | A | 402 | G | C3'-C2'-C1' | -5.45 | 97.14 | 101.50 |
| 1 | A | 542 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 1 | A | 615 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 1 | A | 499 | A | C1'-O4'-C4' | -5.43 | 105.56 | 109.90 |
| 1 | A | 356 | A | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 1 | A | 119 | A | OP2-P-O3' | 5.42 | 117.13 | 105.20 |
| 1 | A | 1065 | U | C2'-C3'-O3' | 5.42 | 122.37 | 113.70 |
| 1 | A | 242 | C | O4'-C1'-N1 | 5.41 | 112.52 | 108.20 |
| 1 | A | 595 | G | C3'-C2'-C1' | 5.41 | 105.82 | 101.50 |
| 1 | A | 48 | C | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 1 | A | 820 | U | O3'-P-O5' | -5.38 | 93.77 | 104.00 |
| 1 | A | 591 | U | C3'-C2'-C1' | -5.38 | 97.20 | 101.50 |
| 1 | A | 387 | U | C1'-O4'-C4' | -5.37 | 105.60 | 109.90 |
| 1 | A | 403 | C | C3'-C2'-C1' | -5.37 | 97.20 | 101.50 |
| 1 | A | 1530 | G | C1'-O4'-C4' | -5.37 | 105.61 | 109.90 |
| 1 | A | 125 | U | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 1 | A | 804 | U | OP2-P-O3' | 5.37 | 117.00 | 105.20 |
| 1 | A | 1256 | A | C3'-C2'-C1' | 5.37 | 105.79 | 101.50 |
| 1 | A | 951 | G | C4'-C3'-C2' | -5.36 | 97.24 | 102.60 |
| 1 | A | 652 | U | C1'-O4'-C4' | -5.36 | 105.61 | 109.90 |
| 1 | A | 1212 | U | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 1 | A | 28 | G | C4'-C3'-C2' | -5.34 | 97.26 | 102.60 |
| 1 | A | 1532 | U | O4'-C4'-C3' | -5.34 | 98.66 | 104.00 |
| 1 | A | 680 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 1 | A | 679 | C | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 1 | A | 1331 | G | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 1 | A | 792 | A | C1'-O4'-C4' | -5.32 | 105.64 | 109.90 |
| 1 | A | 792 | A | O4'-C1'-N9 | 5.29 | 112.44 | 108.20 |
| 1 | A | 332 | G | C4'-C3'-C2' | -5.29 | 97.31 | 102.60 |
| 1 | A | 38 | G | OP2-P-O3' | -5.29 | 93.57 | 105.20 |
| 1 | A | 74 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 1 | A | 541 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 1 | A | 883 | C | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 1 | A | 366 | C | C3'-C2'-C1' | 5.27 | 105.71 | 101.50 |
| 1 | A | 332 | G | C3'-C2'-C1' | -5.26 | 97.29 | 101.50 |
| 1 | A | 1452 | C | N1-C1'-C2' | 5.26 | 120.84 | 114.00 |
| 1 | A | 1302 | U | P-O3'-C3' | 5.26 | 126.01 | 119.70 |
| 1 | A | 574 | A | N7-C8-N9 | 5.24 | 116.42 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1158 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 1 | A | 576 | G | C1'-O4'-C4' | -5.22 | 105.72 | 109.90 |
| 1 | A | 819 | A | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 1 | A | 1285 | A | C1'-O4'-C4' | -5.22 | 105.73 | 109.90 |
| 1 | A | 147 | G | C3'-C2'-C1' | -5.22 | 97.33 | 101.50 |
| 1 | A | 904 | C | C3'-C2'-C1' | -5.21 | 97.33 | 101.50 |
| 1 | A | 858 | G | OP2-P-O3' | 5.21 | 116.66 | 105.20 |
| 1 | A | 918 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 1 | A | 1365 | G | N9-C1'-C2' | -5.20 | 106.28 | 112.00 |
| 1 | A | 204 | U | C2-N1-C1' | 5.19 | 123.93 | 117.70 |
| 1 | A | 137 | C | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 1 | A | 1304 | G | C1'-O4'-C4' | -5.18 | 105.75 | 109.90 |
| 1 | A | 859 | A | C4'-C3'-C2' | -5.18 | 97.42 | 102.60 |
| 1 | A | 345 | C | P-O3'-C3' | 5.18 | 125.92 | 119.70 |
| 1 | A | 511 | C | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 7 | D | 31 | CYS | CA-CB-SG | 5.17 | 123.31 | 114.00 |
| 1 | A | 1201 | A | C1'-O4'-C4' | -5.17 | 105.77 | 109.90 |
| 1 | A | 1533 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 1 | A | 421 | U | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 1 | A | 10 | A | C4'-C3'-C2' | -5.13 | 97.47 | 102.60 |
| 1 | A | 314 | C | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 1 | A | 25 | C | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 1 | A | 135 | C | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 1 | A | 827 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 1 | A | 21 | G | C3'-C2'-C1' | -5.12 | 97.40 | 101.50 |
| 1 | A | 258 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 1 | A | 702 | A | C3'-C2'-C1' | 5.12 | 105.59 | 101.50 |
| 1 | A | 1078 | U | O4'-C1'-N1 | 5.12 | 112.29 | 108.20 |
| 1 | A | 65 | U | P-O3'-C3' | 5.11 | 125.84 | 119.70 |
| 1 | A | 814 | A | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | A | 1315 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 1 | A | 1362 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 1 | A | 849 | C | C4'-C3'-C2' | -5.10 | 97.50 | 102.60 |
| 1 | A | 44 | G | C3'-C2'-C1' | -5.10 | 97.42 | 101.50 |
| 1 | A | 1339 | A | C3'-C2'-C1' | -5.09 | 97.43 | 101.50 |
| 1 | A | 1485 | U | O4'-C4'-C3' | -5.08 | 98.92 | 104.00 |
| 1 | A | 908 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 1 | A | 813 | U | O3'-P-O5' | 5.07 | 113.64 | 104.00 |
| 1 | A | 509 | A | C3'-C2'-C1' | -5.07 | 97.44 | 101.50 |
| 1 | A | 1498 | U | C3'-C2'-C1' | 5.07 | 105.56 | 101.50 |
| 1 | A | 903 | G | O4'-C4'-C3' | -5.07 | 98.93 | 104.00 |
| 1 | A | 1020 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 911 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 1 | A | 1361 | G | OP1-P-O3' | 5.06 | 116.33 | 105.20 |
| 1 | A | 38 | G | C4'-C3'-C2' | -5.05 | 97.55 | 102.60 |
| 19 | P | 6 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 1 | A | 1196 | U | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | A | 289 | G | O4'-C1'-N9 | 5.04 | 112.24 | 108.20 |
| 1 | A | 271 | C | O4'-C1'-N1 | 5.04 | 112.23 | 108.20 |
| 1 | A | 308 | C | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 8 | E | 144 | THR | O-C-N | -5.04 | 114.64 | 122.70 |
| 1 | A | 960 | U | C2-N1-C1' | 5.04 | 123.74 | 117.70 |
| 1 | A | 1346 | A | C1'-O4'-C4' | -5.03 | 105.88 | 109.90 |
| 6 | C | 91 | LEU | CA-CB-CG | 5.03 | 126.87 | 115.30 |
| 1 | A | 615 | C | C3'-C2'-C1' | -5.03 | 97.48 | 101.50 |
| 1 | A | 656 | C | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | A | 1514 | C | C5-C6-N1 | 5.03 | 123.51 | 121.00 |
| 1 | A | 918 | A | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 1 | A | 412 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 1 | A | 1158 | C | C2-N1-C1' | 5.02 | 124.33 | 118.80 |
| 1 | A | 1540 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 1 | A | 972 | C | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 1 | A | 1003 | G | O3'-P-O5' | 5.02 | 113.54 | 104.00 |
| 1 | A | 41 | G | C1'-O4'-C4' | -5.02 | 105.89 | 109.90 |
| 1 | A | 351 | G | O3'-P-O5' | 5.02 | 113.53 | 104.00 |
| 1 | A | 434 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 1 | A | 24 | U | O4'-C1'-N1 | 5.01 | 112.20 | 108.20 |
| 1 | A | 508 | C | C3'-C2'-C1' | 5.00 | 105.50 | 101.50 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3 | W | 37 | YYG | C15 |

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 6 | C | 18 | TRP | Mainchain |
| 14 | K | 112 | THR | Mainchain |
| 20 | Q | 40 | LYS | Mainchain |
| 3 | W | 16 | U | Sidechain |
| 3 | W | 17 | U | Sidechain |
| 3 | W | 18 | G | Sidechain |
| 3 | W | 19 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | W | 62 | A | Sidechain |

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 | 32551 | 0 | 16464 | 2019 | 0 |
| 2 | V | 1622 | 0 | 820 | 134 | 0 |
| 3 | W | 1638 | 0 | 836 | 141 | 0 |
| 4 | X | 136 | 0 | 63 | 22 | 0 |
| 5 | B | 1900 | 0 | 1950 | 92 | 0 |
| 6 | C | 1612 | 0 | 1675 | 113 | 0 |
| 7 | D | 1703 | 0 | 1760 | 288 | 0 |
| 8 | E | 1146 | 0 | 1206 | 59 | 0 |
| 9 | F | 843 | 0 | 857 | 49 | 0 |
| 10 | G | 1257 | 0 | 1295 | 94 | 0 |
| 11 | H | 1116 | 0 | 1177 | 99 | 0 |
| 12 | I | 1011 | 0 | 1040 | 89 | 0 |
| 13 | J | 794 | 0 | 840 | 105 | 0 |
| 14 | K | 885 | 0 | 904 | 55 | 0 |
| 15 | L | 970 | 0 | 1056 | 74 | 0 |
| 16 | M | 997 | 0 | 1070 | 175 | 0 |
| 17 | N | 492 | 0 | 529 | 95 | 0 |
| 18 | O | 734 | 0 | 771 | 30 | 0 |
| 19 | P | 700 | 0 | 720 | 78 | 0 |
| 20 | Q | 857 | 0 | 928 | 53 | 0 |
| 21 | R | 597 | 0 | 668 | 52 | 0 |
| 22 | S | 647 | 0 | 672 | 215 | 0 |
| 23 | T | 762 | 0 | 859 | 33 | 0 |
| 24 | U | 208 | 0 | 221 | 75 | 0 |
| 25 | Y | 365 | 0 | 0 | 0 | 0 |
| All | All | 55543 | 0 | 38381 | 3223 | 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 35.

All (3223) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1320:C:C1' | 22:S:73:GLU:HG2 | 1.23 | 1.60 |
| 1:A:409:G:H5'' | 7:D:25:ARG:CB | 1.29 | 1.57 |
| 16:M:92:HIS:CD2 | 16:M:98:VAL:HG21 | 1.42 | 1.55 |
| 1:A:986:A:C1' | 22:S:55:LYS:HA | 1.31 | 1.54 |
| 3:W:37:YYG:H192 | 10:G:84:ASN:CA | 1.12 | 1.54 |
| 16:M:23:TYR:CE2 | 16:M:70:LEU:HD22 | 1.46 | 1.48 |
| 1:A:409:G:C5' | 7:D:25:ARG:HB2 | 1.42 | 1.45 |
| 1:A:1329:A:H5'' | 16:M:26:GLY:N | 1.27 | 1.45 |
| 7:D:15:GLU:CG | 7:D:63:LYS:HB3 | 1.48 | 1.43 |
| 7:D:15:GLU:HG2 | 7:D:63:LYS:CB | 1.47 | 1.42 |
| 7:D:187:ARG:C | 7:D:188:LEU:N | 1.72 | 1.42 |
| 1:A:1221:G:H5' | 22:S:36:ARG:NH1 | 1.13 | 1.42 |
| 16:M:92:HIS:NE2 | 16:M:98:VAL:HG21 | 1.34 | 1.40 |
| 1:A:986:A:H1' | 22:S:55:LYS:CA | 1.53 | 1.39 |
| 7:D:23:GLY:C | 7:D:112:VAL:HG12 | 1.44 | 1.36 |
| 1:A:1318:A:H5' | 22:S:10:PHE:CB | 1.55 | 1.36 |
| 16:M:91:ARG:HH12 | 16:M:103:THR:CG2 | 1.39 | 1.35 |
| 3:W:1:G:N2 | 3:W:2:C:H41 | 1.22 | 1.35 |
| 16:M:91:ARG:NH1 | 16:M:103:THR:HG21 | 1.37 | 1.34 |
| 5:B:112:VAL:C | 5:B:113:HIS:N | 1.79 | 1.34 |
| 2:V:30:G:O2' | 12:I:127:LYS:NZ | 1.56 | 1.34 |
| 1:A:1320:C:H1' | 22:S:73:GLU:CG | 1.57 | 1.34 |
| 1:A:1500:A:H5'' | 1:A:1508:G:C5' | 1.58 | 1.34 |
| 1:A:953:G:O2' | 16:M:125:ARG:HA | 1.25 | 1.33 |
| 17:N:24:CYS:CB | 17:N:40:CYS:H | 1.40 | 1.33 |
| 1:A:1308:U:C5' | 16:M:110:ARG:HH22 | 1.41 | 1.33 |
| 1:A:986:A:C2 | 22:S:52:TYR:CE2 | 1.95 | 1.32 |
| 2:V:30:G:C2' | 12:I:127:LYS:NZ | 1.93 | 1.31 |
| 15:L:23:LYS:C | 15:L:24:VAL:CA | 2.00 | 1.31 |
| 15:L:23:LYS:O | 15:L:24:VAL:N | 1.63 | 1.31 |
| 1:A:302:G:N3 | 1:A:556:C:H4' | 1.45 | 1.30 |
| 1:A:1319:A:H4' | 22:S:70:LYS:NZ | 1.45 | 1.30 |
| 3:W:37:YYG:H192 | 10:G:84:ASN:N | 1.41 | 1.29 |
| 3:W:1:G:N2 | 3:W:2:C:N4 | 1.77 | 1.29 |
| 1:A:408:A:H5'' | 7:D:22:LYS:O | 1.12 | 1.29 |
| 1:A:1219:U:O2' | 22:S:34:TRP:HB3 | 1.24 | 1.29 |
| 7:D:23:GLY:HA2 | 7:D:112:VAL:C | 1.52 | 1.28 |
| 1:A:1220:G:H21 | 22:S:54:GLY:CA | 1.46 | 1.27 |
| 1:A:39:G:N7 | 1:A:547:A:H8 | 1.32 | 1.26 |
| 1:A:979:C:H5'' | 1:A:1222:G:O6 | 1.14 | 1.26 |
| 1:A:979:C:OP1 | 1:A:1223:C:N4 | 1.67 | 1.26 |
| 1:A:409:G:OP2 | 7:D:22:LYS:HE2 | 1.33 | 1.24 |
| 1:A:1221:G:O2' | 22:S:77:THR:HG23 | 1.35 | 1.23 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1224:G:N2 | 1:A:1362:C:C2 | 2.03 | 1.23 |
| 1:A:25:C:O3' | 1:A:26:A:P | 1.96 | 1.23 |
| 1:A:1329:A:C5' | 16:M:26:GLY:N | 2.02 | 1.23 |
| 3:W:72:C:O2' | 3:W:73:A:C5' | 1.86 | 1.23 |
| 1:A:31:G:O2' | 1:A:46:G:H5' | 1.39 | 1.23 |
| 15:L:23:LYS:CA | 15:L:24:VAL:N | 2.01 | 1.22 |
| 1:A:1298:C:O3' | 1:A:1299:A:P | 1.97 | 1.22 |
| 1:A:1221:G:C5' | 22:S:36:ARG:NH1 | 2.02 | 1.21 |
| 1:A:303:A:O2' | 1:A:555:C:O2' | 1.59 | 1.21 |
| 1:A:820:U:O3' | 1:A:821:G:P | 1.99 | 1.20 |
| 1:A:1268:A:O2' | 24:U:20:LYS:CA | 1.89 | 1.20 |
| 1:A:979:C:C5' | 1:A:1222:G:O6 | 1.90 | 1.20 |
| 1:A:1328:C:C5' | 16:M:28:ALA:HB1 | 1.70 | 1.20 |
| 2:V:7:U:O3' | 2:V:8:U:P | 1.98 | 1.20 |
| 1:A:671:G:H5' | 9:F:77:ARG:NH2 | 1.55 | 1.20 |
| 1:A:1320:C:N3 | 22:S:72:GLY:HA3 | 1.56 | 1.19 |
| 1:A:1223:C:OP2 | 22:S:78:ARG:NH2 | 1.72 | 1.19 |
| 1:A:546:G:O3' | 1:A:547:A:P | 1.99 | 1.19 |
| 1:A:901:A:O2' | 1:A:1513:A:OP1 | 1.62 | 1.18 |
| 16:M:91:ARG:NH1 | 16:M:103:THR:CG2 | 2.02 | 1.18 |
| 1:A:1219:U:O2 | 22:S:34:TRP:CD1 | 1.96 | 1.18 |
| 3:W:72:C:O2' | 3:W:73:A:H5' | 1.38 | 1.18 |
| 1:A:409:G:OP2 | 7:D:22:LYS:CE | 1.90 | 1.18 |
| 3:W:37:YYG:C15 | 10:G:84:ASN:H | 1.57 | 1.18 |
| 8:E:144:THR:C | 8:E:145:LYS:N | 1.96 | 1.18 |
| 7:D:3:ARG:HG3 | 7:D:118:ARG:NH1 | 1.57 | 1.17 |
| 1:A:1500:A:C5' | 1:A:1508:G:H5'' | 1.75 | 1.17 |
| 1:A:576:G:O3' | 1:A:577:G:P | 2.03 | 1.16 |
| 1:A:1320:C:C1' | 22:S:73:GLU:CG | 2.19 | 1.15 |
| 16:M:23:TYR:HE2 | 16:M:70:LEU:CD2 | 1.58 | 1.15 |
| 1:A:29:G:O2' | 1:A:295:C:H4' | 1.44 | 1.15 |
| 1:A:1313:U:C5 | 22:S:4:SER:HB3 | 1.81 | 1.15 |
| 1:A:1269:A:N3 | 1:A:1326:C:H1' | 1.62 | 1.15 |
| 3:W:72:C:O2' | 3:W:73:A:C4' | 1.95 | 1.15 |
| 1:A:953:G:O2' | 16:M:124:PRO:O | 1.62 | 1.14 |
| 1:A:952:U:O2 | 16:M:126:LYS:O | 1.64 | 1.14 |
| 1:A:1198:G:O2' | 13:J:54:PHE:HE2 | 1.29 | 1.14 |
| 13:J:51:ARG:HB2 | 13:J:59:SER:HB3 | 1.15 | 1.14 |
| 2:V:73:A:O3' | 2:V:74:C:P | 2.05 | 1.13 |
| 7:D:15:GLU:CD | 7:D:63:LYS:HB3 | 1.67 | 1.13 |
| 1:A:394:G:O3' | 1:A:395:C:P | 2.05 | 1.13 |
| 16:M:92:HIS:CD2 | 16:M:98:VAL:CG2 | 2.32 | 1.13 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1340:A:P | 3:W:34:G:O2' | 2.06 | 1.13 |
| 1:A:703:G:O3' | 1:A:704:A:P | 2.07 | 1.12 |
| 1:A:953:G:H1' | 16:M:125:ARG:C | 1.69 | 1.12 |
| 6:C:9:GLY:CA | 17:N:49:HIS:O | 1.97 | 1.12 |
| 3:W:25:C:N4 | 3:W:45:G:C2 | 2.17 | 1.12 |
| 1:A:39:G:N7 | 1:A:547:A:C8 | 2.18 | 1.11 |
| 3:W:37:YYG:C16 | 10:G:84:ASN:H | 1.62 | 1.11 |
| 7:D:3:ARG:HH22 | 7:D:74:GLN:NE2 | 1.49 | 1.11 |
| 3:W:37:YYG:C19 | 10:G:84:ASN:HA | 1.65 | 1.11 |
| 1:A:1268:A:O2' | 24:U:20:LYS:N | 1.83 | 1.11 |
| 1:A:1317:C:O2' | 22:S:10:PHE:CE1 | 2.04 | 1.11 |
| 17:N:24:CYS:HB2 | 17:N:40:CYS:H | 1.00 | 1.11 |
| 1:A:1361:G:O3' | 1:A:361(A):C:P | 2.09 | 1.10 |
| 1:A:1224:G:N2 | 1:A:1362:C:O2 | 1.80 | 1.10 |
| 1:A:1329:A:OP1 | 16:M:26:GLY:C | 1.89 | 1.10 |
| 1:A:937:A:O3' | 1:A:938:A:P | 2.09 | 1.09 |
| 7:D:9:CYS:SG | 7:D:31:CYS:HA | 1.91 | 1.09 |
| 7:D:21:LEU:O | 7:D:113:SER:HB2 | 1.51 | 1.09 |
| 1:A:410:G:OP2 | 7:D:25:ARG:CZ | 2.00 | 1.09 |
| 9:F:94:GLN:HB3 | 21:R:32:ARG:HH11 | 1.14 | 1.09 |
| 1:A:115:G:O3' | 1:A:116:A:P | 2.09 | 1.09 |
| 7:D:22:LYS:C | 7:D:113:SER:HB3 | 1.72 | 1.08 |
| 2:V:34:G:H2' | 2:V:35:A:H5'' | 1.31 | 1.08 |
| 1:A:404:U:C4 | 7:D:2:GLY:HA2 | 1.89 | 1.08 |
| 1:A:1308:U:H5' | 16:M:110:ARG:HH22 | 0.95 | 1.08 |
| 1:A:1329:A:C5' | 16:M:26:GLY:H | 1.65 | 1.08 |
| 1:A:1318:A:H5' | 22:S:10:PHE:HB3 | 1.29 | 1.08 |
| 3:W:25:C:N3 | 3:W:26:G:C2 | 2.21 | 1.08 |
| 5:B:185:ILE:HG22 | 5:B:199:TYR:HB2 | 1.34 | 1.08 |
| 1:A:1319:A:H4' | 22:S:70:LYS:CE | 1.82 | 1.08 |
| 1:A:1328:C:H5'' | 16:M:28:ALA:CB | 1.84 | 1.07 |
| 1:A:815:A:O2' | 1:A:1527:C:H1' | 1.52 | 1.07 |
| 1:A:939:G:P | 10:G:102:ARG:HH12 | 1.75 | 1.07 |
| 1:A:1107:C:O3' | 1:A:1108:G:P | 2.12 | 1.07 |
| 7:D:22:LYS:C | 7:D:113:SER:CB | 2.23 | 1.07 |
| 7:D:24:GLU:HB2 | 7:D:112:VAL:HG11 | 1.23 | 1.07 |
| 7:D:21:LEU:HD22 | 7:D:114:ARG:HG3 | 1.37 | 1.07 |
| 8:E:78:HIS:HB2 | 11:H:104:ARG:HD2 | 1.34 | 1.07 |
| 1:A:1046:A:O3' | 1:A:1047:G:P | 2.12 | 1.07 |
| 1:A:1224:G:N1 | 1:A:1362:C:N3 | 2.02 | 1.06 |
| 3:W:37:YYG:C19 | 10:G:83:ALA:C | 2.21 | 1.06 |
| 1:A:671:G:C5' | 9:F:77:ARG:HH21 | 1.67 | 1.06 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:957:U:H4' | 22:S:79:THR:HB | 1.11 | 1.06 |
| 1:A:1313:U:C5 | 22:S:4:SER:CB | 2.39 | 1.06 |
| 1:A:695:A:H2 | 1:A:787:A:H4' | 1.16 | 1.06 |
| 1:A:1328:C:C5' | 16:M:28:ALA:CB | 2.33 | 1.06 |
| 1:A:1313:U:H5 | 22:S:4:SER:HB3 | 1.13 | 1.06 |
| 3:W:25:C:C2 | 3:W:26:G:C2 | 2.43 | 1.06 |
| 7:D:23:GLY:HA2 | 7:D:112:VAL:O | 1.54 | 1.06 |
| 1:A:406:G:H4' | 7:D:5:ILE:HG21 | 1.36 | 1.06 |
| 1:A:1318:A:H5' | 22:S:10:PHE:HB2 | 1.28 | 1.06 |
| 1:A:922:G:N3 | 1:A:1398:A:H2 | 1.52 | 1.06 |
| 1:A:764:C:H2' | 1:A:765:G:C8 | 1.91 | 1.06 |
| 16:M:91:ARG:CD | 16:M:96:LEU:HD12 | 1.86 | 1.05 |
| 1:A:116:A:N1 | 1:A:313:A:O2' | 1.88 | 1.05 |
| 1:A:1400:C:C2 | 2:V:34:G:N2 | 2.24 | 1.05 |
| 1:A:1405:G:N2 | 1:A:1518:A:N3 | 2.04 | 1.05 |
| 1:A:1224:G:O3' | 1:A:1225:A:P | 2.13 | 1.05 |
| 7:D:15:GLU:HG2 | 7:D:63:LYS:HB2 | 1.32 | 1.05 |
| 3:W:25:C:C4 | 3:W:26:G:N1 | 2.24 | 1.05 |
| 9:F:89:MET:HG2 | 21:R:76:LEU:HD21 | 1.32 | 1.05 |
| 13:J:46:ARG:HH11 | 17:N:59:ALA:HB1 | 1.19 | 1.05 |
| 1:A:116:A:N6 | 1:A:313:A:H1' | 1.70 | 1.05 |
| 1:A:1268:A:O2' | 24:U:20:LYS:HA | 1.55 | 1.05 |
| 1:A:1220:G:H21 | 22:S:54:GLY:HA2 | 0.94 | 1.04 |
| 9:F:95:GLU:HB2 | 9:F:96:PRO:CD | 1.88 | 1.04 |
| 1:A:1317:C:O2' | 22:S:10:PHE:CZ | 2.07 | 1.04 |
| 2:V:40:C:H2' | 2:V:41:U:H5'' | 1.36 | 1.04 |
| 3:W:39:PSU:H4' | 14:K:54:ARG:HH22 | 1.18 | 1.04 |
| 7:D:23:GLY:HA2 | 7:D:113:SER:N | 1.71 | 1.04 |
| 1:A:1340:A:OP1 | 3:W:34:G:O2' | 1.75 | 1.04 |
| 3:W:25:C:N3 | 3:W:26:G:N1 | 2.06 | 1.04 |
| 2:V:35:A:N6 | 4:X:117:U:O4 | 1.90 | 1.04 |
| 1:A:1220:G:N2 | 22:S:54:GLY:HA2 | 1.71 | 1.03 |
| 1:A:1268:A:C4' | 24:U:20:LYS:HA | 1.88 | 1.03 |
| 16:M:66:LEU:HA | 16:M:70:LEU:HD12 | 1.39 | 1.03 |
| 3:W:72:C:O2' | 3:W:73:A:O4' | 1.74 | 1.03 |
| 1:A:986:A:C2 | 22:S:52:TYR:HE2 | 1.35 | 1.03 |
| 1:A:764:C:H2' | 1:A:765:G:H8 | 1.20 | 1.03 |
| 1:A:37:U:N3 | 1:A:397:A:N1 | 2.05 | 1.03 |
| 7:D:3:ARG:HG3 | 7:D:118:ARG:HH11 | 1.07 | 1.03 |
| 3:W:25:C:C2 | 3:W:26:G:C4 | 2.46 | 1.03 |
| 16:M:91:ARG:CZ | 16:M:103:THR:HG21 | 1.89 | 1.03 |
| 1:A:1315:U:OP2 | 22:S:6:LYS:HD2 | 1.58 | 1.03 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:116:A:H61 | 1:A:313:A:H1' | 0.86 | 1.03 |
| 1:A:129(A):G:O2' | 1:A:190(E):U:H3' | 1.58 | 1.03 |
| 1:A:1320:C:O2 | 22:S:72:GLY:C | 1.97 | 1.03 |
| 16:M:92:HIS:NE2 | 16:M:98:VAL:CG2 | 2.20 | 1.03 |
| 7:D:99:SER:HB3 | 7:D:139:ARG:HG3 | 1.39 | 1.03 |
| 1:A:1268:A:H4' | 24:U:20:LYS:CA | 1.87 | 1.03 |
| 1:A:116:A:H61 | 1:A:313:A:C1' | 1.71 | 1.03 |
| 1:A:1314:C:N4 | 22:S:4:SER:OG | 1.92 | 1.03 |
| 1:A:1288:A:N1 | 1:A:1371:G:H1' | 1.74 | 1.03 |
| 1:A:1308:U:H5' | 16:M:110:ARG:NH2 | 1.72 | 1.02 |
| 2:V:73:A:H3' | 2:V:74:C:P | 1.99 | 1.02 |
| 1:A:1004:A:C8 | 1:A:1025:U:O4 | 2.11 | 1.02 |
| 1:A:988:G:H4' | 1:A:1014:A:H61 | 1.17 | 1.02 |
| 1:A:1014:A:C2 | 22:S:34:TRP:CE3 | 2.48 | 1.02 |
| 3:W:25:C:C5 | 3:W:26:G:C6 | 2.48 | 1.02 |
| 1:A:1259:C:O2 | 1:A:1283:G:H1' | 1.59 | 1.02 |
| 17:N:24:CYS:HB2 | 17:N:40:CYS:N | 1.75 | 1.01 |
| 1:A:983:A:C8 | 1:A:1201:A:N1 | 2.27 | 1.01 |
| 3:W:9:A:H1' | 3:W:45:G:H2' | 1.06 | 1.01 |
| 1:A:1329:A:O2' | 16:M:24:GLY:HA2 | 1.61 | 1.01 |
| 1:A:922:G:N3 | 1:A:1398:A:C2 | 2.29 | 1.01 |
| 1:A:1221:G:C5' | 22:S:36:ARG:HH12 | 1.65 | 1.01 |
| 1:A:1313:U:O4 | 22:S:4:SER:OG | 1.79 | 1.00 |
| 1:A:427:U:H5' | 7:D:41:GLY:HA2 | 1.43 | 1.00 |
| 3:W:37:YYG:C16 | 10:G:84:ASN:N | 2.21 | 1.00 |
| 1:A:408:A:C5' | 7:D:22:LYS:O | 2.08 | 1.00 |
| 13:J:45:ARG:NH2 | 17:N:36:PHE:HE2 | 1.60 | 1.00 |
| 1:A:541:G:H4' | 7:D:42:GLN:HB2 | 1.38 | 1.00 |
| 1:A:986:A:H4' | 22:S:55:LYS:HG3 | 1.44 | 1.00 |
| 2:V:73:A:C3' | 2:V:74:C:P | 2.49 | 1.00 |
| 1:A:826:C:H5' | 11:H:12:ARG:HE | 1.25 | 1.00 |
| 3:W:25:C:C4 | 3:W:26:G:C6 | 2.49 | 1.00 |
| 1:A:889:A:N6 | 1:A:908:A:N7 | 2.11 | 0.99 |
| 1:A:1237:C:O3' | 1:A:1238:A:P | 2.20 | 0.99 |
| 7:D:3:ARG:CG | 7:D:118:ARG:NH1 | 2.25 | 0.99 |
| 1:A:462:G:H21 | 19:P:82:GLN:HE21 | 1.05 | 0.99 |
| 1:A:600:C:OP1 | 11:H:97:VAL:HB | 1.61 | 0.99 |
| 1:A:1269:A:O4' | 1:A:1326:C:H4' | 1.62 | 0.98 |
| 1:A:1328:C:P | 16:M:28:ALA:HB2 | 2.01 | 0.98 |
| 1:A:1318:A:C5' | 22:S:10:PHE:HB3 | 1.93 | 0.98 |
| 1:A:22:G:O2' | 1:A:913:A:N1 | 1.94 | 0.98 |
| 7:D:23:GLY:O | 7:D:112:VAL:HG12 | 1.62 | 0.98 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 16:M:91:ARG:HD3 | 16:M:96:LEU:CD1 | 1.92 | 0.98 |
| 1:A:404:U:O4 | 7:D:2:GLY:HA2 | 1.63 | 0.98 |
| 9:F:95:GLU:HB2 | 9:F:96:PRO:HD3 | 1.42 | 0.98 |
| 1:A:1319:A:H4' | 22:S:70:LYS:HZ3 | 1.24 | 0.97 |
| 1:A:1095:U:OP2 | 1:A:1108:G:N1 | 1.96 | 0.97 |
| 2:V:34:G:C2' | 2:V:35:A:H5'' | 1.93 | 0.97 |
| 13:J:10:GLY:HA3 | 13:J:16:LEU:HD21 | 1.45 | 0.97 |
| 1:A:876:G:H1' | 11:H:11:THR:HG21 | 1.45 | 0.97 |
| 1:A:1317:C:O2' | 22:S:10:PHE:CD1 | 2.18 | 0.97 |
| 3:W:9:A:H1' | 3:W:45:G:C2' | 1.92 | 0.97 |
| 1:A:450:G:H4' | 19:P:42:ARG:HG2 | 1.45 | 0.97 |
| 1:A:1219:U:O2' | 22:S:34:TRP:CB | 2.13 | 0.97 |
| 1:A:953:G:O2' | 16:M:125:ARG:CA | 2.12 | 0.97 |
| 1:A:1250:A:H4' | 12:I:67:GLY:C | 1.84 | 0.97 |
| 1:A:1340:A:OP1 | 3:W:34:G:C2' | 2.13 | 0.97 |
| 17:N:24:CYS:CB | 17:N:40:CYS:N | 2.25 | 0.97 |
| 7:D:78:LEU:HD21 | 7:D:139:ARG:HH21 | 1.26 | 0.96 |
| 6:C:91:LEU:HD11 | 6:C:99:VAL:HG22 | 1.45 | 0.96 |
| 1:A:1286:A:N6 | 1:A:1354:C:H5'' | 1.79 | 0.96 |
| 1:A:652:U:H1' | 1:A:653:A:H2 | 1.30 | 0.96 |
| 1:A:1268:A:C2' | 24:U:20:LYS:HA | 1.95 | 0.96 |
| 1:A:1328:C:H5'' | 16:M:28:ALA:HB1 | 0.98 | 0.96 |
| 1:A:1189:C:O2' | 6:C:176:HIS:HD2 | 1.49 | 0.96 |
| 1:A:1320:C:H42 | 22:S:36:ARG:HG3 | 1.28 | 0.95 |
| 1:A:463:A:OP2 | 19:P:75:ARG:NH2 | 1.99 | 0.95 |
| 1:A:1061:G:H5' | 13:J:59:SER:OG | 1.67 | 0.95 |
| 1:A:1221:G:H5' | 22:S:36:ARG:HH11 | 1.31 | 0.95 |
| 1:A:1268:A:H4' | 24:U:20:LYS:HA | 1.41 | 0.95 |
| 1:A:302:G:C2 | 1:A:556:C:H4' | 2.01 | 0.95 |
| 4:X:120:G:H2' | 4:X:121:A:C8 | 2.01 | 0.95 |
| 3:W:1:G:H22 | 3:W:2:C:N4 | 1.65 | 0.95 |
| 1:A:939:G:OP1 | 10:G:102:ARG:NH1 | 1.99 | 0.95 |
| 1:A:1061:G:OP1 | 13:J:59:SER:HA | 1.67 | 0.94 |
| 1:A:991:U:O3' | 1:A:992:U:P | 2.25 | 0.94 |
| 1:A:1222:G:H5' | 22:S:77:THR:HG21 | 1.50 | 0.94 |
| 1:A:1308:U:C5' | 16:M:110:ARG:NH2 | 2.27 | 0.94 |
| 9:F:62:TRP:CD1 | 21:R:35:ARG:NH2 | 2.36 | 0.94 |
| 6:C:9:GLY:HA2 | 17:N:49:HIS:O | 1.68 | 0.94 |
| 1:A:21:G:N3 | 1:A:915:A:N6 | 2.16 | 0.94 |
| 4:X:120:G:H2' | 4:X:121:A:H8 | 1.29 | 0.94 |
| 11:H:21:LYS:O | 11:H:63:LEU:HD11 | 1.67 | 0.94 |
| 1:A:1156:G:O3' | 1:A:1157:A:P | 2.25 | 0.94 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1329:A:OP1 | 16:M:26:GLY:O | 1.86 | 0.94 |
| 16:M:66:LEU:C | 16:M:70:LEU:HB2 | 1.88 | 0.94 |
| 1:A:889:A:H4' | 1:A:890:G:H4' | 1.44 | 0.94 |
| 1:A:1037:C:N3 | 1:A:1038:C:C5 | 2.36 | 0.94 |
| 1:A:219:C:O3' | 1:A:220:G:P | 2.26 | 0.94 |
| 16:M:91:ARG:HD3 | 16:M:96:LEU:HD12 | 0.99 | 0.94 |
| 1:A:1270:C:OP1 | 24:U:24:ARG:NH2 | 2.01 | 0.94 |
| 1:A:1067:A:O3' | 1:A:1068:G:P | 2.25 | 0.93 |
| 1:A:1320:C:O4' | 22:S:73:GLU:HG2 | 1.67 | 0.93 |
| 1:A:406:G:H21 | 7:D:119:GLN:HE22 | 1.14 | 0.93 |
| 7:D:3:ARG:CG | 7:D:118:ARG:HH11 | 1.81 | 0.93 |
| 1:A:541:G:C4' | 7:D:42:GLN:HE21 | 1.79 | 0.93 |
| 1:A:302:G:H2' | 1:A:556:C:H5'' | 1.48 | 0.93 |
| 7:D:187:ARG:CA | 7:D:188:LEU:N | 2.32 | 0.93 |
| 1:A:1222:G:OP1 | 1:A:1321:C:H2' | 1.69 | 0.93 |
| 1:A:1327:C:H5'' | 24:U:20:LYS:HE2 | 1.47 | 0.93 |
| 1:A:1070:U:O4 | 1:A:1085:U:C5 | 2.21 | 0.93 |
| 1:A:1222:G:OP2 | 1:A:1322:C:C5 | 2.22 | 0.93 |
| 1:A:1222:G:OP1 | 1:A:1321:C:C2' | 2.17 | 0.93 |
| 1:A:1222:G:OP2 | 1:A:1322:C:C4 | 2.22 | 0.93 |
| 3:W:37:YYG:C21 | 10:G:84:ASN:N | 2.28 | 0.92 |
| 1:A:1268:A:C3' | 24:U:20:LYS:HA | 1.99 | 0.92 |
| 1:A:790:A:O5' | 2:V:38:A:O2' | 1.86 | 0.92 |
| 1:A:410:G:P | 7:D:25:ARG:NE | 2.42 | 0.92 |
| 1:A:1221:G:O2' | 22:S:77:THR:CG2 | 2.17 | 0.92 |
| 1:A:986:A:H2 | 22:S:52:TYR:CE2 | 1.62 | 0.92 |
| 7:D:98:GLU:OE2 | 7:D:103:ASN:ND2 | 2.02 | 0.92 |
| 1:A:22:G:H1' | 1:A:914:A:N6 | 1.83 | 0.92 |
| 1:A:1270:C:P | 24:U:24:ARG:NH2 | 2.43 | 0.92 |
| 1:A:1326:C:H5'' | 24:U:19:GLY:CA | 2.00 | 0.92 |
| 1:A:1037:C:C4 | 1:A:1038:C:C5 | 2.58 | 0.92 |
| 1:A:498:U:O2 | 1:A:547:A:N6 | 2.03 | 0.92 |
| 13:J:46:ARG:NH1 | 17:N:59:ALA:HB1 | 1.85 | 0.92 |
| 7:D:21:LEU:CD2 | 7:D:114:ARG:HG3 | 2.00 | 0.92 |
| 1:A:1329:A:H5'' | 16:M:26:GLY:CA | 1.98 | 0.92 |
| 1:A:1327:C:H5'' | 24:U:20:LYS:CE | 1.99 | 0.92 |
| 1:A:695:A:C2 | 1:A:787:A:H4' | 2.04 | 0.92 |
| 7:D:23:GLY:CA | 7:D:112:VAL:C | 2.39 | 0.91 |
| 6:C:18:TRP:NE1 | 17:N:53:LEU:O | 2.01 | 0.91 |
| 1:A:1255:G:H21 | 1:A:1258:G:N2 | 1.68 | 0.91 |
| 9:F:46:ARG:HH12 | 21:R:37:VAL:HG11 | 1.35 | 0.91 |
| 1:A:1314:C:H41 | 22:S:4:SER:C | 1.73 | 0.91 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:21:G:C2 | 1:A:915:A:N6 | 2.38 | 0.91 |
| 1:A:302:G:N3 | 1:A:556:C:C4' | 2.32 | 0.91 |
| 1:A:1329:A:H5' | 16:M:26:GLY:H | 1.34 | 0.91 |
| 1:A:426:G:O2' | 7:D:42:GLN:HA | 1.70 | 0.91 |
| 9:F:60:PHE:CZ | 21:R:78:LEU:HD21 | 2.06 | 0.91 |
| 1:A:1319:A:C4' | 22:S:70:LYS:NZ | 2.32 | 0.90 |
| 1:A:1320:C:N4 | 22:S:36:ARG:HG3 | 1.84 | 0.90 |
| 1:A:462:G:H21 | 19:P:82:GLN:NE2 | 1.68 | 0.90 |
| 1:A:1014:A:N3 | 22:S:34:TRP:CE3 | 2.38 | 0.90 |
| 1:A:986:A:C4' | 22:S:55:LYS:HG3 | 2.01 | 0.90 |
| 7:D:23:GLY:N | 7:D:113:SER:HB3 | 1.87 | 0.90 |
| 1:A:1314:C:N4 | 22:S:4:SER:O | 2.05 | 0.90 |
| 1:A:1205:U:O2' | 6:C:195:VAL:HG23 | 1.71 | 0.90 |
| 6:C:12:LEU:CD2 | 17:N:51:GLY:HA3 | 2.00 | 0.90 |
| 1:A:1206:G:O4' | 6:C:194:GLY:HA2 | 1.71 | 0.90 |
| 1:A:1268:A:H4' | 24:U:20:LYS:O | 1.70 | 0.90 |
| 3:W:25:C:N1 | 3:W:26:G:C5 | 2.40 | 0.90 |
| 3:W:41:U:H5' | 3:W:41:U:H6 | 1.34 | 0.90 |
| 1:A:1030:C:O3' | 1:A:30(A):G:P | 2.29 | 0.90 |
| 1:A:1115:C:H1' | 17:N:61:TRP:O | 1.71 | 0.90 |
| 1:A:426:G:O2' | 7:D:42:GLN:CA | 2.19 | 0.90 |
| 1:A:781:A:O2' | 1:A:1522:U:O2 | 1.89 | 0.90 |
| 1:A:1500:A:H5'' | 1:A:1508:G:H5'' | 0.91 | 0.90 |
| 1:A:1230:C:O2' | 16:M:126:LYS:HE2 | 1.72 | 0.90 |
| 1:A:1318:A:C5' | 22:S:10:PHE:CB | 2.46 | 0.90 |
| 1:A:1221:G:H5' | 22:S:36:ARG:HH12 | 1.11 | 0.90 |
| 1:A:1328:C:O5' | 16:M:28:ALA:CB | 2.19 | 0.90 |
| 3:W:25:C:N4 | 3:W:45:G:N2 | 2.19 | 0.90 |
| 1:A:1190:G:H5' | 6:C:176:HIS:NE2 | 1.87 | 0.90 |
| 1:A:1222:G:OP2 | 1:A:1322:C:N4 | 2.05 | 0.89 |
| 3:W:33:U:C2 | 3:W:35:A:H5' | 2.06 | 0.89 |
| 6:C:48:TYR:OH | 6:C:122:GLU:OE1 | 1.89 | 0.89 |
| 1:A:1269:A:H5' | 24:U:19:GLY:C | 1.92 | 0.89 |
| 1:A:41:G:H2' | 1:A:42:G:C8 | 2.05 | 0.89 |
| 1:A:1325:C:H4' | 24:U:17:THR:HB | 1.54 | 0.89 |
| 1:A:25:C:H4' | 1:A:524:G:H21 | 1.37 | 0.89 |
| 1:A:677:U:H3 | 1:A:713:G:H1 | 1.19 | 0.89 |
| 1:A:977:A:C5 | 1:A:1224:G:OP1 | 2.25 | 0.89 |
| 7:D:24:GLU:N | 7:D:112:VAL:HG12 | 1.88 | 0.89 |
| 6:C:12:LEU:HD21 | 17:N:51:GLY:HA3 | 1.52 | 0.89 |
| 1:A:1037:C:C2 | 1:A:1038:C:C6 | 2.60 | 0.89 |
| 1:A:376:G:O2' | 19:P:28:ARG:HB3 | 1.72 | 0.89 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 16:M:97:PRO:HG2 | 16:M:103:THR:HG22 | 1.52 | 0.89 |
| 7:D:187:ARG:C | 7:D:188:LEU:CA | 2.42 | 0.89 |
| 3:W:25:C:C2 | 3:W:26:G:N3 | 2.41 | 0.89 |
| 9:F:89:MET:HG2 | 21:R:76:LEU:CD2 | 2.03 | 0.89 |
| 7:D:14:ARG:HD2 | 7:D:66:ARG:HH12 | 1.37 | 0.89 |
| 1:A:247:G:OP2 | 20:Q:99:SER:HB2 | 1.73 | 0.88 |
| 1:A:393:A:OP2 | 19:P:12:LYS:HD3 | 1.73 | 0.88 |
| 1:A:1224:G:C2 | 1:A:1362:C:N3 | 2.41 | 0.88 |
| 16:M:91:ARG:HH12 | 16:M:103:THR:HG21 | 1.02 | 0.88 |
| 1:A:1314:C:N4 | 22:S:4:SER:CB | 2.37 | 0.88 |
| 6:C:16:ARG:HH22 | 6:C:184:TYR:H | 1.17 | 0.88 |
| 1:A:671:G:H5' | 9:F:77:ARG:HH21 | 0.76 | 0.88 |
| 1:A:958:A:C2 | 22:S:55:LYS:HB2 | 2.09 | 0.88 |
| 1:A:1339:A:O2' | 2:V:40:C:O2 | 1.92 | 0.88 |
| 7:D:23:GLY:N | 7:D:113:SER:CB | 2.37 | 0.87 |
| 1:A:1347:G:H8 | 12:I:107:ARG:HB3 | 1.38 | 0.87 |
| 7:D:23:GLY:CA | 7:D:113:SER:HB3 | 2.05 | 0.87 |
| 5:B:32:ILE:HD11 | 5:B:40:HIS:HB3 | 1.57 | 0.87 |
| 1:A:243:A:H4' | 1:A:244:U:H5' | 1.57 | 0.87 |
| 1:A:410:G:OP2 | 7:D:25:ARG:NE | 2.05 | 0.87 |
| 1:A:546:G:HO2' | 1:A:548:G:HO2' | 0.88 | 0.87 |
| 1:A:1287:A:H61 | 1:A:1371:G:C4' | 1.86 | 0.87 |
| 7:D:49:ARG:O | 7:D:51:PRO:HD3 | 1.74 | 0.87 |
| 1:A:815:A:H2 | 1:A:1528:U:H1' | 1.37 | 0.87 |
| 1:A:1221:G:OP1 | 1:A:1320:C:N4 | 2.08 | 0.87 |
| 2:V:37:G:N2 | 4:X:116:U:C2 | 2.43 | 0.87 |
| 1:A:426:G:H1' | 7:D:42:GLN:HG3 | 1.55 | 0.87 |
| 1:A:891:U:H2' | 1:A:892:A:H8 | 1.36 | 0.87 |
| 1:A:944:G:C6 | 1:A:1337:G:H2' | 2.10 | 0.87 |
| 3:W:10:G:N7 | 3:W:45:G:O2' | 2.05 | 0.87 |
| 1:A:266:G:H22 | 1:A:270:A:H62 | 1.20 | 0.87 |
| 1:A:32:A:H2' | 1:A:33:A:C8 | 2.10 | 0.87 |
| 7:D:9:CYS:SG | 7:D:31:CYS:CA | 2.63 | 0.87 |
| 7:D:15:GLU:HG2 | 7:D:63:LYS:HB3 | 1.06 | 0.87 |
| 1:A:986:A:C1' | 22:S:55:LYS:CA | 2.27 | 0.86 |
| 7:D:8:VAL:HB | 7:D:115:ARG:CZ | 2.05 | 0.86 |
| 1:A:31:G:C5 | 1:A:306:G:H1' | 2.10 | 0.86 |
| 1:A:1014:A:O3' | 22:S:14:HIS:CE1 | 2.28 | 0.86 |
| 1:A:1221:G:C4' | 22:S:36:ARG:HH12 | 1.87 | 0.86 |
| 1:A:958:A:N3 | 22:S:55:LYS:HB2 | 1.90 | 0.86 |
| 7:D:23:GLY:CA | 7:D:112:VAL:O | 2.23 | 0.86 |
| 16:M:92:HIS:CE1 | 16:M:98:VAL:HG21 | 2.11 | 0.86 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-------------------|-------------|----------|
| 7:D:127:THR:HB | 7:D:147:ALA:HB3 | 1.58 | 0.86 |
| 1:A:1276:G:O2' | 1:A:1282:C:H4' | 1.76 | 0.86 |
| 1:A:957:U:H4' | 22:S:79:THR:CB | 2.03 | 0.86 |
| 1:A:1277:C:O2' | 1:A:1282:C:C2 | 2.27 | 0.86 |
| 1:A:1308:U:H5'' | 16:M:110:ARG:HH22 | 1.41 | 0.86 |
| 20:Q:8:GLY:HA3 | 20:Q:22:LEU:O | 1.75 | 0.85 |
| 1:A:495:U:H2' | 1:A:496:A:H5' | 1.59 | 0.85 |
| 1:A:815:A:C2 | 1:A:1528:U:H1' | 2.12 | 0.85 |
| 16:M:23:TYR:CE2 | 16:M:70:LEU:CD2 | 2.43 | 0.85 |
| 1:A:1277:C:C1' | 1:A:1282:C:H1' | 2.06 | 0.85 |
| 1:A:562:C:H1' | 15:L:15:ARG:HD2 | 1.56 | 0.85 |
| 1:A:1004:A:H3' | 1:A:1025:U:C2 | 2.10 | 0.85 |
| 1:A:986:A:O4' | 22:S:55:LYS:HA | 1.76 | 0.85 |
| 3:W:25:C:C6 | 3:W:26:G:C6 | 2.63 | 0.85 |
| 1:A:410:G:P | 7:D:25:ARG:HE | 2.00 | 0.85 |
| 1:A:1340:A:C4' | 2:V:31:A:O2' | 2.21 | 0.85 |
| 1:A:585:G:O2' | 1:A:879:C:H5'' | 1.76 | 0.85 |
| 1:A:668:G:N3 | 18:O:46:HIS:NE2 | 2.24 | 0.85 |
| 3:W:39:PSU:H4' | 14:K:54:ARG:NH2 | 1.92 | 0.85 |
| 7:D:23:GLY:O | 7:D:112:VAL:O | 1.95 | 0.85 |
| 1:A:983:A:O3' | 1:A:984:C:P | 2.34 | 0.85 |
| 1:A:1270:C:P | 24:U:24:ARG:HH22 | 1.98 | 0.85 |
| 1:A:1291:G:H4' | 12:I:38:GLN:O | 1.76 | 0.85 |
| 1:A:559:A:H4' | 1:A:560:U:O5' | 1.75 | 0.84 |
| 1:A:947:G:H4' | 1:A:1332:A:H2 | 1.41 | 0.84 |
| 1:A:1014:A:C2 | 22:S:34:TRP:CD2 | 2.65 | 0.84 |
| 1:A:1320:C:C2 | 22:S:72:GLY:C | 2.50 | 0.84 |
| 16:M:66:LEU:C | 16:M:67:GLU:N | 2.31 | 0.84 |
| 1:A:409:G:C5' | 7:D:25:ARG:CB | 2.19 | 0.84 |
| 1:A:1317:C:O2' | 22:S:10:PHE:CE2 | 2.24 | 0.84 |
| 1:A:403:C:N4 | 1:A:547:A:H5' | 1.92 | 0.84 |
| 2:V:37:G:C2 | 4:X:116:U:N3 | 2.46 | 0.84 |
| 1:A:1339:A:C2 | 2:V:31:A:H1' | 2.13 | 0.84 |
| 1:A:375:U:O3' | 19:P:6:LEU:HD22 | 1.77 | 0.84 |
| 1:A:1340:A:OP1 | 3:W:34:G:H2' | 1.78 | 0.84 |
| 1:A:1058:G:OP1 | 6:C:199:LYS:HE3 | 1.76 | 0.84 |
| 3:W:72:C:C2' | 3:W:73:A:C5' | 2.55 | 0.84 |
| 1:A:1375:A:OP1 | 10:G:12:LEU:HD21 | 1.77 | 0.84 |
| 7:D:22:LYS:C | 7:D:113:SER:HB2 | 1.95 | 0.84 |
| 1:A:1328:C:P | 16:M:28:ALA:CB | 2.66 | 0.84 |
| 2:V:30:G:C3' | 12:I:127:LYS:NZ | 2.29 | 0.84 |
| 1:A:1220:G:O2' | 22:S:36:ARG:HD3 | 1.76 | 0.84 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:409:G:O3' | 7:D:25:ARG:HG3 | 1.78 | 0.84 |
| 7:D:31:CYS:O | 7:D:33:MET:N | 2.10 | 0.84 |
| 1:A:39:G:C8 | 1:A:498:U:C4 | 2.66 | 0.84 |
| 1:A:1318:A:H4' | 22:S:10:PHE:HB3 | 1.58 | 0.83 |
| 1:A:377:G:OP1 | 19:P:3:LYS:HD2 | 1.78 | 0.83 |
| 14:K:110:ASP:HB3 | 21:R:85:LEU:HB3 | 1.60 | 0.83 |
| 1:A:953:G:O3' | 16:M:124:PRO:O | 1.96 | 0.83 |
| 13:J:64:GLU:HG2 | 17:N:59:ALA:HA | 1.57 | 0.83 |
| 1:A:1277:C:H1' | 1:A:1282:C:H1' | 1.60 | 0.83 |
| 1:A:1220:G:N2 | 22:S:54:GLY:CA | 2.32 | 0.83 |
| 1:A:405:U:OP2 | 7:D:5:ILE:HD12 | 1.77 | 0.83 |
| 1:A:25:C:H4' | 1:A:524:G:N2 | 1.94 | 0.83 |
| 1:A:1400:C:C5 | 2:V:34:G:N1 | 2.46 | 0.83 |
| 1:A:47:C:H4' | 1:A:48:C:C5' | 2.08 | 0.83 |
| 1:A:1286:A:H62 | 1:A:1354:C:H5'' | 1.39 | 0.83 |
| 7:D:22:LYS:O | 7:D:113:SER:HB3 | 1.77 | 0.83 |
| 6:C:9:GLY:N | 17:N:49:HIS:O | 2.10 | 0.83 |
| 3:W:25:C:O2 | 3:W:26:G:N3 | 2.11 | 0.83 |
| 3:W:9:A:C1' | 3:W:45:G:H2' | 2.02 | 0.83 |
| 1:A:20:U:N3 | 1:A:916:G:C2 | 2.47 | 0.83 |
| 1:A:768:A:OP1 | 1:A:804:U:H5'' | 1.79 | 0.83 |
| 1:A:31:G:O2' | 1:A:46:G:C5' | 2.25 | 0.83 |
| 3:W:25:C:C5 | 3:W:26:G:O6 | 2.32 | 0.83 |
| 2:V:35:A:N1 | 4:X:118:C:N4 | 2.03 | 0.83 |
| 1:A:37:U:O2 | 1:A:397:A:N6 | 2.09 | 0.83 |
| 1:A:1004:A:H5'' | 1:A:1025:U:C5 | 2.14 | 0.83 |
| 1:A:674:G:H2' | 1:A:675:A:H8 | 1.44 | 0.83 |
| 1:A:958:A:C1' | 22:S:55:LYS:HD2 | 2.08 | 0.83 |
| 1:A:1320:C:O4' | 22:S:73:GLU:CG | 2.25 | 0.83 |
| 1:A:436:C:H2' | 1:A:437:U:C6 | 2.14 | 0.83 |
| 3:W:33:U:O2 | 3:W:35:A:H3' | 1.79 | 0.83 |
| 1:A:397:A:C6 | 1:A:548:G:C5 | 2.67 | 0.83 |
| 1:A:397:A:N6 | 1:A:548:G:C5 | 2.47 | 0.82 |
| 1:A:541:G:H4' | 7:D:42:GLN:HE21 | 1.44 | 0.82 |
| 1:A:597:G:H21 | 11:H:94:TYR:HE2 | 1.24 | 0.82 |
| 1:A:1223:C:P | 22:S:78:ARG:HH21 | 2.02 | 0.82 |
| 1:A:1223:C:P | 22:S:78:ARG:NH2 | 2.51 | 0.82 |
| 1:A:953:G:C2' | 16:M:125:ARG:HA | 2.09 | 0.82 |
| 7:D:3:ARG:NH2 | 7:D:74:GLN:NE2 | 2.27 | 0.82 |
| 1:A:1347:G:H22 | 1:A:1373:G:H2' | 1.42 | 0.82 |
| 1:A:1391:U:H2' | 1:A:1392:G:H8 | 1.45 | 0.82 |
| 15:L:23:LYS:O | 15:L:24:VAL:CA | 2.17 | 0.82 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 6:C:91:LEU:HD21 | 6:C:99:VAL:H | 1.44 | 0.82 |
| 1:A:1400:C:C6 | 2:V:34:G:N1 | 2.48 | 0.82 |
| 20:Q:22:LEU:HD12 | 20:Q:23:VAL:O | 1.80 | 0.82 |
| 1:A:1014:A:C2 | 22:S:34:TRP:CZ3 | 2.67 | 0.82 |
| 1:A:1220:G:H4' | 22:S:36:ARG:HG2 | 1.59 | 0.82 |
| 3:W:37:YYG:N20 | 10:G:84:ASN:N | 2.28 | 0.82 |
| 17:N:24:CYS:HB3 | 17:N:40:CYS:H | 1.42 | 0.82 |
| 1:A:397:A:C5 | 1:A:548:G:N7 | 2.48 | 0.82 |
| 1:A:1205:U:H4' | 6:C:195:VAL:CG2 | 2.09 | 0.82 |
| 3:W:37:YYG:H192 | 10:G:84:ASN:HA | 0.82 | 0.82 |
| 5:B:174:VAL:O | 5:B:178:ARG:HB2 | 1.79 | 0.82 |
| 1:A:1004:A:H5'' | 1:A:1025:U:C6 | 2.15 | 0.81 |
| 1:A:110:C:O2' | 19:P:25:ARG:O | 1.98 | 0.81 |
| 1:A:194:C:O2' | 23:T:68:LYS:HD3 | 1.81 | 0.81 |
| 1:A:1269:A:O4' | 1:A:1326:C:C4' | 2.28 | 0.81 |
| 1:A:1375:A:OP1 | 10:G:28:ASN:ND2 | 2.13 | 0.81 |
| 11:H:18:ARG:HG3 | 11:H:18:ARG:HH11 | 1.44 | 0.81 |
| 1:A:1224:G:N2 | 1:A:1362:C:N3 | 2.28 | 0.81 |
| 1:A:1313:U:C4 | 22:S:4:SER:CB | 2.63 | 0.81 |
| 18:O:87:ILE:O | 18:O:88:ARG:HB2 | 1.78 | 0.81 |
| 1:A:1500:A:H5'' | 1:A:1508:G:H5' | 1.63 | 0.81 |
| 1:A:815:A:O2' | 1:A:1527:C:C1' | 2.29 | 0.81 |
| 1:A:406:G:C4' | 7:D:5:ILE:HG21 | 2.11 | 0.81 |
| 3:W:37:YYG:C15 | 10:G:84:ASN:N | 2.42 | 0.81 |
| 1:A:1330:U:P | 16:M:25:ILE:O | 2.39 | 0.81 |
| 3:W:65:G:H3' | 3:W:66:A:P | 2.21 | 0.81 |
| 7:D:21:LEU:O | 7:D:113:SER:CB | 2.28 | 0.81 |
| 1:A:1268:A:H4' | 24:U:20:LYS:C | 1.99 | 0.81 |
| 1:A:597:G:N2 | 11:H:94:TYR:HE2 | 1.79 | 0.81 |
| 1:A:736:C:OP1 | 21:R:72:ARG:NH2 | 2.14 | 0.81 |
| 1:A:375:U:H4' | 19:P:17:TYR:CE2 | 2.16 | 0.81 |
| 1:A:483:C:O2 | 19:P:13:HIS:HE1 | 1.63 | 0.80 |
| 21:R:73:ALA:HB1 | 21:R:79:LEU:HD11 | 1.63 | 0.80 |
| 5:B:54:THR:HG21 | 5:B:201:ILE:HD11 | 1.62 | 0.80 |
| 1:A:20:U:C4 | 1:A:916:G:N1 | 2.50 | 0.80 |
| 1:A:737:A:H4' | 9:F:72:VAL:HG11 | 1.63 | 0.80 |
| 1:A:1319:A:C4' | 22:S:70:LYS:HZ3 | 1.94 | 0.80 |
| 2:V:37:G:N2 | 4:X:116:U:N3 | 2.28 | 0.80 |
| 1:A:1222:G:P | 1:A:1321:C:O2 | 2.40 | 0.80 |
| 1:A:575:G:N2 | 1:A:880:C:O2 | 2.14 | 0.80 |
| 13:J:64:GLU:HB3 | 17:N:59:ALA:HB2 | 1.60 | 0.80 |
| 1:A:1329:A:H5'' | 16:M:25:ILE:C | 2.02 | 0.80 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1329:A:O2' | 16:M:24:GLY:CA | 2.30 | 0.80 |
| 3:W:25:C:C6 | 3:W:26:G:C5 | 2.70 | 0.80 |
| 1:A:1315:U:OP2 | 22:S:6:LYS:CD | 2.28 | 0.80 |
| 16:M:91:ARG:HH12 | 16:M:103:THR:CB | 1.94 | 0.80 |
| 7:D:3:ARG:HH22 | 7:D:74:GLN:CD | 1.85 | 0.80 |
| 13:J:11:PHE:CE2 | 17:N:55:GLY:HA3 | 2.16 | 0.80 |
| 1:A:1220:G:H5' | 22:S:36:ARG:H | 1.46 | 0.80 |
| 16:M:98:VAL:HG23 | 16:M:110:ARG:HH21 | 1.46 | 0.80 |
| 1:A:1229:A:C2 | 16:M:125:ARG:O | 2.35 | 0.80 |
| 1:A:1070:U:C4 | 1:A:1085:U:C4 | 2.69 | 0.80 |
| 1:A:1405:G:O4' | 1:A:1519:A:H4' | 1.80 | 0.80 |
| 2:V:34:G:C3' | 2:V:35:A:H5'' | 2.11 | 0.80 |
| 20:Q:21:VAL:HG12 | 20:Q:23:VAL:HG23 | 1.63 | 0.80 |
| 1:A:1320:C:H5'' | 22:S:3:ARG:CZ | 2.11 | 0.80 |
| 7:D:24:GLU:CB | 7:D:112:VAL:HG11 | 2.08 | 0.80 |
| 13:J:51:ARG:HB2 | 13:J:59:SER:CB | 2.07 | 0.80 |
| 1:A:1288:A:N6 | 1:A:1371:G:O2' | 2.14 | 0.80 |
| 1:A:767:A:N6 | 1:A:813:U:H3 | 1.79 | 0.80 |
| 1:A:250:A:H4' | 1:A:251:G:O5' | 1.82 | 0.80 |
| 15:L:117:ARG:CZ | 15:L:124:LYS:HD2 | 2.12 | 0.80 |
| 7:D:23:GLY:C | 7:D:112:VAL:CG1 | 2.40 | 0.79 |
| 1:A:958:A:N6 | 22:S:77:THR:O | 2.14 | 0.79 |
| 1:A:1061:G:H1' | 13:J:56:HIS:HE1 | 1.48 | 0.79 |
| 9:F:94:GLN:HB3 | 21:R:32:ARG:NH1 | 1.96 | 0.79 |
| 1:A:41:G:H2' | 1:A:42:G:H8 | 1.47 | 0.79 |
| 1:A:958:A:O4' | 22:S:55:LYS:NZ | 2.14 | 0.79 |
| 1:A:976:G:H2' | 1:A:361(A):C:H42 | 1.48 | 0.79 |
| 7:D:23:GLY:HA2 | 7:D:113:SER:CA | 2.12 | 0.79 |
| 1:A:302:G:H21 | 1:A:556:C:C4' | 1.95 | 0.79 |
| 13:J:45:ARG:NH2 | 17:N:36:PHE:CE2 | 2.47 | 0.79 |
| 1:A:22:G:C1' | 1:A:914:A:N6 | 2.46 | 0.79 |
| 1:A:1320:C:N3 | 22:S:72:GLY:CA | 2.44 | 0.79 |
| 1:A:1062:U:OP1 | 13:J:58:ASP:OD2 | 2.01 | 0.79 |
| 1:A:829:G:O2' | 5:B:26:PRO:HG2 | 1.81 | 0.79 |
| 1:A:404:U:C4 | 7:D:2:GLY:CA | 2.65 | 0.79 |
| 20:Q:15:MET:HB3 | 20:Q:18:THR:HB | 1.64 | 0.79 |
| 1:A:428:G:O2' | 7:D:36:ARG:NH1 | 2.15 | 0.79 |
| 1:A:15:G:O6 | 1:A:1396:A:N6 | 2.15 | 0.79 |
| 1:A:60:A:H62 | 1:A:110:C:N4 | 1.79 | 0.79 |
| 19:P:20:VAL:HG11 | 19:P:32:TYR:HB2 | 1.64 | 0.79 |
| 1:A:881:G:OP2 | 15:L:9:GLN:CD | 2.20 | 0.79 |
| 1:A:957:U:C4' | 22:S:79:THR:HB | 2.05 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:W:72:C:C2' | 3:W:73:A:O4' | 2.31 | 0.79 |
| 3:W:25:C:C2 | 3:W:26:G:C5 | 2.71 | 0.79 |
| 1:A:1255:G:N2 | 1:A:1277:C:O2 | 2.16 | 0.79 |
| 3:W:37:YYG:H243 | 10:G:85:TYR:CE2 | 2.18 | 0.79 |
| 19:P:6:LEU:HB2 | 19:P:17:TYR:HB3 | 1.63 | 0.79 |
| 1:A:1060:C:C5' | 13:J:51:ARG:HB3 | 2.13 | 0.78 |
| 1:A:1400:C:C4 | 2:V:34:G:C2 | 2.71 | 0.78 |
| 19:P:20:VAL:HG11 | 19:P:32:TYR:CB | 2.13 | 0.78 |
| 1:A:1327:C:H5' | 24:U:20:LYS:HB3 | 1.66 | 0.78 |
| 6:C:11:ARG:HG2 | 6:C:15:THR:O | 1.82 | 0.78 |
| 1:A:1317:C:O2' | 22:S:10:PHE:CG | 2.36 | 0.78 |
| 1:A:953:G:C2' | 16:M:124:PRO:O | 2.31 | 0.78 |
| 10:G:150:ALA:HA | 14:K:59:TYR:CB | 2.12 | 0.78 |
| 3:W:37:YYG:C19 | 10:G:84:ASN:CB | 2.56 | 0.78 |
| 1:A:403:C:H42 | 1:A:547:A:H5' | 1.49 | 0.78 |
| 1:A:1230:C:O2' | 16:M:126:LYS:CE | 2.31 | 0.78 |
| 5:B:180:LEU:O | 5:B:181:PHE:HB2 | 1.81 | 0.78 |
| 19:P:20:VAL:CG1 | 19:P:32:TYR:HB2 | 2.13 | 0.78 |
| 1:A:453:A:H4' | 19:P:72:ARG:HG3 | 1.64 | 0.78 |
| 6:C:106:VAL:HG12 | 6:C:108:ASN:N | 1.99 | 0.78 |
| 16:M:92:HIS:CE1 | 16:M:110:ARG:NH2 | 2.51 | 0.78 |
| 1:A:667:G:O2' | 18:O:49:ASP:OD1 | 2.02 | 0.78 |
| 7:D:141:ARG:HB3 | 7:D:142:PRO:HD2 | 1.66 | 0.78 |
| 1:A:576:G:N7 | 1:A:881:G:H1' | 1.99 | 0.78 |
| 7:D:98:GLU:CD | 7:D:103:ASN:HD21 | 1.88 | 0.78 |
| 3:W:1:G:H21 | 3:W:2:C:N4 | 1.80 | 0.77 |
| 2:V:30:G:H2' | 12:I:127:LYS:NZ | 1.98 | 0.77 |
| 1:A:571:U:H3' | 1:A:572:A:C5' | 2.14 | 0.77 |
| 12:I:11:LYS:HG3 | 12:I:108:VAL:HG11 | 1.66 | 0.77 |
| 2:V:70:C:H2' | 2:V:71:G:H8 | 1.48 | 0.77 |
| 1:A:20:U:O4' | 1:A:572:A:N1 | 2.18 | 0.77 |
| 1:A:361(A):C:O3' | 1:A:1362:C:P | 2.42 | 0.77 |
| 16:M:94:ARG:C | 16:M:95:GLY:N | 2.38 | 0.77 |
| 6:C:18:TRP:HB3 | 6:C:20:SER:O | 1.83 | 0.77 |
| 2:V:5:A:H2' | 2:V:6:U:H6 | 1.48 | 0.77 |
| 1:A:1107:C:P | 6:C:172:ARG:HG2 | 2.25 | 0.77 |
| 7:D:98:GLU:O | 7:D:99:SER:C | 2.12 | 0.77 |
| 21:R:53:ARG:HD2 | 21:R:58:LEU:O | 1.84 | 0.77 |
| 7:D:17:VAL:HG11 | 7:D:197:PRO:HG2 | 1.67 | 0.77 |
| 1:A:953:G:H1' | 16:M:125:ARG:CA | 2.14 | 0.77 |
| 1:A:562:C:O2' | 15:L:15:ARG:HB3 | 1.85 | 0.77 |
| 6:C:106:VAL:HG12 | 6:C:108:ASN:H | 1.48 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1326:C:H5'' | 24:U:19:GLY:HA2 | 1.63 | 0.77 |
| 7:D:14:ARG:CG | 7:D:66:ARG:NH1 | 2.48 | 0.77 |
| 1:A:886:G:N2 | 1:A:912:C:H1' | 1.99 | 0.77 |
| 1:A:1317:C:O2' | 22:S:10:PHE:CD2 | 2.37 | 0.77 |
| 1:A:1256:A:H61 | 1:A:1278:U:H1' | 1.50 | 0.77 |
| 1:A:1376:U:H2' | 1:A:1377:A:C8 | 2.20 | 0.77 |
| 16:M:23:TYR:CD2 | 16:M:70:LEU:HD22 | 2.19 | 0.76 |
| 3:W:72:C:C2' | 3:W:73:A:H5' | 2.13 | 0.76 |
| 1:A:31:G:C2 | 1:A:306:G:O2' | 2.38 | 0.76 |
| 1:A:403:C:OP2 | 7:D:3:ARG:NH2 | 2.18 | 0.76 |
| 1:A:757:U:H5' | 1:A:822:C:O2 | 1.85 | 0.76 |
| 1:A:876:G:C1' | 11:H:11:THR:HG21 | 2.13 | 0.76 |
| 1:A:1250:A:N3 | 1:A:1370:G:O2' | 2.19 | 0.76 |
| 9:F:46:ARG:NH1 | 21:R:37:VAL:HG11 | 2.01 | 0.76 |
| 1:A:1319:A:H4' | 22:S:70:LYS:HE2 | 1.66 | 0.76 |
| 17:N:40:CYS:O | 17:N:43:CYS:SG | 2.44 | 0.76 |
| 1:A:509:A:C8 | 7:D:54:TYR:HE2 | 2.03 | 0.76 |
| 1:A:745:C:H1' | 1:A:836:G:O2' | 1.85 | 0.76 |
| 3:W:7:U:O3' | 3:W:8:U:P | 2.43 | 0.76 |
| 1:A:1318:A:C4' | 22:S:10:PHE:HB3 | 2.16 | 0.76 |
| 1:A:953:G:C3' | 16:M:124:PRO:O | 2.33 | 0.76 |
| 1:A:31:G:H1' | 1:A:46:G:C5' | 2.14 | 0.76 |
| 2:V:48:C:O2 | 2:V:48:C:H2' | 1.84 | 0.76 |
| 1:A:1404:C:O2 | 1:A:1519:A:O2' | 2.03 | 0.76 |
| 7:D:98:GLU:O | 7:D:100:ARG:N | 2.19 | 0.76 |
| 1:A:22:G:O2' | 1:A:913:A:C2 | 2.35 | 0.76 |
| 1:A:18:C:C2 | 1:A:918:A:C2 | 2.73 | 0.76 |
| 1:A:986:A:H4' | 22:S:55:LYS:CG | 2.15 | 0.76 |
| 6:C:18:TRP:CD1 | 17:N:51:GLY:O | 2.38 | 0.76 |
| 1:A:651:C:O3' | 1:A:652:U:P | 2.44 | 0.76 |
| 1:A:977:A:N7 | 1:A:1224:G:OP1 | 2.19 | 0.75 |
| 1:A:891:U:H2' | 1:A:892:A:C8 | 2.21 | 0.75 |
| 8:E:51:VAL:HB | 8:E:52:PRO:HD3 | 1.67 | 0.75 |
| 1:A:1329:A:H4' | 16:M:24:GLY:C | 2.07 | 0.75 |
| 2:V:40:C:C2' | 2:V:41:U:H5'' | 2.15 | 0.75 |
| 1:A:20:U:O4' | 1:A:572:A:C2 | 2.38 | 0.75 |
| 1:A:585:G:N3 | 1:A:879:C:H4' | 2.02 | 0.75 |
| 1:A:668:G:H5' | 18:O:48:LYS:O | 1.85 | 0.75 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.21 | 0.75 |
| 9:F:7:ASN:ND2 | 21:R:34:TYR:CZ | 2.55 | 0.75 |
| 1:A:1400:C:C5 | 2:V:34:G:C6 | 2.74 | 0.75 |
| 20:Q:44:ALA:CB | 20:Q:59:ILE:HD11 | 2.16 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:429:U:P | 7:D:13:ARG:HE | 2.09 | 0.75 |
| 20:Q:87:LYS:O | 20:Q:91:ARG:HB3 | 1.87 | 0.75 |
| 8:E:95:ALA:HB3 | 8:E:96:PRO:HD3 | 1.68 | 0.75 |
| 1:A:826:C:H4' | 11:H:12:ARG:HG2 | 1.67 | 0.75 |
| 1:A:1182:G:H4' | 1:A:1183:A:O5' | 1.85 | 0.75 |
| 1:A:1268:A:H2 | 1:A:1327:C:H1' | 1.51 | 0.75 |
| 7:D:187:ARG:C | 7:D:188:LEU:C | 2.46 | 0.75 |
| 1:A:426:G:O2' | 7:D:42:GLN:CB | 2.35 | 0.75 |
| 2:V:66:A:H2' | 2:V:67:A:C8 | 2.22 | 0.75 |
| 13:J:45:ARG:HH21 | 17:N:36:PHE:HE2 | 1.34 | 0.75 |
| 1:A:693:G:H2' | 1:A:694:A:C8 | 2.22 | 0.75 |
| 3:W:37:YYG:H192 | 10:G:83:ALA:C | 1.96 | 0.75 |
| 1:A:541:G:C4' | 7:D:42:GLN:NE2 | 2.50 | 0.75 |
| 1:A:1073:U:N3 | 1:A:1074:G:N7 | 2.35 | 0.75 |
| 7:D:21:LEU:C | 7:D:113:SER:HB2 | 2.07 | 0.74 |
| 1:A:1269:A:H5' | 24:U:19:GLY:O | 1.87 | 0.74 |
| 15:L:23:LYS:C | 15:L:24:VAL:N | 0.70 | 0.74 |
| 5:B:163:PHE:HA | 5:B:185:ILE:O | 1.87 | 0.74 |
| 1:A:1095:U:H5' | 1:A:1109:C:C2 | 2.22 | 0.74 |
| 1:A:426:G:H4' | 7:D:42:GLN:HA | 1.67 | 0.74 |
| 9:F:62:TRP:CB | 21:R:35:ARG:HH12 | 1.99 | 0.74 |
| 10:G:150:ALA:HA | 14:K:59:TYR:CG | 2.22 | 0.74 |
| 2:V:73:A:O3' | 2:V:74:C:OP2 | 2.05 | 0.74 |
| 7:D:15:GLU:CG | 7:D:63:LYS:CB | 2.26 | 0.74 |
| 1:A:1201:A:H4' | 1:A:1202:G:H5'' | 1.69 | 0.74 |
| 7:D:109:GLY:HA3 | 7:D:165:MET:HG3 | 1.68 | 0.74 |
| 1:A:1327:C:C5' | 24:U:20:LYS:HE2 | 2.17 | 0.74 |
| 1:A:403:C:OP2 | 7:D:74:GLN:NE2 | 2.20 | 0.74 |
| 11:H:36:LEU:HA | 11:H:39:LEU:HB2 | 1.69 | 0.74 |
| 1:A:1156:G:O2' | 1:A:1179:A:N6 | 2.20 | 0.74 |
| 1:A:988:G:H4' | 1:A:1014:A:N6 | 1.99 | 0.74 |
| 1:A:1320:C:O4' | 22:S:73:GLU:OE2 | 2.06 | 0.74 |
| 1:A:1060:C:H4' | 13:J:52:GLY:N | 2.02 | 0.74 |
| 1:A:375:U:HO2' | 19:P:17:TYR:HE2 | 1.34 | 0.74 |
| 1:A:405:U:OP2 | 7:D:5:ILE:CD1 | 2.35 | 0.74 |
| 3:W:10:G:O6 | 3:W:45:G:N3 | 2.21 | 0.74 |
| 16:M:92:HIS:CE1 | 16:M:98:VAL:CG2 | 2.70 | 0.74 |
| 1:A:1269:A:H1' | 1:A:1326:C:O4' | 1.87 | 0.74 |
| 1:A:1340:A:P | 3:W:34:G:HO2' | 2.10 | 0.74 |
| 15:L:54:LYS:CG | 15:L:75:HIS:HE1 | 2.01 | 0.74 |
| 16:M:94:ARG:N | 16:M:95:GLY:N | 2.35 | 0.74 |
| 1:A:39:G:C8 | 1:A:547:A:C8 | 2.76 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:450:G:OP1 | 19:P:43:LYS:NZ | 2.21 | 0.74 |
| 1:A:509:A:H8 | 7:D:54:TYR:HE2 | 1.35 | 0.74 |
| 1:A:266:G:N2 | 1:A:270:A:H62 | 1.85 | 0.73 |
| 2:V:4:G:H2' | 2:V:5:A:C8 | 2.23 | 0.73 |
| 1:A:31:G:C2' | 1:A:46:G:H5' | 2.18 | 0.73 |
| 1:A:47:C:H4' | 1:A:48:C:H5'' | 1.69 | 0.73 |
| 1:A:900:A:H2' | 1:A:901:A:C8 | 2.23 | 0.73 |
| 1:A:20:U:C2 | 1:A:916:G:N2 | 2.56 | 0.73 |
| 1:A:137:C:O2' | 19:P:61:SER:O | 2.06 | 0.73 |
| 1:A:1320:C:H4' | 22:S:3:ARG:NH2 | 2.03 | 0.73 |
| 16:M:91:ARG:O | 16:M:96:LEU:HG | 1.88 | 0.73 |
| 1:A:953:G:H1' | 16:M:125:ARG:O | 1.89 | 0.73 |
| 1:A:1259:C:O2' | 1:A:1284:C:O4' | 2.06 | 0.73 |
| 3:W:65:G:O3' | 3:W:66:A:P | 2.45 | 0.73 |
| 3:W:37:YYG:H31 | 3:W:37:YYG:C1' | 2.19 | 0.73 |
| 16:M:23:TYR:O | 16:M:67:GLU:N | 2.21 | 0.73 |
| 1:A:1107:C:C3' | 1:A:1108:G:P | 2.77 | 0.73 |
| 7:D:78:LEU:CD2 | 7:D:139:ARG:HH21 | 2.01 | 0.73 |
| 1:A:634:C:H2' | 1:A:635:G:H8 | 1.52 | 0.73 |
| 7:D:24:GLU:HB2 | 7:D:112:VAL:CG1 | 2.12 | 0.73 |
| 15:L:23:LYS:O | 15:L:24:VAL:HA | 1.88 | 0.73 |
| 1:A:1259:C:H2' | 1:A:1283:G:O2' | 1.88 | 0.73 |
| 1:A:450:G:C4' | 19:P:42:ARG:HG2 | 2.18 | 0.73 |
| 4:X:119:U:H2' | 4:X:120:G:C8 | 2.23 | 0.73 |
| 7:D:185:PHE:HE2 | 7:D:189:PRO:HD3 | 1.54 | 0.73 |
| 1:A:1357:A:O2' | 17:N:34:TYR:CE2 | 2.41 | 0.73 |
| 1:A:1229:A:O3' | 2:V:30:G:H5'' | 1.89 | 0.73 |
| 1:A:983:A:C3' | 1:A:984:C:P | 2.77 | 0.73 |
| 1:A:1298:C:H5'' | 1:A:1299:A:OP1 | 1.89 | 0.73 |
| 9:F:62:TRP:CB | 21:R:35:ARG:NH1 | 2.52 | 0.73 |
| 1:A:54:C:N4 | 1:A:352:C:H2' | 2.04 | 0.73 |
| 11:H:44:PHE:O | 11:H:64:LYS:HB3 | 1.88 | 0.73 |
| 1:A:1313:U:C5 | 22:S:4:SER:HB2 | 2.22 | 0.73 |
| 1:A:1277:C:H1' | 1:A:1282:C:O2 | 1.89 | 0.73 |
| 1:A:1156:G:H1' | 1:A:1179:A:H61 | 1.53 | 0.73 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.23 | 0.73 |
| 1:A:1095:U:H5' | 1:A:1109:C:N3 | 2.04 | 0.73 |
| 10:G:74:GLU:HG2 | 10:G:75:VAL:H | 1.52 | 0.73 |
| 1:A:551:U:H5' | 15:L:119:LYS:HE2 | 1.69 | 0.73 |
| 1:A:762:C:H2' | 1:A:763:G:C8 | 2.24 | 0.73 |
| 5:B:145:LEU:O | 5:B:149:LEU:HB2 | 1.88 | 0.73 |
| 1:A:696:A:N3 | 1:A:786:G:O2' | 2.22 | 0.73 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:375:U:C4' | 19:P:17:TYR:CE2 | 2.71 | 0.73 |
| 20:Q:44:ALA:HB2 | 20:Q:59:ILE:HD11 | 1.70 | 0.73 |
| 1:A:1219:U:O2' | 22:S:34:TRP:C | 2.26 | 0.72 |
| 1:A:986:A:H1' | 22:S:55:LYS:HA | 0.75 | 0.72 |
| 6:C:150:LYS:HB2 | 6:C:173:VAL:HG21 | 1.70 | 0.72 |
| 10:G:77:SER:HB3 | 10:G:84:ASN:HB3 | 1.71 | 0.72 |
| 13:J:63:PHE:HE2 | 17:N:49:HIS:CE1 | 2.06 | 0.72 |
| 1:A:1037:C:N3 | 1:A:1038:C:C6 | 2.56 | 0.72 |
| 1:A:1060:C:H5'' | 13:J:51:ARG:HB3 | 1.72 | 0.72 |
| 19:P:13:HIS:O | 19:P:15:PRO:HD3 | 1.88 | 0.72 |
| 5:B:170:GLU:HG3 | 5:B:173:ALA:HB3 | 1.70 | 0.72 |
| 7:D:11:LEU:C | 7:D:13:ARG:H | 1.93 | 0.72 |
| 20:Q:67:LYS:O | 20:Q:68:ARG:HB2 | 1.90 | 0.72 |
| 1:A:1237:C:C3' | 1:A:1238:A:P | 2.78 | 0.72 |
| 1:A:1320:C:O4' | 22:S:73:GLU:CD | 2.27 | 0.72 |
| 1:A:815:A:N1 | 1:A:1508:G:N2 | 2.37 | 0.72 |
| 7:D:78:LEU:HD21 | 7:D:139:ARG:NH2 | 2.02 | 0.72 |
| 1:A:436:C:H2' | 1:A:437:U:N1 | 2.05 | 0.72 |
| 1:A:1225:A:O2' | 22:S:80:TYR:HB2 | 1.90 | 0.72 |
| 1:A:361(A):C:O3' | 1:A:1362:C:H5'' | 1.89 | 0.72 |
| 3:W:37:YYG:H31 | 3:W:37:YYG:C2' | 2.20 | 0.72 |
| 1:A:1268:A:H1' | 24:U:20:LYS:HB3 | 1.71 | 0.72 |
| 1:A:983:A:C8 | 1:A:1201:A:C2 | 2.77 | 0.72 |
| 1:A:1095:U:OP1 | 1:A:1108:G:N2 | 2.23 | 0.72 |
| 1:A:571:U:O4 | 1:A:865:A:N1 | 2.22 | 0.72 |
| 1:A:568:G:N3 | 1:A:574:A:H2 | 1.87 | 0.72 |
| 1:A:1320:C:H1' | 22:S:73:GLU:HG2 | 0.72 | 0.72 |
| 1:A:542:G:OP1 | 7:D:41:GLY:HA2 | 1.89 | 0.72 |
| 1:A:22:G:H1' | 1:A:914:A:C6 | 2.24 | 0.72 |
| 1:A:652:U:H1' | 1:A:653:A:C2 | 2.21 | 0.72 |
| 1:A:162:A:N3 | 1:A:348:G:H4' | 2.05 | 0.72 |
| 1:A:407:G:H4' | 7:D:115:ARG:HB3 | 1.70 | 0.71 |
| 1:A:1015:A:OP1 | 22:S:14:HIS:CE1 | 2.43 | 0.71 |
| 1:A:1061:G:H5' | 13:J:59:SER:HG | 1.53 | 0.71 |
| 11:H:27:PRO:HB2 | 11:H:32:LYS:HZ3 | 1.55 | 0.71 |
| 1:A:18:C:H42 | 1:A:917:G:H1 | 1.36 | 0.71 |
| 1:A:20:U:C2 | 1:A:916:G:C2 | 2.78 | 0.71 |
| 7:D:17:VAL:CG1 | 7:D:197:PRO:HG2 | 2.20 | 0.71 |
| 1:A:1325:C:OP1 | 24:U:15:ARG:NE | 2.23 | 0.71 |
| 1:A:1268:A:H1' | 24:U:20:LYS:CB | 2.20 | 0.71 |
| 1:A:31:G:C4 | 1:A:306:G:H1' | 2.24 | 0.71 |
| 1:A:1255:G:N2 | 1:A:1258:G:N2 | 2.37 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:483:C:O2 | 19:P:13:HIS:CE1 | 2.42 | 0.71 |
| 2:V:14:A:H2' | 2:V:15:G:H8 | 1.55 | 0.71 |
| 1:A:965:A:O2' | 1:A:966:G:H5'' | 1.91 | 0.71 |
| 1:A:1320:C:C2 | 22:S:72:GLY:HA3 | 2.24 | 0.71 |
| 3:W:72:C:HO2' | 3:W:73:A:C4' | 1.93 | 0.71 |
| 5:B:75:LYS:HA | 5:B:78:GLN:HB2 | 1.73 | 0.71 |
| 1:A:405:U:P | 7:D:5:ILE:CD1 | 2.78 | 0.71 |
| 16:M:92:HIS:CG | 16:M:98:VAL:HG21 | 2.20 | 0.71 |
| 1:A:397:A:C6 | 1:A:548:G:N7 | 2.59 | 0.71 |
| 7:D:185:PHE:CE2 | 7:D:189:PRO:HD3 | 2.25 | 0.71 |
| 8:E:9:LYS:HD2 | 8:E:112:LEU:HD23 | 1.72 | 0.71 |
| 16:M:91:ARG:O | 16:M:96:LEU:N | 2.24 | 0.71 |
| 1:A:1289:A:H2 | 1:A:1372:U:H4' | 1.55 | 0.71 |
| 20:Q:15:MET:CB | 20:Q:18:THR:HB | 2.21 | 0.71 |
| 1:A:1015:A:OP1 | 22:S:14:HIS:HE1 | 1.74 | 0.71 |
| 1:A:20:U:O4' | 1:A:572:A:C6 | 2.44 | 0.71 |
| 23:T:67:ALA:HA | 23:T:72:LEU:O | 1.91 | 0.71 |
| 1:A:1269:A:H5' | 24:U:19:GLY:CA | 2.21 | 0.70 |
| 1:A:1329:A:H4' | 16:M:24:GLY:O | 1.90 | 0.70 |
| 6:C:16:ARG:NH2 | 6:C:184:TYR:H | 1.89 | 0.70 |
| 1:A:279:A:H5' | 1:A:280:C:H3' | 1.73 | 0.70 |
| 10:G:150:ALA:HA | 14:K:59:TYR:HB3 | 1.72 | 0.70 |
| 1:A:136:C:O2' | 19:P:63:GLY:HA3 | 1.92 | 0.70 |
| 16:M:91:ARG:NH1 | 16:M:103:THR:HG22 | 2.05 | 0.70 |
| 1:A:302:G:N3 | 1:A:556:C:C5' | 2.54 | 0.70 |
| 1:A:1298:C:C3' | 1:A:1299:A:P | 2.79 | 0.70 |
| 7:D:98:GLU:C | 7:D:100:ARG:N | 2.35 | 0.70 |
| 1:A:19:C:O2 | 1:A:917:G:C2 | 2.43 | 0.70 |
| 1:A:1278:U:OP1 | 1:A:1281:U:H5 | 1.74 | 0.70 |
| 13:J:34:VAL:HG12 | 13:J:36:GLY:H | 1.56 | 0.70 |
| 1:A:1320:C:H1' | 22:S:73:GLU:CB | 2.21 | 0.70 |
| 7:D:20:TYR:O | 7:D:22:LYS:N | 2.23 | 0.70 |
| 1:A:463:A:H5'' | 19:P:80:PHE:HB3 | 1.73 | 0.70 |
| 7:D:22:LYS:HG3 | 7:D:115:ARG:NH2 | 2.07 | 0.70 |
| 1:A:1269:A:H4' | 24:U:18:TYR:O | 1.91 | 0.70 |
| 1:A:952:U:O2 | 16:M:126:LYS:C | 2.29 | 0.70 |
| 1:A:642:A:C2 | 11:H:113:SER:O | 2.44 | 0.70 |
| 1:A:1104:G:O2' | 5:B:111:ARG:NH2 | 2.24 | 0.70 |
| 1:A:976:G:H2' | 1:A:361(A):C:N4 | 2.05 | 0.70 |
| 7:D:27:TYR:HH | 7:D:106:TYR:HH | 1.37 | 0.70 |
| 7:D:31:CYS:C | 7:D:33:MET:H | 1.95 | 0.70 |
| 1:A:1328:C:O3' | 16:M:28:ALA:HB3 | 1.89 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:769:G:H21 | 1:A:900:A:H61 | 1.38 | 0.70 |
| 2:V:36:A:N6 | 4:X:117:U:N3 | 2.38 | 0.70 |
| 1:A:1095:U:P | 1:A:1108:G:H22 | 2.15 | 0.70 |
| 3:W:65:G:C3' | 3:W:66:A:P | 2.79 | 0.70 |
| 1:A:1086:U:H2' | 1:A:1087:G:C8 | 2.26 | 0.70 |
| 1:A:1098:C:H4' | 1:A:1167:A:H2 | 1.55 | 0.70 |
| 1:A:25:C:C4' | 1:A:524:G:H21 | 2.03 | 0.70 |
| 1:A:1255:G:O2' | 1:A:1258:G:H1' | 1.92 | 0.70 |
| 1:A:1320:C:O2 | 22:S:73:GLU:N | 2.25 | 0.70 |
| 1:A:958:A:N9 | 22:S:55:LYS:HD2 | 2.07 | 0.70 |
| 1:A:1229:A:O2' | 16:M:125:ARG:NH1 | 2.24 | 0.70 |
| 1:A:302:G:N2 | 1:A:556:C:C4' | 2.54 | 0.70 |
| 1:A:1314:C:H41 | 22:S:4:SER:CB | 2.04 | 0.70 |
| 2:V:69:U:H2' | 2:V:70:C:C6 | 2.27 | 0.70 |
| 10:G:145:ALA:O | 10:G:146:GLU:HB3 | 1.90 | 0.70 |
| 19:P:11:SER:H | 19:P:14:ASN:HB3 | 1.55 | 0.70 |
| 1:A:408:A:OP1 | 7:D:22:LYS:HA | 1.92 | 0.70 |
| 1:A:1060:C:O4' | 13:J:52:GLY:HA3 | 1.92 | 0.70 |
| 3:W:25:C:C4 | 3:W:45:G:N2 | 2.60 | 0.70 |
| 1:A:1224:G:C8 | 1:A:1322:C:OP1 | 2.45 | 0.70 |
| 1:A:1219:U:C2' | 22:S:34:TRP:HB3 | 2.21 | 0.70 |
| 7:D:22:LYS:HG3 | 7:D:115:ARG:HH22 | 1.56 | 0.70 |
| 9:F:7:ASN:ND2 | 21:R:34:TYR:CE1 | 2.60 | 0.70 |
| 15:L:45:PRO:HD2 | 15:L:50:SER:HA | 1.74 | 0.70 |
| 1:A:958:A:H1' | 22:S:55:LYS:HD2 | 1.72 | 0.69 |
| 1:A:1500:A:OP1 | 1:A:1505:G:P | 2.50 | 0.69 |
| 1:A:950:U:H1' | 1:A:971:G:C4 | 2.26 | 0.69 |
| 15:L:28:LYS:HB2 | 15:L:30:ALA:HB2 | 1.72 | 0.69 |
| 1:A:361(A):C:C3' | 1:A:1362:C:H5'' | 2.22 | 0.69 |
| 3:W:37:YYG:H243 | 10:G:85:TYR:CD2 | 2.26 | 0.69 |
| 1:A:1277:C:O4' | 1:A:1282:C:H1' | 1.91 | 0.69 |
| 1:A:518:C:H2' | 1:A:530:G:C8 | 2.27 | 0.69 |
| 20:Q:81:ARG:HG2 | 20:Q:84:LEU:HG | 1.74 | 0.69 |
| 6:C:18:TRP:CD1 | 17:N:54:PRO:HA | 2.27 | 0.69 |
| 1:A:566:G:H8 | 1:A:566:G:O5' | 1.75 | 0.69 |
| 1:A:586:C:H1' | 1:A:878:G:O2' | 1.92 | 0.69 |
| 21:R:80:PRO:O | 21:R:82:THR:N | 2.23 | 0.69 |
| 1:A:427:U:H5' | 7:D:41:GLY:CA | 2.19 | 0.69 |
| 13:J:90:LEU:H | 13:J:91:PRO:HD2 | 1.56 | 0.69 |
| 1:A:1268:A:C4' | 24:U:20:LYS:CA | 2.58 | 0.69 |
| 7:D:3:ARG:NH2 | 7:D:74:GLN:CD | 2.44 | 0.69 |
| 3:W:65:G:O3' | 3:W:66:A:H5' | 1.90 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:W:14:A:C5 | 3:W:22:G:C2 | 2.81 | 0.69 |
| 1:A:988:G:C4' | 1:A:1014:A:H61 | 2.02 | 0.69 |
| 7:D:12:CYS:O | 7:D:33:MET:HB3 | 1.92 | 0.69 |
| 3:W:34:G:OP1 | 3:W:34:G:H8 | 1.75 | 0.69 |
| 20:Q:40:LYS:HD3 | 20:Q:42:TYR:HE1 | 1.57 | 0.69 |
| 1:A:1060:C:H5' | 13:J:52:GLY:H | 1.57 | 0.69 |
| 17:N:27:CYS:SG | 17:N:43:CYS:N | 2.60 | 0.69 |
| 1:A:586:C:H5' | 1:A:879:C:OP1 | 1.92 | 0.69 |
| 2:V:4:G:H2' | 2:V:5:A:H8 | 1.54 | 0.69 |
| 8:E:152:ARG:HA | 11:H:64:LYS:HZ1 | 1.57 | 0.69 |
| 1:A:1492:A:H2' | 1:A:1493:A:O4' | 1.93 | 0.69 |
| 7:D:62:GLN:HE22 | 7:D:65:ARG:HH11 | 1.40 | 0.69 |
| 6:C:156:ARG:HB2 | 6:C:196:LEU:HD22 | 1.75 | 0.69 |
| 1:A:1320:C:C2 | 22:S:72:GLY:CA | 2.76 | 0.69 |
| 3:W:37:YYG:N20 | 3:W:37:YYG:H101 | 2.07 | 0.69 |
| 18:O:45:VAL:O | 18:O:46:HIS:HB2 | 1.93 | 0.69 |
| 9:F:62:TRP:CG | 21:R:35:ARG:NH1 | 2.59 | 0.69 |
| 1:A:813:U:H2' | 1:A:814:A:H8 | 1.58 | 0.69 |
| 2:V:60:C:H5' | 2:V:61:C:OP2 | 1.93 | 0.69 |
| 1:A:778:G:H2' | 1:A:779:C:C6 | 2.28 | 0.69 |
| 8:E:16:THR:O | 8:E:26:PHE:HB2 | 1.92 | 0.69 |
| 1:A:983:A:C8 | 1:A:1201:A:C6 | 2.81 | 0.68 |
| 1:A:757:U:O3' | 1:A:821:G:N2 | 2.25 | 0.68 |
| 1:A:1248:A:N3 | 12:I:70:LYS:NZ | 2.38 | 0.68 |
| 21:R:53:ARG:HH11 | 21:R:59:SER:HA | 1.58 | 0.68 |
| 3:W:37:YYG:H31 | 3:W:37:YYG:H1' | 1.74 | 0.68 |
| 1:A:1061:G:H1' | 13:J:56:HIS:CE1 | 2.28 | 0.68 |
| 1:A:113:G:H21 | 1:A:353:A:H2' | 1.58 | 0.68 |
| 1:A:426:G:C4' | 7:D:42:GLN:HA | 2.22 | 0.68 |
| 1:A:559:A:H4' | 1:A:560:U:C5' | 2.23 | 0.68 |
| 18:O:28:GLN:O | 18:O:32:LEU:HG | 1.94 | 0.68 |
| 2:V:19:G:H5' | 2:V:20:G:OP2 | 1.93 | 0.68 |
| 1:A:988:G:O2' | 1:A:1015:A:N6 | 2.25 | 0.68 |
| 1:A:409:G:OP2 | 7:D:22:LYS:CD | 2.40 | 0.68 |
| 7:D:12:CYS:CB | 7:D:31:CYS:O | 2.41 | 0.68 |
| 7:D:70:ILE:CD1 | 7:D:100:ARG:CZ | 2.70 | 0.68 |
| 1:A:953:G:O2' | 16:M:124:PRO:C | 2.31 | 0.68 |
| 1:A:1269:A:C2 | 1:A:1326:C:O2 | 2.46 | 0.68 |
| 1:A:13:U:H3 | 1:A:21:G:H1 | 1.39 | 0.68 |
| 1:A:1250:A:OP1 | 12:I:66:ARG:HG2 | 1.93 | 0.68 |
| 13:J:11:PHE:CD2 | 17:N:55:GLY:HA3 | 2.28 | 0.68 |
| 5:B:124:SER:HB2 | 5:B:125:PRO:HD2 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:D:152:SER:O | 7:D:158:ILE:HG13 | 1.93 | 0.68 |
| 11:H:97:VAL:HG13 | 11:H:98:LYS:H | 1.57 | 0.68 |
| 1:A:143:A:H4' | 1:A:144:G:C8 | 2.28 | 0.68 |
| 1:A:587:G:OP1 | 11:H:92:ARG:NH2 | 2.26 | 0.68 |
| 8:E:80:ILE:HD13 | 8:E:138:ALA:HB1 | 1.75 | 0.68 |
| 12:I:53:VAL:HB | 12:I:58:ARG:HH22 | 1.59 | 0.68 |
| 1:A:1319:A:H4' | 22:S:70:LYS:HZ1 | 1.53 | 0.68 |
| 7:D:187:ARG:HA | 7:D:188:LEU:N | 2.07 | 0.68 |
| 1:A:584:G:H1 | 1:A:757:U:H3 | 1.40 | 0.68 |
| 11:H:23:SER:HB2 | 11:H:60:ARG:HD2 | 1.76 | 0.68 |
| 1:A:1221:G:O3' | 22:S:77:THR:HG21 | 1.93 | 0.68 |
| 1:A:1061:G:O4' | 13:J:56:HIS:CE1 | 2.47 | 0.68 |
| 1:A:1405:G:H1' | 1:A:1519:A:C4' | 2.24 | 0.68 |
| 7:D:14:ARG:HG2 | 7:D:66:ARG:NH1 | 2.08 | 0.68 |
| 8:E:103:GLY:O | 8:E:107:ARG:HB2 | 1.94 | 0.68 |
| 9:F:50:TYR:CE1 | 21:R:77:GLY:HA2 | 2.29 | 0.68 |
| 1:A:1269:A:H2 | 1:A:1326:C:O2 | 1.77 | 0.68 |
| 13:J:53:PRO:O | 13:J:54:PHE:HB3 | 1.93 | 0.68 |
| 1:A:562:C:H1' | 15:L:15:ARG:CD | 2.23 | 0.68 |
| 1:A:1320:C:O2 | 22:S:72:GLY:O | 2.10 | 0.67 |
| 1:A:1268:A:C1' | 24:U:20:LYS:CB | 2.71 | 0.67 |
| 1:A:1224:G:HO3' | 1:A:1225:A:P | 2.15 | 0.67 |
| 1:A:397:A:N7 | 1:A:548:G:C8 | 2.62 | 0.67 |
| 1:A:813:U:OP1 | 1:A:904:C:H5' | 1.94 | 0.67 |
| 1:A:123:C:H5'' | 1:A:311:C:O2' | 1.94 | 0.67 |
| 1:A:1289:A:C2 | 1:A:1372:U:H4' | 2.29 | 0.67 |
| 1:A:946:A:H61 | 1:A:1235:U:H3 | 1.41 | 0.67 |
| 10:G:153:HIS:CE1 | 14:K:58:PRO:HG2 | 2.29 | 0.67 |
| 5:B:239:VAL:HG12 | 5:B:240:GLN:H | 1.60 | 0.67 |
| 5:B:61:LEU:HA | 5:B:64:ARG:HD2 | 1.76 | 0.67 |
| 1:A:1220:G:O2' | 22:S:52:TYR:O | 2.11 | 0.67 |
| 1:A:975:A:C4 | 1:A:1357:A:H2 | 2.12 | 0.67 |
| 1:A:1340:A:OP1 | 3:W:34:G:N3 | 2.28 | 0.67 |
| 1:A:129(A):G:N1 | 1:A:190(D):U:H4' | 2.08 | 0.67 |
| 1:A:32:A:H2' | 1:A:33:A:H8 | 1.60 | 0.67 |
| 1:A:590:C:H5'' | 11:H:30:ARG:CD | 2.24 | 0.67 |
| 1:A:29:G:HO2' | 1:A:295:C:H4' | 1.56 | 0.67 |
| 1:A:529:G:C6 | 15:L:49:ASN:ND2 | 2.63 | 0.67 |
| 1:A:1222:G:H5' | 22:S:77:THR:CG2 | 2.24 | 0.67 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.43 | 0.67 |
| 1:A:781:A:H4' | 1:A:1522:U:O2' | 1.94 | 0.67 |
| 16:M:23:TYR:HD2 | 16:M:70:LEU:HD13 | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1061:G:C1' | 13:J:56:HIS:CE1 | 2.78 | 0.67 |
| 1:A:815:A:HO2' | 1:A:1527:C:C1' | 2.07 | 0.67 |
| 1:A:1189:C:O2' | 6:C:176:HIS:CD2 | 2.40 | 0.67 |
| 1:A:598:U:H4' | 11:H:94:TYR:HB3 | 1.76 | 0.67 |
| 1:A:453:A:H4' | 19:P:72:ARG:CG | 2.25 | 0.67 |
| 1:A:1073:U:C4 | 1:A:1074:G:N7 | 2.62 | 0.67 |
| 1:A:759:A:H5' | 1:A:759:A:H8 | 1.59 | 0.67 |
| 2:V:69:U:H2' | 2:V:70:C:H6 | 1.59 | 0.67 |
| 3:W:7:U:HO3' | 3:W:8:U:P | 2.18 | 0.67 |
| 1:A:1328:C:OP1 | 16:M:28:ALA:CB | 2.43 | 0.67 |
| 1:A:31:G:H1' | 1:A:46:G:H5' | 1.76 | 0.67 |
| 3:W:44:A:C2' | 3:W:45:G:H5' | 2.25 | 0.67 |
| 1:A:1347:G:H3' | 12:I:108:VAL:HA | 1.76 | 0.67 |
| 1:A:189:G:H1 | 1:A:190(J):U:H3 | 1.40 | 0.67 |
| 1:A:315:A:H1' | 1:A:353:A:N1 | 2.10 | 0.67 |
| 7:D:22:LYS:CA | 7:D:113:SER:HB2 | 2.25 | 0.66 |
| 1:A:1498:U:H1' | 1:A:1499:A:C8 | 2.30 | 0.66 |
| 1:A:811:C:OP1 | 1:A:898:G:H5' | 1.93 | 0.66 |
| 1:A:950:U:H3 | 1:A:1231:G:H1 | 1.42 | 0.66 |
| 1:A:1070:U:O4 | 1:A:1085:U:C4 | 2.47 | 0.66 |
| 1:A:523:A:C2 | 15:L:91:LYS:HB3 | 2.30 | 0.66 |
| 1:A:1198:G:O2' | 13:J:54:PHE:CE2 | 2.20 | 0.66 |
| 3:W:25:C:C2 | 3:W:26:G:C6 | 2.83 | 0.66 |
| 1:A:1426:C:H42 | 1:A:1474:G:H1 | 1.43 | 0.66 |
| 2:V:70:C:H2' | 2:V:71:G:C8 | 2.29 | 0.66 |
| 1:A:1287:A:H61 | 1:A:1371:G:H4' | 1.60 | 0.66 |
| 1:A:1182:G:O2' | 1:A:1183:A:OP2 | 2.11 | 0.66 |
| 13:J:24:VAL:HA | 13:J:34:VAL:HG11 | 1.76 | 0.66 |
| 1:A:292:G:C5 | 1:A:293:G:H1' | 2.30 | 0.66 |
| 2:V:35:A:N6 | 4:X:117:U:C4 | 2.63 | 0.66 |
| 1:A:1256:A:OP2 | 1:A:1279:A:N6 | 2.29 | 0.66 |
| 1:A:1119:C:OP1 | 12:I:83:ARG:NH1 | 2.29 | 0.66 |
| 3:W:37:YYG:H191 | 10:G:83:ALA:C | 2.16 | 0.66 |
| 1:A:1339:A:C2 | 2:V:31:A:C1' | 2.77 | 0.66 |
| 1:A:1189:C:H5'' | 1:A:1190:G:OP2 | 1.95 | 0.66 |
| 1:A:1236:A:H4' | 1:A:1304:G:H4' | 1.76 | 0.66 |
| 18:O:24:SER:O | 18:O:28:GLN:HG2 | 1.95 | 0.66 |
| 1:A:143:A:O3' | 1:A:144:G:H8 | 1.79 | 0.66 |
| 1:A:1242:C:O2' | 1:A:1303:C:H5'' | 1.96 | 0.66 |
| 7:D:19:LEU:HD22 | 7:D:67:ILE:HG12 | 1.77 | 0.66 |
| 1:A:1059:C:H2' | 13:J:52:GLY:HA2 | 1.75 | 0.66 |
| 8:E:144:THR:O | 8:E:147:ASP:HB2 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:890:G:O2' | 1:A:891:U:C6 | 2.47 | 0.66 |
| 19:P:7:ALA:H | 19:P:18:ARG:H | 1.42 | 0.66 |
| 8:E:81:GLU:HA | 8:E:89:ILE:O | 1.94 | 0.66 |
| 1:A:965:A:OP1 | 1:A:1198:G:H5'' | 1.95 | 0.66 |
| 2:V:8:U:O2 | 2:V:48:C:H1' | 1.96 | 0.66 |
| 2:V:66:A:H2' | 2:V:67:A:H8 | 1.59 | 0.66 |
| 1:A:939:G:H5'' | 10:G:102:ARG:CZ | 2.26 | 0.66 |
| 11:H:27:PRO:O | 11:H:32:LYS:HD2 | 1.95 | 0.66 |
| 1:A:738:C:C5' | 9:F:70:ASP:HA | 2.25 | 0.66 |
| 1:A:975:A:C4 | 1:A:1357:A:C2 | 2.84 | 0.66 |
| 1:A:406:G:H21 | 7:D:119:GLN:NE2 | 1.90 | 0.66 |
| 2:V:36:A:C6 | 4:X:117:U:N3 | 2.64 | 0.66 |
| 1:A:1070:U:OP1 | 8:E:18:ARG:NH1 | 2.28 | 0.66 |
| 1:A:761:G:O2' | 20:Q:104:LYS:HA | 1.96 | 0.66 |
| 1:A:409:G:H5'' | 7:D:25:ARG:CG | 2.21 | 0.66 |
| 1:A:17:U:C2 | 1:A:919:A:C2 | 2.84 | 0.66 |
| 5:B:101:MET:HA | 5:B:108:ILE:HG13 | 1.78 | 0.66 |
| 1:A:1014:A:N1 | 22:S:34:TRP:CZ3 | 2.64 | 0.66 |
| 1:A:985:C:H2' | 1:A:986:A:H8 | 1.61 | 0.66 |
| 7:D:23:GLY:CA | 7:D:113:SER:CB | 2.74 | 0.66 |
| 8:E:144:THR:O | 8:E:147:ASP:N | 2.29 | 0.66 |
| 6:C:7:PRO:O | 6:C:11:ARG:HB2 | 1.95 | 0.66 |
| 15:L:102:ARG:HB3 | 15:L:109:GLY:HA2 | 1.78 | 0.66 |
| 1:A:1358:U:H5'' | 17:N:34:TYR:HA | 1.79 | 0.65 |
| 7:D:23:GLY:C | 7:D:112:VAL:O | 2.35 | 0.65 |
| 3:W:37:YYG:C21 | 10:G:84:ASN:H | 2.02 | 0.65 |
| 6:C:18:TRP:CD1 | 17:N:53:LEU:O | 2.48 | 0.65 |
| 7:D:14:ARG:CD | 7:D:66:ARG:HH12 | 2.07 | 0.65 |
| 6:C:38:ARG:HB3 | 6:C:94:LEU:HD21 | 1.78 | 0.65 |
| 1:A:1220:G:C4' | 22:S:36:ARG:HG2 | 2.26 | 0.65 |
| 1:A:407:G:H8 | 1:A:407:G:O5' | 1.79 | 0.65 |
| 7:D:24:GLU:N | 7:D:112:VAL:CG1 | 2.59 | 0.65 |
| 1:A:1313:U:O4 | 22:S:4:SER:CB | 2.44 | 0.65 |
| 1:A:789:U:O2 | 1:A:792:A:H8 | 1.77 | 0.65 |
| 1:A:1320:C:C4' | 22:S:73:GLU:OE2 | 2.44 | 0.65 |
| 1:A:757:U:OP1 | 1:A:822:C:O2' | 2.07 | 0.65 |
| 1:A:1004:A:H3' | 1:A:1025:U:N3 | 2.10 | 0.65 |
| 1:A:1347:G:N2 | 1:A:1373:G:H2' | 2.10 | 0.65 |
| 8:E:29:GLY:HA2 | 8:E:46:GLY:O | 1.97 | 0.65 |
| 1:A:720:C:C5 | 1:A:721:G:H2' | 2.30 | 0.65 |
| 1:A:1313:U:H5 | 22:S:4:SER:CB | 1.89 | 0.65 |
| 1:A:426:G:C2' | 7:D:42:GLN:HA | 2.25 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1205:U:H4' | 6:C:195:VAL:HG21 | 1.78 | 0.65 |
| 20:Q:22:LEU:HD11 | 20:Q:24:GLU:HG2 | 1.77 | 0.65 |
| 21:R:70:ILE:O | 21:R:74:ARG:HD2 | 1.96 | 0.65 |
| 2:V:43:G:H2' | 2:V:44:A:H8 | 1.60 | 0.65 |
| 1:A:1326:C:C5' | 24:U:19:GLY:HA2 | 2.26 | 0.65 |
| 1:A:1053:G:H8 | 1:A:1053:G:H5'' | 1.61 | 0.65 |
| 2:V:47:U:H1' | 2:V:50:U:OP1 | 1.97 | 0.65 |
| 1:A:1269:A:H5' | 24:U:19:GLY:HA2 | 1.79 | 0.65 |
| 1:A:1061:G:OP1 | 13:J:51:ARG:HD2 | 1.96 | 0.65 |
| 1:A:302:G:N2 | 1:A:556:C:O4' | 2.27 | 0.65 |
| 7:D:96:LEU:HG | 7:D:139:ARG:CZ | 2.26 | 0.65 |
| 6:C:50:ALA:HB1 | 6:C:70:VAL:HG11 | 1.79 | 0.65 |
| 1:A:1255:G:H21 | 1:A:1258:G:H21 | 1.45 | 0.65 |
| 1:A:429:U:OP1 | 7:D:13:ARG:NE | 2.29 | 0.65 |
| 1:A:1015:A:P | 22:S:14:HIS:CE1 | 2.90 | 0.65 |
| 1:A:815:A:OP2 | 1:A:816:A:H8 | 1.80 | 0.65 |
| 1:A:1405:G:C1' | 1:A:1519:A:H4' | 2.27 | 0.65 |
| 1:A:375:U:O2' | 19:P:17:TYR:HE2 | 1.78 | 0.65 |
| 1:A:247:G:OP2 | 20:Q:99:SER:CB | 2.42 | 0.65 |
| 1:A:776:G:N2 | 1:A:802:A:OP2 | 2.29 | 0.65 |
| 1:A:1220:G:H4' | 22:S:36:ARG:CG | 2.27 | 0.65 |
| 1:A:1325:C:OP1 | 24:U:15:ARG:HG2 | 1.97 | 0.65 |
| 21:R:74:ARG:HG2 | 21:R:81:PHE:HB3 | 1.78 | 0.65 |
| 1:A:564:C:H4' | 11:H:91:ARG:NH2 | 2.12 | 0.65 |
| 1:A:1250:A:H4' | 12:I:67:GLY:CA | 2.27 | 0.65 |
| 1:A:451:A:H61 | 1:A:480:U:H2' | 1.62 | 0.65 |
| 2:V:14:A:H2' | 2:V:15:G:C8 | 2.31 | 0.65 |
| 13:J:38:ILE:HG13 | 13:J:38:ILE:O | 1.97 | 0.65 |
| 7:D:12:CYS:HB3 | 7:D:31:CYS:O | 1.96 | 0.64 |
| 1:A:575:G:N2 | 1:A:880:C:C2 | 2.61 | 0.64 |
| 1:A:713:G:H2' | 1:A:714:G:C8 | 2.33 | 0.64 |
| 3:W:14:A:C6 | 3:W:22:G:C2 | 2.85 | 0.64 |
| 14:K:18:ARG:HH21 | 14:K:37:GLY:HA2 | 1.62 | 0.64 |
| 1:A:394:G:C3' | 1:A:395:C:P | 2.86 | 0.64 |
| 1:A:1107:C:H3' | 1:A:1108:G:P | 2.37 | 0.64 |
| 1:A:642:A:N7 | 11:H:115:SER:HA | 2.13 | 0.64 |
| 1:A:948:C:O5' | 1:A:948:C:H6 | 1.80 | 0.64 |
| 6:C:157:ILE:HD12 | 6:C:164:ARG:HG3 | 1.79 | 0.64 |
| 1:A:1014:A:OP2 | 22:S:18:LYS:NZ | 2.30 | 0.64 |
| 1:A:986:A:H1' | 22:S:55:LYS:N | 2.12 | 0.64 |
| 1:A:404:U:C5 | 7:D:2:GLY:HA2 | 2.32 | 0.64 |
| 1:A:1268:A:O2' | 24:U:19:GLY:C | 2.36 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1499:A:OP1 | 1:A:1505:G:OP2 | 2.16 | 0.64 |
| 13:J:11:PHE:CZ | 17:N:55:GLY:HA3 | 2.31 | 0.64 |
| 1:A:31:G:H1' | 1:A:46:G:H5'' | 1.78 | 0.64 |
| 1:A:369:C:H42 | 1:A:392:G:H1 | 1.44 | 0.64 |
| 12:I:103:THR:HG22 | 12:I:105:ASP:H | 1.62 | 0.64 |
| 1:A:1219:U:HO2' | 22:S:34:TRP:HB3 | 1.55 | 0.64 |
| 1:A:1060:C:H2' | 1:A:1061:G:H8 | 1.63 | 0.64 |
| 1:A:600:C:H4' | 11:H:128:GLY:O | 1.97 | 0.64 |
| 1:A:1190:G:H5' | 6:C:176:HIS:CE1 | 2.33 | 0.64 |
| 1:A:542:G:OP1 | 7:D:41:GLY:CA | 2.45 | 0.64 |
| 1:A:463:A:H4' | 19:P:80:PHE:O | 1.98 | 0.64 |
| 1:A:674:G:H2' | 1:A:675:A:C8 | 2.32 | 0.64 |
| 1:A:1319:A:P | 22:S:5:LEU:HD22 | 2.38 | 0.64 |
| 1:A:1328:C:OP1 | 16:M:28:ALA:HB2 | 1.98 | 0.64 |
| 1:A:939:G:H5'' | 10:G:102:ARG:NH2 | 2.13 | 0.64 |
| 1:A:18:C:N3 | 1:A:918:A:C2 | 2.65 | 0.64 |
| 1:A:3(A):G:N1 | 1:A:1038:C:H1' | 2.12 | 0.64 |
| 1:A:1115:C:O4' | 17:N:61:TRP:HA | 1.98 | 0.64 |
| 11:H:18:ARG:HG3 | 11:H:18:ARG:NH1 | 2.13 | 0.64 |
| 15:L:70:ILE:HG12 | 15:L:100:ILE:HD11 | 1.79 | 0.64 |
| 1:A:801:U:H2' | 1:A:802:A:H8 | 1.62 | 0.64 |
| 1:A:65:U:H4' | 1:A:66:G:H5' | 1.78 | 0.64 |
| 3:W:37:YYG:O18 | 10:G:83:ALA:C | 2.32 | 0.64 |
| 6:C:91:LEU:HD11 | 6:C:99:VAL:CG2 | 2.22 | 0.64 |
| 1:A:463:A:P | 19:P:75:ARG:HH22 | 2.19 | 0.64 |
| 1:A:1125:U:H2' | 1:A:1281:U:O2 | 1.97 | 0.64 |
| 1:A:975:A:C5 | 1:A:1357:A:H2 | 2.15 | 0.64 |
| 3:W:25:C:C2 | 3:W:26:G:N1 | 2.62 | 0.64 |
| 13:J:64:GLU:CG | 17:N:59:ALA:HA | 2.28 | 0.64 |
| 1:A:22:G:C2' | 1:A:913:A:C2 | 2.81 | 0.64 |
| 21:R:46:GLU:HB3 | 21:R:85:LEU:HD13 | 1.79 | 0.64 |
| 14:K:99:GLN:HG2 | 14:K:105:VAL:HG11 | 1.78 | 0.64 |
| 1:A:1221:G:H5'' | 1:A:1321:C:O2 | 1.98 | 0.63 |
| 7:D:23:GLY:CA | 7:D:113:SER:N | 2.57 | 0.63 |
| 16:M:15:VAL:O | 16:M:19:LEU:HG | 1.98 | 0.63 |
| 2:V:36:A:N6 | 4:X:117:U:C4 | 2.66 | 0.63 |
| 1:A:940:C:H2' | 1:A:941:G:C8 | 2.33 | 0.63 |
| 1:A:20:U:C4 | 1:A:916:G:C2 | 2.86 | 0.63 |
| 1:A:1373:G:H5'' | 12:I:42:ARG:HH21 | 1.63 | 0.63 |
| 1:A:985:C:H2' | 1:A:986:A:C8 | 2.32 | 0.63 |
| 16:M:91:ARG:NH2 | 16:M:103:THR:HG21 | 2.13 | 0.63 |
| 1:A:1318:A:O2' | 22:S:37:ARG:O | 2.15 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:953:G:H1' | 16:M:125:ARG:HA | 1.78 | 0.63 |
| 1:A:522:C:H2' | 1:A:523:A:H8 | 1.62 | 0.63 |
| 2:V:57:G:H2' | 2:V:58:A:H5'' | 1.80 | 0.63 |
| 1:A:1221:G:H4' | 22:S:36:ARG:HH12 | 1.61 | 0.63 |
| 1:A:986:A:N9 | 22:S:54:GLY:O | 2.31 | 0.63 |
| 3:W:37:YYG:H191 | 10:G:79:ARG:HD3 | 1.79 | 0.63 |
| 1:A:815:A:HO2' | 1:A:1527:C:H1' | 1.61 | 0.63 |
| 3:W:45:G:O3' | 3:W:46:G:H5' | 1.97 | 0.63 |
| 1:A:1025:U:H2' | 1:A:1026:G:C8 | 2.33 | 0.63 |
| 1:A:1156:G:C1' | 1:A:1179:A:H61 | 2.10 | 0.63 |
| 1:A:768:A:OP1 | 1:A:804:U:C5' | 2.45 | 0.63 |
| 1:A:46:G:O3' | 1:A:47:C:P | 2.57 | 0.63 |
| 1:A:1418:A:H8 | 1:A:1419:G:O4' | 1.79 | 0.63 |
| 14:K:61:ALA:HB1 | 14:K:94:ALA:HB2 | 1.81 | 0.63 |
| 1:A:1203:C:OP1 | 17:N:2:ALA:N | 2.32 | 0.63 |
| 6:C:12:LEU:HD11 | 17:N:51:GLY:CA | 2.29 | 0.63 |
| 1:A:1326:C:OP1 | 24:U:12:LYS:NZ | 2.31 | 0.63 |
| 1:A:1237:C:O2' | 1:A:1300:G:N2 | 2.32 | 0.63 |
| 1:A:789:U:O2 | 1:A:792:A:C8 | 2.51 | 0.63 |
| 1:A:36:C:H4' | 15:L:117:ARG:NH2 | 2.14 | 0.63 |
| 7:D:10:ARG:O | 7:D:13:ARG:HB2 | 1.99 | 0.63 |
| 2:V:61:C:H2' | 2:V:62:A:H8 | 1.64 | 0.63 |
| 3:W:1:G:N2 | 3:W:2:C:C4 | 2.61 | 0.63 |
| 1:A:983:A:H5' | 1:A:984:C:P | 2.39 | 0.63 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.33 | 0.63 |
| 1:A:949:A:H4' | 1:A:1364:U:H3 | 1.64 | 0.63 |
| 1:A:703:G:HO3' | 1:A:704:A:P | 2.21 | 0.63 |
| 1:A:1400:C:N3 | 2:V:34:G:C2 | 2.67 | 0.63 |
| 1:A:940:C:H2' | 1:A:941:G:H8 | 1.63 | 0.63 |
| 1:A:1259:C:O2' | 1:A:1284:C:C4' | 2.47 | 0.63 |
| 1:A:944:G:C3' | 1:A:945:G:H5' | 2.29 | 0.63 |
| 8:E:17:ALA:HA | 8:E:26:PHE:HB3 | 1.78 | 0.63 |
| 1:A:529:G:C5 | 15:L:49:ASN:ND2 | 2.67 | 0.63 |
| 1:A:979:C:OP1 | 1:A:1222:G:C6 | 2.51 | 0.63 |
| 1:A:947:G:H4' | 1:A:1332:A:C2 | 2.30 | 0.63 |
| 10:G:149:ARG:HD2 | 14:K:59:TYR:CZ | 2.32 | 0.63 |
| 15:L:54:LYS:HG2 | 15:L:75:HIS:CE1 | 2.34 | 0.63 |
| 5:B:103:THR:O | 5:B:104:ASN:HB2 | 1.99 | 0.63 |
| 1:A:1014:A:C4 | 22:S:34:TRP:CE3 | 2.86 | 0.62 |
| 1:A:1320:C:C6 | 22:S:70:LYS:HD2 | 2.33 | 0.62 |
| 1:A:408:A:OP1 | 7:D:115:ARG:CZ | 2.46 | 0.62 |
| 1:A:764:C:C2' | 1:A:765:G:H8 | 2.03 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:25:C:H4' | 1:A:524:G:C2 | 2.33 | 0.62 |
| 1:A:564:C:O2' | 11:H:91:ARG:NH1 | 2.32 | 0.62 |
| 1:A:315:A:H1' | 1:A:353:A:C2 | 2.34 | 0.62 |
| 13:J:64:GLU:CB | 17:N:59:ALA:HB2 | 2.28 | 0.62 |
| 1:A:1285:A:H4' | 1:A:1286:A:O5' | 1.98 | 0.62 |
| 1:A:1278:U:OP1 | 1:A:1281:U:C5 | 2.51 | 0.62 |
| 1:A:398:C:H2' | 1:A:399:G:C8 | 2.34 | 0.62 |
| 1:A:1224:G:C6 | 1:A:1322:C:H4' | 2.33 | 0.62 |
| 1:A:571:U:O2 | 1:A:917:G:H4' | 1.99 | 0.62 |
| 1:A:946:A:N3 | 1:A:1333:A:H2 | 1.97 | 0.62 |
| 10:G:149:ARG:HD2 | 14:K:59:TYR:OH | 1.98 | 0.62 |
| 1:A:1498:U:H1' | 1:A:1499:A:N7 | 2.14 | 0.62 |
| 17:N:24:CYS:HB2 | 17:N:39:LEU:HA | 1.81 | 0.62 |
| 1:A:813:U:H2' | 1:A:814:A:C8 | 2.34 | 0.62 |
| 1:A:1073:U:C2 | 1:A:1074:G:C8 | 2.87 | 0.62 |
| 1:A:568:G:N2 | 1:A:574:A:C2 | 2.65 | 0.62 |
| 1:A:1124:G:OP1 | 13:J:35:SER:OG | 2.15 | 0.62 |
| 3:W:44:A:O2' | 3:W:45:G:H5' | 2.00 | 0.62 |
| 1:A:1366:C:OP2 | 12:I:117:HIS:NE2 | 2.32 | 0.62 |
| 23:T:23:ARG:HA | 23:T:26:ASN:HD21 | 1.64 | 0.62 |
| 1:A:1339:A:H2 | 2:V:31:A:C1' | 2.13 | 0.62 |
| 1:A:1528:U:H2' | 1:A:1530:G:H5' | 1.81 | 0.62 |
| 20:Q:40:LYS:HD3 | 20:Q:42:TYR:CE1 | 2.34 | 0.62 |
| 3:W:25:C:O2 | 3:W:26:G:C4 | 2.50 | 0.62 |
| 1:A:184:G:H4' | 1:A:224:C:H4' | 1.82 | 0.62 |
| 1:A:1339:A:H2 | 2:V:31:A:H1' | 1.63 | 0.62 |
| 1:A:965:A:O2' | 1:A:966:G:C5' | 2.47 | 0.62 |
| 1:A:323:U:H3 | 1:A:327:A:H62 | 1.45 | 0.62 |
| 10:G:71:PRO:HG2 | 10:G:91:VAL:HG11 | 1.82 | 0.62 |
| 1:A:1222:G:OP1 | 1:A:1321:C:O2' | 2.15 | 0.62 |
| 1:A:1357:A:O2' | 17:N:34:TYR:HE2 | 1.82 | 0.62 |
| 1:A:302:G:C2 | 1:A:556:C:C4' | 2.76 | 0.62 |
| 1:A:296:U:H4' | 1:A:556:C:O2 | 1.99 | 0.62 |
| 1:A:819:A:C6 | 1:A:1529:G:C5 | 2.87 | 0.62 |
| 1:A:1406:U:O2 | 1:A:1517:G:N2 | 2.29 | 0.62 |
| 1:A:1250:A:H4' | 12:I:67:GLY:O | 1.98 | 0.62 |
| 4:X:119:U:H2' | 4:X:120:G:H8 | 1.61 | 0.62 |
| 10:G:111:ARG:HD2 | 10:G:123:GLU:HB2 | 1.81 | 0.62 |
| 3:W:37:YYG:H101 | 3:W:37:YYG:C21 | 2.30 | 0.62 |
| 1:A:1197:G:H2' | 1:A:1198:G:H5' | 1.80 | 0.62 |
| 1:A:953:G:C1' | 16:M:125:ARG:HA | 2.29 | 0.62 |
| 1:A:120:A:C8 | 1:A:120:A:H3' | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:51:A:N1 | 1:A:314:C:O2' | 2.32 | 0.62 |
| 20:Q:67:LYS:O | 20:Q:68:ARG:CB | 2.46 | 0.62 |
| 1:A:521:G:O6 | 15:L:49:ASN:ND2 | 2.33 | 0.62 |
| 1:A:66:G:N2 | 1:A:172:A:C2 | 2.67 | 0.62 |
| 18:O:36:ILE:HD11 | 18:O:60:VAL:HG22 | 1.81 | 0.62 |
| 1:A:410:G:OP2 | 7:D:25:ARG:NH2 | 2.32 | 0.62 |
| 1:A:1395:C:O2 | 1:A:1398:A:O2' | 2.17 | 0.62 |
| 3:W:72:C:H2' | 3:W:73:A:H8 | 1.64 | 0.62 |
| 1:A:409:G:OP2 | 7:D:22:LYS:NZ | 2.33 | 0.62 |
| 1:A:946:A:N3 | 1:A:1333:A:C2 | 2.67 | 0.62 |
| 1:A:523:A:H2 | 15:L:91:LYS:HB3 | 1.65 | 0.62 |
| 16:M:23:TYR:CD2 | 16:M:70:LEU:HD13 | 2.35 | 0.61 |
| 1:A:1198:G:HO2' | 13:J:54:PHE:HE2 | 0.63 | 0.61 |
| 8:E:79:GLU:HG3 | 8:E:93:PRO:HD2 | 1.82 | 0.61 |
| 14:K:99:GLN:HA | 14:K:105:VAL:HG21 | 1.82 | 0.61 |
| 14:K:65:ALA:HB1 | 14:K:98:LEU:HG | 1.81 | 0.61 |
| 1:A:1037:C:H2' | 1:A:1038:C:O4' | 1.99 | 0.61 |
| 3:W:40:C:H2' | 3:W:41:U:H5' | 1.82 | 0.61 |
| 1:A:574:A:N3 | 1:A:883:C:H1' | 2.15 | 0.61 |
| 3:W:72:C:H2' | 3:W:73:A:O4' | 1.99 | 0.61 |
| 1:A:1406:U:C1' | 1:A:1518:A:O2' | 2.48 | 0.61 |
| 1:A:1148:U:O4' | 12:I:16:ARG:HD2 | 2.00 | 0.61 |
| 12:I:32:ASP:HB3 | 12:I:35:GLU:HB2 | 1.83 | 0.61 |
| 1:A:1400:C:N3 | 2:V:34:G:N2 | 2.49 | 0.61 |
| 1:A:3(A):G:H1 | 1:A:1038:C:H1' | 1.65 | 0.61 |
| 1:A:595:G:H2' | 1:A:641:U:O4 | 2.01 | 0.61 |
| 1:A:1269:A:C1' | 1:A:1326:C:O4' | 2.48 | 0.61 |
| 1:A:1313:U:C4 | 22:S:4:SER:HB3 | 2.32 | 0.61 |
| 1:A:22:G:C2 | 1:A:914:A:N7 | 2.69 | 0.61 |
| 1:A:877:C:O2' | 11:H:89:PRO:HG2 | 1.99 | 0.61 |
| 15:L:54:LYS:HG3 | 15:L:75:HIS:HE1 | 1.65 | 0.61 |
| 16:M:24:GLY:O | 16:M:29:ARG:HD2 | 2.01 | 0.61 |
| 15:L:54:LYS:HG2 | 15:L:75:HIS:HE1 | 1.65 | 0.61 |
| 1:A:408:A:OP2 | 7:D:115:ARG:NH1 | 2.34 | 0.61 |
| 5:B:102:LEU:HD23 | 5:B:177:ALA:HB2 | 1.83 | 0.61 |
| 18:O:3:ILE:HG21 | 18:O:34:LEU:HD21 | 1.83 | 0.61 |
| 1:A:1226:C:OP2 | 16:M:103:THR:OG1 | 2.09 | 0.61 |
| 7:D:15:GLU:CD | 7:D:63:LYS:CB | 2.56 | 0.61 |
| 1:A:983:A:H3' | 1:A:984:C:P | 2.40 | 0.61 |
| 4:X:116:U:H2' | 4:X:117:U:C6 | 2.35 | 0.61 |
| 1:A:1004:A:N9 | 1:A:1025:U:O4 | 2.34 | 0.61 |
| 9:F:69:GLU:O | 9:F:72:VAL:HG23 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 23:T:87:LYS:O | 23:T:91:LEU:HG | 2.01 | 0.61 |
| 16:M:24:GLY:CA | 16:M:70:LEU:CD1 | 2.79 | 0.61 |
| 8:E:11:ILE:HD11 | 8:E:108:ALA:HB2 | 1.83 | 0.61 |
| 7:D:18:LYS:HA | 7:D:33:MET:CE | 2.31 | 0.61 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.47 | 0.61 |
| 1:A:20:U:H1' | 1:A:572:A:C4 | 2.36 | 0.61 |
| 1:A:947:G:C4' | 1:A:1332:A:H2 | 2.13 | 0.61 |
| 15:L:37:CYS:O | 15:L:79:GLU:HA | 2.01 | 0.61 |
| 7:D:8:VAL:HB | 7:D:115:ARG:NH1 | 2.16 | 0.60 |
| 1:A:15:G:O6 | 1:A:1396:A:C6 | 2.54 | 0.60 |
| 1:A:1405:G:H1' | 1:A:1519:A:O4' | 2.01 | 0.60 |
| 9:F:23:LYS:HA | 9:F:26:ILE:HD12 | 1.83 | 0.60 |
| 1:A:186:C:H1' | 23:T:81:LYS:HE2 | 1.81 | 0.60 |
| 1:A:1320:C:C4' | 22:S:73:GLU:CD | 2.69 | 0.60 |
| 7:D:24:GLU:O | 7:D:27:TYR:HB2 | 2.02 | 0.60 |
| 1:A:1327:C:H5'' | 24:U:20:LYS:HE3 | 1.83 | 0.60 |
| 1:A:405:U:O4 | 7:D:2:GLY:N | 2.33 | 0.60 |
| 3:W:37:YYG:C19 | 10:G:83:ALA:O | 2.50 | 0.60 |
| 1:A:1403:C:H1' | 1:A:1500:A:N1 | 2.17 | 0.60 |
| 1:A:47:C:H4' | 1:A:48:C:H5' | 1.83 | 0.60 |
| 1:A:541:G:C5' | 7:D:42:GLN:HE21 | 2.14 | 0.60 |
| 6:C:48:TYR:OH | 6:C:122:GLU:CD | 2.40 | 0.60 |
| 1:A:944:G:O6 | 1:A:1337:G:H2' | 2.00 | 0.60 |
| 1:A:627:G:H2' | 1:A:628:G:H8 | 1.64 | 0.60 |
| 1:A:1193:G:O2' | 8:E:25:ARG:NH2 | 2.34 | 0.60 |
| 1:A:1268:A:O2' | 24:U:20:LYS:CB | 2.48 | 0.60 |
| 13:J:49:VAL:HG11 | 17:N:45:ARG:HB2 | 1.84 | 0.60 |
| 1:A:92:C:H2' | 1:A:93:G:H8 | 1.66 | 0.60 |
| 1:A:1014:A:N3 | 22:S:34:TRP:CD2 | 2.67 | 0.60 |
| 16:M:92:HIS:CE1 | 16:M:110:ARG:CZ | 2.84 | 0.60 |
| 1:A:950:U:O4' | 1:A:971:G:C2 | 2.55 | 0.60 |
| 1:A:1277:C:H4' | 1:A:1282:C:O4' | 2.02 | 0.60 |
| 1:A:541:G:O4' | 7:D:42:GLN:NE2 | 2.34 | 0.60 |
| 1:A:1342:C:H2' | 1:A:1343:G:H8 | 1.66 | 0.60 |
| 10:G:66:VAL:HG12 | 10:G:70:LYS:HE2 | 1.84 | 0.60 |
| 1:A:361(A):C:O3' | 1:A:1362:C:C5' | 2.50 | 0.60 |
| 14:K:58:PRO:HA | 14:K:90:GLY:HA3 | 1.82 | 0.60 |
| 1:A:801:U:H2' | 1:A:802:A:C8 | 2.37 | 0.60 |
| 1:A:64:G:H4' | 1:A:65:U:H5'' | 1.82 | 0.60 |
| 1:A:1353:G:OP1 | 24:U:10:ARG:NH2 | 2.34 | 0.60 |
| 14:K:40:ILE:HG23 | 14:K:75:TYR:HD2 | 1.66 | 0.60 |
| 1:A:1490:C:H5'' | 1:A:1490:C:H6 | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:D:23:GLY:O | 7:D:112:VAL:CG1 | 2.45 | 0.60 |
| 2:V:20:G:H2' | 2:V:20:G:N3 | 2.14 | 0.60 |
| 8:E:39:GLY:HA2 | 8:E:69:VAL:HB | 1.84 | 0.60 |
| 1:A:920:U:O4' | 1:A:1080:A:C6 | 2.54 | 0.60 |
| 7:D:3:ARG:HH22 | 7:D:74:GLN:HE22 | 1.45 | 0.60 |
| 16:M:19:LEU:HD13 | 16:M:25:ILE:HG21 | 1.82 | 0.60 |
| 13:J:61:GLU:OE1 | 17:N:49:HIS:HE1 | 1.84 | 0.60 |
| 1:A:15:G:C6 | 1:A:1396:A:C6 | 2.90 | 0.60 |
| 1:A:1276:G:O2' | 1:A:1282:C:C4' | 2.49 | 0.60 |
| 1:A:586:C:O2' | 1:A:878:G:H4' | 2.01 | 0.60 |
| 1:A:1366:C:P | 12:I:117:HIS:HE2 | 2.25 | 0.60 |
| 1:A:112:G:H5' | 1:A:389:A:H4' | 1.82 | 0.60 |
| 16:M:87:TYR:HB2 | 22:S:73:GLU:O | 2.00 | 0.60 |
| 1:A:375:U:H6 | 1:A:375:U:O5' | 1.85 | 0.60 |
| 20:Q:22:LEU:HD11 | 20:Q:24:GLU:CG | 2.31 | 0.60 |
| 1:A:1374:A:O2' | 10:G:31:MET:SD | 2.52 | 0.60 |
| 1:A:944:G:O6 | 1:A:1337:G:H8 | 1.84 | 0.60 |
| 1:A:324:G:N2 | 1:A:327:A:C8 | 2.70 | 0.60 |
| 21:R:36:ASN:HB3 | 21:R:40:LEU:HG | 1.83 | 0.60 |
| 5:B:91:PRO:HG3 | 5:B:155:LEU:H | 1.66 | 0.60 |
| 1:A:689:C:H6 | 1:A:689:C:O5' | 1.84 | 0.60 |
| 1:A:1358:U:OP1 | 17:N:34:TYR:HA | 2.02 | 0.59 |
| 1:A:1156:G:H1' | 1:A:1179:A:N6 | 2.17 | 0.59 |
| 7:D:55:ALA:O | 7:D:59:ARG:HG2 | 2.02 | 0.59 |
| 1:A:454:C:H3' | 1:A:455:C:H6 | 1.67 | 0.59 |
| 1:A:755:G:H2' | 1:A:756:C:C6 | 2.36 | 0.59 |
| 1:A:290:C:H6 | 1:A:290:C:O5' | 1.84 | 0.59 |
| 12:I:78:LYS:HD3 | 12:I:101:PHE:HE2 | 1.66 | 0.59 |
| 1:A:1320:C:C2 | 22:S:73:GLU:N | 2.70 | 0.59 |
| 1:A:1325:C:H4' | 24:U:17:THR:CB | 2.30 | 0.59 |
| 1:A:1060:C:H4' | 13:J:51:ARG:HB3 | 1.84 | 0.59 |
| 1:A:1312:G:O6 | 22:S:2:PRO:O | 2.20 | 0.59 |
| 6:C:23:TYR:HD2 | 6:C:24:ALA:N | 2.01 | 0.59 |
| 1:A:1229:A:H2 | 16:M:125:ARG:O | 1.85 | 0.59 |
| 3:W:72:C:C2' | 3:W:73:A:O5' | 2.49 | 0.59 |
| 1:A:19:C:C2 | 1:A:917:G:C2 | 2.91 | 0.59 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 2.01 | 0.59 |
| 3:W:65:G:C2' | 3:W:66:A:H5' | 2.32 | 0.59 |
| 1:A:380:G:N2 | 1:A:382:A:H3' | 2.18 | 0.59 |
| 1:A:355:C:H1' | 1:A:388:G:H2' | 1.84 | 0.59 |
| 7:D:12:CYS:HB2 | 7:D:31:CYS:O | 2.03 | 0.59 |
| 1:A:1269:A:C5' | 24:U:19:GLY:HA2 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1400:C:C2 | 2:V:34:G:C2 | 2.90 | 0.59 |
| 10:G:102:ARG:HG2 | 10:G:106:GLN:HE22 | 1.67 | 0.59 |
| 1:A:943:U:OP1 | 1:A:945:G:O6 | 2.21 | 0.59 |
| 1:A:104:G:P | 23:T:18:GLN:HE21 | 2.26 | 0.59 |
| 1:A:1441:G:H1' | 1:A:1461:G:H22 | 1.67 | 0.59 |
| 8:E:28:PHE:CD1 | 8:E:28:PHE:N | 2.69 | 0.59 |
| 7:D:70:ILE:HD11 | 7:D:100:ARG:CZ | 2.32 | 0.59 |
| 13:J:16:LEU:HB3 | 13:J:70:ARG:HE | 1.66 | 0.59 |
| 1:A:1521:G:H2' | 1:A:1522:U:C6 | 2.38 | 0.59 |
| 1:A:738:C:H4' | 9:F:70:ASP:HA | 1.84 | 0.59 |
| 2:V:43:G:H2' | 2:V:44:A:C8 | 2.37 | 0.59 |
| 1:A:1192:C:C6 | 1:A:1192:C:H3' | 2.37 | 0.59 |
| 1:A:1358:U:H5'' | 17:N:33:VAL:O | 2.02 | 0.59 |
| 1:A:1268:A:C1' | 24:U:20:LYS:HB2 | 2.32 | 0.59 |
| 1:A:1060:C:H2' | 1:A:1061:G:C8 | 2.37 | 0.59 |
| 1:A:375:U:O3' | 19:P:6:LEU:CD2 | 2.48 | 0.59 |
| 1:A:1126:U:OP2 | 1:A:1281:U:C2 | 2.55 | 0.59 |
| 1:A:642:A:C4 | 11:H:114:THR:O | 2.56 | 0.59 |
| 5:B:17:PHE:HD1 | 5:B:18:GLY:N | 2.00 | 0.59 |
| 22:S:55:LYS:HE2 | 22:S:56:GLN:HE21 | 1.66 | 0.59 |
| 3:W:41:U:H2' | 3:W:42:G:O4' | 2.03 | 0.59 |
| 20:Q:5:VAL:HA | 20:Q:59:ILE:O | 2.03 | 0.59 |
| 23:T:72:LEU:HB3 | 23:T:77:ALA:HB2 | 1.83 | 0.59 |
| 13:J:64:GLU:HB3 | 17:N:59:ALA:CB | 2.33 | 0.59 |
| 15:L:54:LYS:HB3 | 15:L:70:ILE:HB | 1.85 | 0.59 |
| 1:A:522:C:H2' | 1:A:523:A:C8 | 2.38 | 0.59 |
| 1:A:989:C:C4' | 1:A:1016:A:H2 | 2.16 | 0.59 |
| 1:A:1319:A:C5' | 22:S:5:LEU:HD22 | 2.33 | 0.59 |
| 12:I:114:TYR:CD1 | 13:J:60:ARG:CB | 2.85 | 0.59 |
| 1:A:758:G:O5' | 1:A:758:G:H8 | 1.85 | 0.59 |
| 1:A:1095:U:O5' | 1:A:1095:U:H6 | 1.86 | 0.59 |
| 5:B:69:LEU:HB2 | 5:B:159:PRO:HB2 | 1.84 | 0.59 |
| 7:D:201:GLN:O | 7:D:205:GLU:HG2 | 2.03 | 0.59 |
| 1:A:932:C:OP1 | 10:G:4:ARG:HG2 | 2.02 | 0.59 |
| 1:A:121:C:H4' | 1:A:122:G:N7 | 2.18 | 0.59 |
| 1:A:377:G:P | 19:P:5:ARG:HH11 | 2.25 | 0.59 |
| 14:K:110:ASP:CB | 21:R:85:LEU:HB3 | 2.31 | 0.59 |
| 1:A:761:G:H2' | 1:A:762:C:C6 | 2.38 | 0.59 |
| 7:D:30:LYS:C | 7:D:32:ALA:H | 2.07 | 0.59 |
| 1:A:1221:G:C4' | 22:S:36:ARG:NH1 | 2.58 | 0.58 |
| 7:D:106:TYR:HA | 7:D:111:ALA:HB3 | 1.85 | 0.58 |
| 1:A:298:A:H3' | 1:A:299:G:H8 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:900:A:H2' | 1:A:901:A:H8 | 1.68 | 0.58 |
| 1:A:1314:C:N4 | 22:S:4:SER:HB2 | 2.18 | 0.58 |
| 2:V:34:G:C3' | 2:V:35:A:C5' | 2.80 | 0.58 |
| 1:A:1084:G:H2' | 1:A:1085:U:C6 | 2.37 | 0.58 |
| 1:A:1406:U:C2 | 1:A:1517:G:N2 | 2.71 | 0.58 |
| 1:A:17:U:C2 | 1:A:919:A:H2 | 2.20 | 0.58 |
| 1:A:794:A:H4' | 1:A:1521:G:O2' | 2.03 | 0.58 |
| 1:A:429:U:P | 7:D:13:ARG:NE | 2.67 | 0.58 |
| 20:Q:57:VAL:HG12 | 20:Q:76:LEU:HA | 1.84 | 0.58 |
| 6:C:180:ALA:HB1 | 6:C:203:PHE:HE1 | 1.66 | 0.58 |
| 1:A:987:G:H21 | 1:A:1014:A:H2 | 1.48 | 0.58 |
| 1:A:361(A):C:C2' | 1:A:1362:C:H5'' | 2.32 | 0.58 |
| 1:A:1226:C:C4 | 16:M:104:ARG:HG3 | 2.37 | 0.58 |
| 1:A:1328:C:C5' | 16:M:28:ALA:HB3 | 2.31 | 0.58 |
| 1:A:21:G:N2 | 1:A:915:A:N6 | 2.50 | 0.58 |
| 5:B:28:PHE:CZ | 5:B:42:ILE:HD11 | 2.39 | 0.58 |
| 11:H:29:SER:HB2 | 11:H:32:LYS:HZ1 | 1.69 | 0.58 |
| 9:F:62:TRP:NE1 | 21:R:35:ARG:NH2 | 2.49 | 0.58 |
| 7:D:173:TRP:CZ3 | 7:D:193:ASP:O | 2.56 | 0.58 |
| 1:A:1342:C:H2' | 1:A:1343:G:C8 | 2.37 | 0.58 |
| 7:D:29:PRO:HB3 | 7:D:34:GLU:HG2 | 1.85 | 0.58 |
| 1:A:977:A:H2' | 1:A:977:A:N3 | 2.18 | 0.58 |
| 1:A:1268:A:O4' | 24:U:20:LYS:HB2 | 2.04 | 0.58 |
| 1:A:1340:A:H4' | 2:V:31:A:O2' | 2.03 | 0.58 |
| 1:A:939:G:OP1 | 10:G:102:ARG:CZ | 2.51 | 0.58 |
| 1:A:991:U:O2' | 1:A:993:G:H1' | 2.02 | 0.58 |
| 1:A:1291:G:H5' | 12:I:40:LEU:HD23 | 1.85 | 0.58 |
| 1:A:1418:A:C8 | 1:A:1419:G:H1' | 2.38 | 0.58 |
| 7:D:102:ASP:HB3 | 7:D:136:PRO:HB3 | 1.84 | 0.58 |
| 7:D:157:LEU:HD23 | 7:D:160:GLN:HG3 | 1.84 | 0.58 |
| 15:L:82:VAL:O | 15:L:83:VAL:HB | 2.01 | 0.58 |
| 1:A:1221:G:H5' | 22:S:36:ARG:CZ | 2.18 | 0.58 |
| 17:N:40:CYS:N | 17:N:43:CYS:SG | 2.77 | 0.58 |
| 1:A:565:U:H3' | 1:A:566:G:C8 | 2.38 | 0.58 |
| 1:A:54:C:H41 | 1:A:352:C:H2' | 1.68 | 0.58 |
| 14:K:12:ARG:NH1 | 14:K:40:ILE:HA | 2.18 | 0.58 |
| 1:A:1468:A:H2' | 1:A:1469:G:O4' | 2.03 | 0.58 |
| 1:A:986:A:C4 | 22:S:54:GLY:O | 2.55 | 0.58 |
| 7:D:8:VAL:CB | 7:D:115:ARG:CZ | 2.79 | 0.58 |
| 1:A:1260:C:H4' | 1:A:1284:C:H5' | 1.86 | 0.58 |
| 1:A:1236:A:H4' | 1:A:1304:G:C5' | 2.33 | 0.58 |
| 1:A:932:C:H4' | 10:G:4:ARG:NH2 | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 14:K:79:SER:HA | 14:K:104:GLN:HB3 | 1.85 | 0.58 |
| 1:A:1220:G:H21 | 22:S:54:GLY:HA3 | 1.58 | 0.58 |
| 1:A:1222:G:H5'' | 22:S:78:ARG:NH2 | 2.18 | 0.58 |
| 1:A:403:C:H42 | 1:A:547:A:C5' | 2.16 | 0.58 |
| 1:A:546:G:C3' | 1:A:547:A:P | 2.90 | 0.58 |
| 1:A:1347:G:C8 | 12:I:107:ARG:HB3 | 2.28 | 0.58 |
| 1:A:886:G:H22 | 1:A:912:C:H1' | 1.68 | 0.58 |
| 1:A:776:G:H22 | 1:A:802:A:P | 2.27 | 0.58 |
| 15:L:82:VAL:O | 15:L:106:ASP:HB2 | 2.03 | 0.58 |
| 19:P:22:THR:HA | 19:P:33:ILE:HG13 | 1.84 | 0.58 |
| 1:A:1219:U:O2 | 22:S:34:TRP:HD1 | 1.77 | 0.58 |
| 1:A:406:G:C5' | 7:D:5:ILE:HG21 | 2.33 | 0.58 |
| 1:A:1060:C:C4' | 13:J:51:ARG:HB3 | 2.33 | 0.58 |
| 15:L:23:LYS:O | 15:L:97:ARG:HD3 | 2.04 | 0.58 |
| 1:A:463:A:P | 19:P:75:ARG:NH2 | 2.75 | 0.58 |
| 1:A:501:C:H1' | 1:A:549:C:H1' | 1.85 | 0.58 |
| 1:A:761:G:H1' | 20:Q:103:GLY:O | 2.04 | 0.58 |
| 1:A:1134:G:H1 | 1:A:1140:C:H42 | 1.52 | 0.58 |
| 7:D:18:LYS:HA | 7:D:33:MET:HE1 | 1.86 | 0.58 |
| 3:W:41:U:H5' | 3:W:41:U:C6 | 2.27 | 0.58 |
| 18:O:45:VAL:O | 18:O:46:HIS:CB | 2.52 | 0.58 |
| 1:A:738:C:H5'' | 9:F:70:ASP:HA | 1.85 | 0.58 |
| 7:D:10:ARG:HG2 | 7:D:40:PRO:HG3 | 1.84 | 0.58 |
| 1:A:1319:A:OP2 | 22:S:5:LEU:HB3 | 2.03 | 0.58 |
| 1:A:988:G:N2 | 1:A:1016:A:H1' | 2.19 | 0.58 |
| 1:A:1060:C:C4' | 13:J:52:GLY:HA3 | 2.34 | 0.58 |
| 1:A:29:G:O2' | 1:A:295:C:C4' | 2.36 | 0.58 |
| 1:A:560:U:H5' | 1:A:566:G:N2 | 2.18 | 0.58 |
| 2:V:73:A:H3' | 2:V:74:C:OP1 | 2.03 | 0.58 |
| 5:B:93:VAL:HG21 | 5:B:97:TRP:HD1 | 1.69 | 0.58 |
| 1:A:1225:A:OP2 | 16:M:104:ARG:HB2 | 2.04 | 0.57 |
| 1:A:409:G:C5' | 7:D:25:ARG:HB3 | 2.24 | 0.57 |
| 1:A:1396:A:N3 | 1:A:1398:A:C2 | 2.72 | 0.57 |
| 1:A:120:A:H3' | 1:A:120:A:H8 | 1.68 | 0.57 |
| 1:A:575:G:OP1 | 1:A:575:G:H4' | 2.03 | 0.57 |
| 1:A:939:G:P | 10:G:102:ARG:NH1 | 2.60 | 0.57 |
| 13:J:64:GLU:OE1 | 17:N:57:ARG:HB3 | 2.04 | 0.57 |
| 1:A:691:G:H1 | 14:K:52:GLY:HA2 | 1.69 | 0.57 |
| 1:A:18:C:N4 | 1:A:917:G:H1 | 2.02 | 0.57 |
| 1:A:1307:U:H2' | 1:A:1308:U:C6 | 2.38 | 0.57 |
| 1:A:815:A:OP2 | 1:A:816:A:C8 | 2.57 | 0.57 |
| 1:A:1220:G:O3' | 22:S:36:ARG:HD3 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1319:A:C3' | 22:S:70:LYS:HZ1 | 2.17 | 0.57 |
| 1:A:1308:U:H5'' | 16:M:110:ARG:NH2 | 2.09 | 0.57 |
| 3:W:37:YYG:C24 | 10:G:85:TYR:CE2 | 2.87 | 0.57 |
| 1:A:31:G:C1' | 1:A:46:G:H5' | 2.34 | 0.57 |
| 3:W:25:C:N3 | 3:W:26:G:C6 | 2.69 | 0.57 |
| 1:A:1406:U:H1' | 1:A:1518:A:O2' | 2.05 | 0.57 |
| 1:A:20:U:C4' | 1:A:572:A:C6 | 2.88 | 0.57 |
| 1:A:22:G:H4' | 1:A:885:G:C8 | 2.39 | 0.57 |
| 1:A:1101:A:O2' | 1:A:1102:A:OP2 | 2.20 | 0.57 |
| 1:A:1481:U:H2' | 1:A:1482:G:C8 | 2.40 | 0.57 |
| 1:A:1222:G:H5'' | 22:S:78:ARG:CZ | 2.34 | 0.57 |
| 1:A:965:A:H1' | 1:A:969:A:C8 | 2.39 | 0.57 |
| 1:A:1237:C:O2 | 1:A:1335:C:H5' | 2.04 | 0.57 |
| 1:A:570:G:H2' | 1:A:571:U:C5 | 2.40 | 0.57 |
| 10:G:26:PHE:HB2 | 10:G:101:LEU:HD22 | 1.86 | 0.57 |
| 11:H:96:GLY:HA2 | 11:H:130:GLY:HA3 | 1.87 | 0.57 |
| 1:A:1269:A:C4' | 1:A:1326:C:H4' | 2.34 | 0.57 |
| 16:M:8:GLU:HG3 | 16:M:22:ILE:HG12 | 1.85 | 0.57 |
| 1:A:314:C:O2' | 1:A:353:A:N1 | 2.36 | 0.57 |
| 1:A:946:A:H2' | 1:A:947:G:H8 | 1.69 | 0.57 |
| 1:A:1376:U:H5'' | 10:G:94:ARG:HH22 | 1.67 | 0.57 |
| 19:P:59:TRP:O | 19:P:64:ALA:HB3 | 2.05 | 0.57 |
| 1:A:1071:C:H5'' | 8:E:49:PRO:HG3 | 1.86 | 0.57 |
| 1:A:1402:C:H2' | 1:A:1403:C:O4' | 2.05 | 0.57 |
| 1:A:46:G:P | 1:A:306:G:H21 | 2.28 | 0.57 |
| 1:A:828:A:N6 | 1:A:858:G:O2' | 2.37 | 0.57 |
| 1:A:574:A:HO2' | 1:A:882:C:C2' | 2.14 | 0.57 |
| 1:A:1098:C:H4' | 1:A:1167:A:C2 | 2.39 | 0.57 |
| 7:D:101:LEU:HD13 | 7:D:138:TYR:CD2 | 2.40 | 0.57 |
| 7:D:170:VAL:HG12 | 7:D:171:GLY:H | 1.70 | 0.57 |
| 1:A:563:A:C5 | 1:A:567:G:H1' | 2.39 | 0.57 |
| 3:W:44:A:H2' | 3:W:45:G:O4' | 2.04 | 0.57 |
| 19:P:7:ALA:O | 19:P:17:TYR:HA | 2.05 | 0.57 |
| 1:A:376:G:P | 19:P:6:LEU:HD22 | 2.45 | 0.57 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.53 | 0.57 |
| 1:A:988:G:N3 | 1:A:1015:A:C2 | 2.73 | 0.57 |
| 1:A:966:G:H2' | 1:A:967:C:C6 | 2.40 | 0.57 |
| 1:A:497:A:O2' | 1:A:498:U:P | 2.63 | 0.57 |
| 2:V:7:U:O4 | 2:V:49:C:N4 | 2.38 | 0.57 |
| 2:V:8:U:H1' | 2:V:48:C:H1' | 1.87 | 0.57 |
| 14:K:110:ASP:HB3 | 21:R:85:LEU:CB | 2.34 | 0.57 |
| 1:A:59:A:H5'' | 1:A:60:A:H5' | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1101:A:HO2' | 1:A:1102:A:P | 2.28 | 0.57 |
| 2:V:19:G:H5' | 2:V:20:G:P | 2.44 | 0.57 |
| 1:A:609:A:H2' | 1:A:610:G:O4' | 2.05 | 0.57 |
| 5:B:46:LYS:HE2 | 5:B:46:LYS:HA | 1.86 | 0.57 |
| 1:A:958:A:C4 | 22:S:55:LYS:HD2 | 2.40 | 0.57 |
| 1:A:983:A:H5' | 1:A:984:C:OP2 | 2.05 | 0.57 |
| 1:A:1107:C:OP1 | 6:C:172:ARG:HG2 | 2.03 | 0.57 |
| 1:A:1287:A:N6 | 1:A:1371:G:H4' | 2.20 | 0.57 |
| 1:A:677:U:H2' | 1:A:678:U:C6 | 2.40 | 0.57 |
| 3:W:64:A:H2' | 3:W:65:G:O4' | 2.04 | 0.57 |
| 1:A:986:A:H2' | 22:S:52:TYR:OH | 2.05 | 0.56 |
| 18:O:63:ARG:HH12 | 18:O:87:ILE:HG12 | 1.70 | 0.56 |
| 1:A:1192:C:H6 | 1:A:1192:C:H3' | 1.70 | 0.56 |
| 1:A:1317:C:C2' | 22:S:10:PHE:CE2 | 2.88 | 0.56 |
| 1:A:17:U:O2 | 1:A:919:A:C2 | 2.58 | 0.56 |
| 5:B:164:VAL:HG21 | 5:B:170:GLU:CB | 2.35 | 0.56 |
| 10:G:69:VAL:HA | 10:G:138:LYS:HD2 | 1.86 | 0.56 |
| 1:A:824:C:H1' | 11:H:1:MET:N | 2.19 | 0.56 |
| 1:A:1320:C:C4 | 22:S:72:GLY:HA3 | 2.37 | 0.56 |
| 1:A:968:A:H5'' | 1:A:969:A:OP2 | 2.05 | 0.56 |
| 1:A:403:C:N4 | 1:A:547:A:C5' | 2.66 | 0.56 |
| 1:A:575:G:N2 | 1:A:880:C:N3 | 2.44 | 0.56 |
| 1:A:1107:C:OP1 | 6:C:172:ARG:HA | 2.06 | 0.56 |
| 1:A:1004:A:H2' | 1:A:1025:U:N3 | 2.20 | 0.56 |
| 1:A:1286:A:N3 | 24:U:22:ARG:NH2 | 2.54 | 0.56 |
| 1:A:826:C:O5' | 1:A:826:C:H6 | 1.87 | 0.56 |
| 1:A:908:A:H2' | 1:A:909:A:H8 | 1.69 | 0.56 |
| 1:A:23:C:H4' | 1:A:913:A:N6 | 2.19 | 0.56 |
| 9:F:60:PHE:HZ | 21:R:78:LEU:HD21 | 1.64 | 0.56 |
| 1:A:903:G:OP1 | 1:A:1512:U:OP1 | 2.23 | 0.56 |
| 20:Q:87:LYS:O | 20:Q:91:ARG:CB | 2.52 | 0.56 |
| 5:B:17:PHE:HD1 | 5:B:18:GLY:H | 1.50 | 0.56 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.39 | 0.56 |
| 1:A:976:G:C5 | 1:A:361(A):C:C5 | 2.93 | 0.56 |
| 1:A:986:A:C2' | 22:S:52:TYR:OH | 2.53 | 0.56 |
| 9:F:62:TRP:HB2 | 21:R:35:ARG:NH1 | 2.20 | 0.56 |
| 1:A:573:A:H2' | 1:A:574:A:C8 | 2.40 | 0.56 |
| 8:E:105:VAL:HB | 8:E:106:PRO:HD3 | 1.86 | 0.56 |
| 1:A:173:U:OP1 | 1:A:198:G:H4' | 2.05 | 0.56 |
| 1:A:1342:C:H4' | 12:I:125:TYR:HB2 | 1.88 | 0.56 |
| 16:M:66:LEU:CA | 16:M:70:LEU:HD12 | 2.24 | 0.56 |
| 1:A:297:G:H5' | 1:A:557:G:H4' | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:450:G:H21 | 19:P:13:HIS:CE1 | 2.22 | 0.56 |
| 9:F:46:ARG:HH12 | 21:R:37:VAL:CG1 | 2.15 | 0.56 |
| 1:A:1205:U:H4' | 6:C:195:VAL:HG23 | 1.87 | 0.56 |
| 1:A:1329:A:OP1 | 16:M:26:GLY:CA | 2.53 | 0.56 |
| 1:A:790:A:P | 2:V:38:A:O2' | 2.64 | 0.56 |
| 1:A:376:G:H5'' | 19:P:5:ARG:HB2 | 1.86 | 0.56 |
| 1:A:1347:G:H22 | 1:A:1373:G:C2' | 2.16 | 0.56 |
| 3:W:14:A:C6 | 3:W:22:G:N3 | 2.74 | 0.56 |
| 1:A:599:C:O2' | 11:H:129:VAL:HA | 2.06 | 0.56 |
| 1:A:1382:C:O5' | 1:A:1382:C:H6 | 1.88 | 0.56 |
| 7:D:21:LEU:HD11 | 7:D:67:ILE:HA | 1.88 | 0.56 |
| 1:A:1330:U:OP1 | 16:M:25:ILE:O | 2.23 | 0.56 |
| 1:A:1237:C:H3' | 1:A:1238:A:P | 2.44 | 0.56 |
| 1:A:878:G:H5' | 11:H:89:PRO:HB2 | 1.87 | 0.56 |
| 21:R:80:PRO:C | 21:R:82:THR:H | 2.08 | 0.56 |
| 7:D:23:GLY:HA3 | 7:D:113:SER:HB3 | 1.88 | 0.56 |
| 1:A:185:A:N3 | 23:T:81:LYS:NZ | 2.53 | 0.56 |
| 1:A:1060:C:C5 | 6:C:2:GLY:O | 2.59 | 0.56 |
| 1:A:818:G:O2' | 1:A:820:U:C5 | 2.59 | 0.56 |
| 7:D:78:LEU:CD2 | 7:D:139:ARG:NH2 | 2.67 | 0.56 |
| 13:J:10:GLY:CA | 13:J:16:LEU:HD21 | 2.28 | 0.56 |
| 1:A:1418:A:C8 | 1:A:1419:G:C1' | 2.89 | 0.56 |
| 20:Q:65:ILE:HG13 | 20:Q:69:LYS:O | 2.04 | 0.56 |
| 14:K:44:SER:H | 14:K:47:VAL:HB | 1.70 | 0.56 |
| 1:A:1317:C:C4 | 17:N:16:PHE:CE1 | 2.94 | 0.56 |
| 1:A:1059:C:C2' | 13:J:52:GLY:HA2 | 2.35 | 0.56 |
| 1:A:1405:G:C1' | 1:A:1519:A:C4' | 2.84 | 0.56 |
| 1:A:946:A:O2' | 1:A:1333:A:C2' | 2.54 | 0.56 |
| 1:A:59:A:H3' | 1:A:60:A:C5' | 2.36 | 0.56 |
| 1:A:573:A:N3 | 1:A:883:C:O2' | 2.29 | 0.56 |
| 1:A:627:G:H2' | 1:A:628:G:C8 | 2.41 | 0.56 |
| 1:A:242:C:C2 | 1:A:285:G:N2 | 2.74 | 0.56 |
| 1:A:1114:C:O2' | 17:N:60:SER:O | 2.24 | 0.56 |
| 1:A:1014:A:H4' | 22:S:14:HIS:CG | 2.41 | 0.55 |
| 2:V:7:U:C4 | 2:V:49:C:C5 | 2.93 | 0.55 |
| 2:V:34:G:H3' | 2:V:35:A:C5' | 2.36 | 0.55 |
| 8:E:80:ILE:HD12 | 8:E:91:LEU:HB3 | 1.88 | 0.55 |
| 1:A:505:G:OP2 | 1:A:534:U:O2' | 2.13 | 0.55 |
| 14:K:33:THR:HA | 14:K:39:PRO:HA | 1.88 | 0.55 |
| 11:H:135:CYS:SG | 11:H:136:GLU:N | 2.78 | 0.55 |
| 2:V:23:A:H2' | 2:V:24:G:C8 | 2.40 | 0.55 |
| 1:A:1358:U:OP1 | 17:N:34:TYR:CA | 2.54 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1107:C:OP1 | 6:C:172:ARG:CB | 2.54 | 0.55 |
| 1:A:590:C:H5'' | 11:H:30:ARG:HD3 | 1.88 | 0.55 |
| 7:D:140:VAL:CG1 | 7:D:144:ASP:HB2 | 2.35 | 0.55 |
| 22:S:40:ILE:HD13 | 22:S:62:ILE:HD13 | 1.88 | 0.55 |
| 1:A:1220:G:C2 | 22:S:54:GLY:HA2 | 2.37 | 0.55 |
| 7:D:31:CYS:HB3 | 7:D:33:MET:SD | 2.46 | 0.55 |
| 2:V:27:C:H2' | 2:V:28:C:C6 | 2.41 | 0.55 |
| 1:A:17:U:H3 | 1:A:918:A:H61 | 1.52 | 0.55 |
| 1:A:1205:U:C4' | 6:C:195:VAL:CG2 | 2.82 | 0.55 |
| 12:I:55:ALA:HB3 | 12:I:58:ARG:NE | 2.22 | 0.55 |
| 7:D:23:GLY:CA | 7:D:113:SER:CA | 2.83 | 0.55 |
| 7:D:20:TYR:C | 7:D:22:LYS:H | 2.09 | 0.55 |
| 16:M:92:HIS:CG | 16:M:98:VAL:CG2 | 2.86 | 0.55 |
| 1:A:1330:U:OP1 | 16:M:20:THR:O | 2.24 | 0.55 |
| 1:A:1269:A:C5' | 24:U:19:GLY:O | 2.53 | 0.55 |
| 2:V:41:U:H2' | 2:V:41:U:O2 | 2.04 | 0.55 |
| 1:A:311:C:H2' | 1:A:312:C:O4' | 2.07 | 0.55 |
| 8:E:147:ASP:HA | 8:E:150:ARG:HB2 | 1.89 | 0.55 |
| 7:D:70:ILE:HD12 | 7:D:100:ARG:CZ | 2.36 | 0.55 |
| 1:A:1236:A:H4' | 1:A:1304:G:H5'' | 1.88 | 0.55 |
| 1:A:1097:C:O2' | 1:A:1168:A:N3 | 2.33 | 0.55 |
| 1:A:952:U:H2' | 16:M:126:LYS:OXT | 2.05 | 0.55 |
| 20:Q:22:LEU:HD13 | 20:Q:39:SER:OG | 2.06 | 0.55 |
| 1:A:1347:G:H3' | 12:I:108:VAL:CA | 2.37 | 0.55 |
| 1:A:955:U:OP1 | 16:M:120:LYS:HD2 | 2.07 | 0.55 |
| 3:W:29:A:O2' | 3:W:30:G:H5' | 2.06 | 0.55 |
| 7:D:26:CYS:O | 7:D:31:CYS:HB2 | 2.06 | 0.55 |
| 1:A:1328:C:P | 24:U:20:LYS:NZ | 2.79 | 0.55 |
| 1:A:1060:C:H5' | 13:J:52:GLY:N | 2.22 | 0.55 |
| 2:V:34:G:H3' | 2:V:35:A:H5'' | 1.88 | 0.55 |
| 9:F:89:MET:CG | 21:R:76:LEU:HD21 | 2.22 | 0.55 |
| 1:A:598:U:H4' | 11:H:94:TYR:CB | 2.36 | 0.55 |
| 5:B:84:GLU:HG3 | 5:B:212:GLN:NE2 | 2.21 | 0.55 |
| 13:J:7:LYS:HB3 | 13:J:97:GLU:HB2 | 1.89 | 0.55 |
| 2:V:59:U:O2 | 2:V:59:U:C2' | 2.55 | 0.55 |
| 1:A:1224:G:C6 | 1:A:1322:C:C4' | 2.89 | 0.55 |
| 1:A:1374:A:H1' | 10:G:31:MET:SD | 2.47 | 0.55 |
| 1:A:1451:A:H3' | 1:A:1451:A:C8 | 2.41 | 0.55 |
| 1:A:563:A:H2 | 15:L:15:ARG:HH12 | 1.55 | 0.55 |
| 1:A:1277:C:H1' | 1:A:1282:C:C2 | 2.41 | 0.55 |
| 1:A:826:C:H5' | 11:H:12:ARG:NE | 2.08 | 0.55 |
| 1:A:1206:G:O4' | 6:C:194:GLY:CA | 2.52 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:375:U:O4' | 19:P:17:TYR:OH | 2.22 | 0.55 |
| 1:A:501:C:H3' | 1:A:501:C:C6 | 2.42 | 0.55 |
| 1:A:642:A:C8 | 11:H:115:SER:HA | 2.40 | 0.55 |
| 1:A:143:A:H4' | 1:A:144:G:H8 | 1.69 | 0.55 |
| 1:A:948:C:H4' | 1:A:1306:A:O3' | 2.06 | 0.55 |
| 1:A:579:G:H4' | 1:A:728:A:H1' | 1.89 | 0.55 |
| 16:M:44:ARG:HB3 | 16:M:46:LYS:HG2 | 1.88 | 0.55 |
| 12:I:37:PHE:N | 12:I:37:PHE:CD2 | 2.74 | 0.55 |
| 1:A:988:G:N3 | 1:A:1015:A:H2 | 2.05 | 0.55 |
| 1:A:922:G:H2' | 1:A:923:A:C8 | 2.41 | 0.55 |
| 1:A:939:G:O2' | 1:A:940:C:O4' | 2.24 | 0.55 |
| 1:A:1237:C:HO2' | 1:A:1300:G:H22 | 1.52 | 0.55 |
| 1:A:3(A):G:C6 | 1:A:1038:C:C2 | 2.95 | 0.55 |
| 9:F:49:ALA:HB2 | 21:R:78:LEU:O | 2.06 | 0.55 |
| 1:A:509:A:C8 | 7:D:54:TYR:CE2 | 2.90 | 0.55 |
| 1:A:1182:G:H4' | 1:A:1183:A:C5' | 2.37 | 0.55 |
| 1:A:1074:G:H2' | 1:A:1075:C:O4' | 2.07 | 0.55 |
| 1:A:868:C:O4' | 1:A:873:A:C6 | 2.60 | 0.55 |
| 6:C:29:TYR:HE2 | 17:N:54:PRO:HG2 | 1.72 | 0.55 |
| 1:A:1259:C:H42 | 1:A:1276:G:H1 | 1.53 | 0.55 |
| 19:P:8:ARG:NH1 | 19:P:11:SER:O | 2.33 | 0.55 |
| 1:A:979:C:OP1 | 1:A:1222:G:O6 | 2.25 | 0.54 |
| 1:A:1326:C:H4' | 24:U:19:GLY:HA2 | 1.88 | 0.54 |
| 1:A:294:U:H2' | 1:A:295:C:C6 | 2.42 | 0.54 |
| 1:A:1107:C:OP1 | 6:C:172:ARG:CG | 2.55 | 0.54 |
| 1:A:18:C:N3 | 1:A:917:G:N2 | 2.48 | 0.54 |
| 1:A:1148:U:O3' | 12:I:14:VAL:HG11 | 2.07 | 0.54 |
| 20:Q:67:LYS:HA | 20:Q:70:ARG:NH2 | 2.22 | 0.54 |
| 1:A:1349:A:OP2 | 12:I:118:LYS:NZ | 2.29 | 0.54 |
| 1:A:160:A:H2' | 1:A:161:A:O4' | 2.07 | 0.54 |
| 1:A:749:C:O2 | 1:A:749:C:H2' | 2.07 | 0.54 |
| 1:A:1225:A:O4' | 22:S:78:ARG:HD3 | 2.06 | 0.54 |
| 16:M:92:HIS:HE1 | 16:M:110:ARG:NH2 | 2.00 | 0.54 |
| 1:A:1259:C:O3' | 1:A:1284:C:H4' | 2.07 | 0.54 |
| 8:E:7:GLU:HB3 | 8:E:112:LEU:HD11 | 1.88 | 0.54 |
| 23:T:41:VAL:O | 23:T:45:GLN:HB2 | 2.07 | 0.54 |
| 15:L:37:CYS:HA | 15:L:57:LYS:O | 2.07 | 0.54 |
| 8:E:15:ARG:HG2 | 8:E:28:PHE:CD2 | 2.43 | 0.54 |
| 13:J:6:ILE:HG22 | 13:J:98:ILE:HG12 | 1.88 | 0.54 |
| 1:A:405:U:OP1 | 7:D:5:ILE:CD1 | 2.56 | 0.54 |
| 1:A:15:G:H4' | 8:E:24:ARG:HH22 | 1.72 | 0.54 |
| 1:A:790:A:C5' | 2:V:38:A:O2' | 2.55 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:279:A:H4' | 1:A:280:C:OP2 | 2.06 | 0.54 |
| 5:B:164:VAL:HG21 | 5:B:170:GLU:HB3 | 1.89 | 0.54 |
| 6:C:150:LYS:HE3 | 6:C:167:TRP:HE1 | 1.71 | 0.54 |
| 11:H:111:ILE:HG22 | 11:H:134:ILE:HD12 | 1.89 | 0.54 |
| 1:A:109:A:N7 | 1:A:326:G:C2 | 2.76 | 0.54 |
| 5:B:96:ARG:H | 5:B:96:ARG:HD2 | 1.72 | 0.54 |
| 1:A:1222:G:OP1 | 1:A:1321:C:O2 | 2.24 | 0.54 |
| 1:A:1269:A:H1' | 1:A:1326:C:C1' | 2.37 | 0.54 |
| 16:M:24:GLY:HA2 | 16:M:70:LEU:HD11 | 1.89 | 0.54 |
| 2:V:7:U:O4 | 2:V:49:C:C4 | 2.61 | 0.54 |
| 1:A:769:G:N2 | 1:A:900:A:H61 | 2.06 | 0.54 |
| 1:A:1354:C:H2' | 1:A:1355:G:C8 | 2.43 | 0.54 |
| 9:F:7:ASN:ND2 | 21:R:34:TYR:OH | 2.27 | 0.54 |
| 7:D:101:LEU:HD13 | 7:D:138:TYR:HD2 | 1.72 | 0.54 |
| 12:I:37:PHE:HD2 | 12:I:37:PHE:N | 2.05 | 0.54 |
| 14:K:72:ALA:O | 14:K:77:MET:HB2 | 2.07 | 0.54 |
| 1:A:1268:A:C2 | 1:A:1327:C:H1' | 2.38 | 0.54 |
| 3:W:72:C:H2' | 3:W:73:A:C8 | 2.43 | 0.54 |
| 1:A:695:A:H2' | 1:A:696:A:C8 | 2.42 | 0.54 |
| 1:A:20:U:C6 | 1:A:916:G:N2 | 2.75 | 0.54 |
| 1:A:280:C:O2 | 20:Q:39:SER:N | 2.36 | 0.54 |
| 1:A:877:C:O3' | 11:H:89:PRO:HD2 | 2.07 | 0.54 |
| 14:K:57:THR:HG23 | 14:K:60:ALA:H | 1.73 | 0.54 |
| 2:V:56:C:C5 | 2:V:57:G:C6 | 2.96 | 0.54 |
| 5:B:103:THR:O | 5:B:104:ASN:CB | 2.54 | 0.54 |
| 10:G:71:PRO:HA | 10:G:138:LYS:HE3 | 1.90 | 0.54 |
| 1:A:325:A:H2' | 1:A:326:G:O4' | 2.07 | 0.54 |
| 1:A:1054:C:H1' | 1:A:1196:U:C5 | 2.41 | 0.54 |
| 6:C:188:LEU:HD12 | 6:C:190:ARG:HG3 | 1.89 | 0.54 |
| 18:O:82:ILE:O | 18:O:86:GLY:N | 2.34 | 0.54 |
| 1:A:1263:C:H42 | 1:A:1272:G:H1 | 1.55 | 0.54 |
| 1:A:1319:A:H5' | 22:S:5:LEU:HD22 | 1.90 | 0.54 |
| 1:A:975:A:C8 | 1:A:1357:A:H2 | 2.25 | 0.54 |
| 1:A:1269:A:C4' | 24:U:19:GLY:HA2 | 2.38 | 0.54 |
| 1:A:1267:C:O2' | 24:U:20:LYS:HD3 | 2.08 | 0.54 |
| 1:A:1085:U:O4' | 1:A:1094:G:N1 | 2.41 | 0.54 |
| 1:A:1004:A:H2' | 1:A:1025:U:H3 | 1.72 | 0.54 |
| 1:A:1127:G:H2' | 1:A:1128:C:C6 | 2.43 | 0.54 |
| 1:A:1372:U:H2' | 1:A:1373:G:O4' | 2.07 | 0.54 |
| 1:A:736:C:OP1 | 21:R:72:ARG:CZ | 2.55 | 0.54 |
| 15:L:100:ILE:H | 15:L:100:ILE:HD13 | 1.72 | 0.54 |
| 1:A:1098:C:C4' | 1:A:1167:A:H2 | 2.20 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 5:B:18:GLY:HA3 | 5:B:41:ILE:HA | 1.90 | 0.54 |
| 1:A:578:C:O2 | 1:A:728:A:H2 | 1.90 | 0.54 |
| 16:M:14:ARG:HA | 16:M:44:ARG:HA | 1.89 | 0.54 |
| 9:F:76:ALA:HB1 | 9:F:80:ARG:HH21 | 1.71 | 0.54 |
| 19:P:4:ILE:HG12 | 19:P:21:VAL:HG13 | 1.88 | 0.54 |
| 1:A:228:A:O4' | 19:P:62:VAL:HG11 | 2.06 | 0.54 |
| 1:A:397:A:N6 | 1:A:548:G:C4 | 2.75 | 0.54 |
| 1:A:695:A:H2 | 1:A:787:A:C4' | 2.06 | 0.54 |
| 1:A:1156:G:C2' | 1:A:1179:A:H61 | 2.20 | 0.54 |
| 6:C:70:VAL:HG12 | 6:C:72:LYS:H | 1.73 | 0.54 |
| 16:M:23:TYR:HB3 | 16:M:67:GLU:HA | 1.90 | 0.54 |
| 1:A:1059:C:O2' | 13:J:53:PRO:HD2 | 2.07 | 0.54 |
| 1:A:765:G:H1 | 1:A:812:C:C2' | 2.20 | 0.54 |
| 1:A:129(A):G:H2' | 1:A:190(E):U:H5'' | 1.89 | 0.54 |
| 1:A:1418:A:N7 | 1:A:1419:G:H1' | 2.23 | 0.54 |
| 1:A:989:C:O4' | 1:A:1016:A:H2 | 1.90 | 0.54 |
| 1:A:1315:U:H3 | 1:A:1319:A:H62 | 1.54 | 0.54 |
| 1:A:988:G:HO2' | 1:A:1015:A:N6 | 2.03 | 0.54 |
| 1:A:1225:A:C4' | 22:S:78:ARG:HD3 | 2.38 | 0.54 |
| 1:A:1060:C:N4 | 6:C:2:GLY:HA3 | 2.23 | 0.54 |
| 1:A:426:G:H4' | 7:D:42:GLN:CA | 2.35 | 0.54 |
| 1:A:1348:U:OP1 | 12:I:109:VAL:HA | 2.08 | 0.54 |
| 1:A:1306:A:H61 | 1:A:1331:G:H1' | 1.73 | 0.54 |
| 1:A:186:C:OP1 | 23:T:78:ALA:HB1 | 2.07 | 0.54 |
| 12:I:96:LEU:HG | 12:I:101:PHE:HB2 | 1.90 | 0.54 |
| 1:A:621:A:H2' | 1:A:622:A:C8 | 2.43 | 0.54 |
| 6:C:178:LEU:O | 6:C:179:ARG:CB | 2.55 | 0.54 |
| 1:A:1222:G:H5'' | 22:S:78:ARG:NE | 2.23 | 0.54 |
| 1:A:1319:A:OP2 | 22:S:5:LEU:HD22 | 2.08 | 0.54 |
| 2:V:31:A:O3' | 12:I:127:LYS:HB2 | 2.08 | 0.54 |
| 1:A:121:C:H41 | 1:A:235:C:H3' | 1.72 | 0.54 |
| 1:A:105:G:H2' | 1:A:106:C:C6 | 2.43 | 0.54 |
| 1:A:345:C:H4' | 1:A:346:G:O5' | 2.07 | 0.54 |
| 14:K:121:PRO:HB2 | 14:K:125:PHE:HB2 | 1.89 | 0.54 |
| 16:M:24:GLY:HA3 | 16:M:70:LEU:CD1 | 2.38 | 0.53 |
| 1:A:1235:U:H5'' | 24:U:3:LYS:HD2 | 1.90 | 0.53 |
| 15:L:42:THR:OG1 | 15:L:52:LEU:HB3 | 2.08 | 0.53 |
| 1:A:188:C:H1' | 23:T:105:SER:O | 2.08 | 0.53 |
| 7:D:123:HIS:HB2 | 7:D:125:HIS:NE2 | 2.23 | 0.53 |
| 3:W:37:YYG:O22 | 10:G:84:ASN:N | 2.41 | 0.53 |
| 1:A:48:C:OP1 | 1:A:115:G:OP1 | 2.26 | 0.53 |
| 1:A:971:G:N2 | 1:A:1363:A:OP2 | 2.40 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:22:G:H2' | 1:A:913:A:C2 | 2.43 | 0.53 |
| 1:A:375:U:O4' | 19:P:17:TYR:CE2 | 2.61 | 0.53 |
| 7:D:30:LYS:C | 7:D:32:ALA:N | 2.61 | 0.53 |
| 13:J:84:GLN:HA | 13:J:88:LEU:HD12 | 1.91 | 0.53 |
| 1:A:1504:G:H3' | 1:A:1504:G:P | 2.48 | 0.53 |
| 7:D:24:GLU:CA | 7:D:112:VAL:CG1 | 2.87 | 0.53 |
| 1:A:1058:G:H2' | 1:A:1059:C:O4' | 2.08 | 0.53 |
| 1:A:563:A:O2' | 1:A:566:G:O2' | 2.25 | 0.53 |
| 1:A:1066:C:H2' | 1:A:1067:A:C8 | 2.43 | 0.53 |
| 1:A:915:A:N7 | 1:A:916:G:C8 | 2.76 | 0.53 |
| 1:A:68:G:H2' | 1:A:69:G:O4' | 2.07 | 0.53 |
| 16:M:92:HIS:HE1 | 16:M:110:ARG:CZ | 2.20 | 0.53 |
| 1:A:1060:C:H5'' | 13:J:51:ARG:HD3 | 1.90 | 0.53 |
| 1:A:775:G:O2' | 1:A:776:G:H5' | 2.08 | 0.53 |
| 1:A:398:C:H2' | 1:A:399:G:H8 | 1.73 | 0.53 |
| 1:A:263:A:H2' | 1:A:264:U:H5' | 1.91 | 0.53 |
| 7:D:159:ARG:O | 7:D:163:GLU:HB3 | 2.08 | 0.53 |
| 3:W:16:U:H1' | 3:W:17:U:OP2 | 2.08 | 0.53 |
| 1:A:1338:G:H21 | 2:V:41:U:H1' | 1.74 | 0.53 |
| 1:A:39:G:C5 | 1:A:498:U:O4 | 2.62 | 0.53 |
| 1:A:25:C:H4' | 1:A:524:G:N3 | 2.23 | 0.53 |
| 1:A:1287:A:N6 | 1:A:1371:G:C4' | 2.66 | 0.53 |
| 1:A:1055:A:H2 | 6:C:194:GLY:HA3 | 1.74 | 0.53 |
| 1:A:375:U:O4' | 19:P:17:TYR:CZ | 2.62 | 0.53 |
| 1:A:1347:G:OP2 | 12:I:107:ARG:HD2 | 2.08 | 0.53 |
| 1:A:640:A:O2' | 11:H:116:LYS:NZ | 2.27 | 0.53 |
| 2:V:18:G:H2' | 2:V:19:G:O5' | 2.09 | 0.53 |
| 1:A:720:C:H6 | 1:A:720:C:O5' | 1.92 | 0.53 |
| 16:M:10:PRO:HG2 | 16:M:18:ALA:HB1 | 1.90 | 0.53 |
| 20:Q:3:LYS:HB3 | 20:Q:61:GLU:O | 2.07 | 0.53 |
| 1:A:831:U:H2' | 1:A:832:C:C6 | 2.43 | 0.53 |
| 1:A:1225:A:OP2 | 1:A:1226:C:H5 | 1.91 | 0.53 |
| 1:A:426:G:C1' | 7:D:42:GLN:HG3 | 2.34 | 0.53 |
| 1:A:667:G:H1 | 1:A:739:C:H42 | 1.57 | 0.53 |
| 1:A:767:A:H1' | 1:A:1525:G:H1' | 1.91 | 0.53 |
| 10:G:146:GLU:O | 10:G:149:ARG:HB2 | 2.08 | 0.53 |
| 1:A:762:C:H2' | 1:A:763:G:H8 | 1.71 | 0.53 |
| 1:A:708:C:H4' | 14:K:37:GLY:HA3 | 1.91 | 0.53 |
| 12:I:114:TYR:CD1 | 13:J:60:ARG:HB3 | 2.44 | 0.53 |
| 2:V:32:C:P | 12:I:127:LYS:HB2 | 2.49 | 0.53 |
| 1:A:311:C:C5 | 1:A:312:C:C5 | 2.96 | 0.53 |
| 1:A:450:G:H1 | 1:A:483:C:H42 | 1.56 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 20:Q:9:VAL:HG12 | 20:Q:56:VAL:HG22 | 1.91 | 0.53 |
| 1:A:726:C:N4 | 1:A:731:G:H1 | 2.07 | 0.53 |
| 6:C:35:GLU:OE2 | 6:C:97:LYS:HG3 | 2.09 | 0.53 |
| 1:A:1219:U:O2 | 22:S:34:TRP:NE1 | 2.39 | 0.53 |
| 13:J:60:ARG:O | 13:J:61:GLU:HB2 | 2.08 | 0.53 |
| 1:A:20:U:N1 | 1:A:916:G:N2 | 2.56 | 0.53 |
| 7:D:141:ARG:HB3 | 7:D:142:PRO:CD | 2.36 | 0.53 |
| 1:A:54:C:C4 | 1:A:352:C:H2' | 2.44 | 0.53 |
| 7:D:58:LEU:HD13 | 7:D:59:ARG:HH11 | 1.73 | 0.53 |
| 11:H:82:HIS:O | 11:H:137:VAL:HA | 2.09 | 0.53 |
| 8:E:36:ASP:O | 8:E:37:ARG:HB2 | 2.09 | 0.53 |
| 1:A:645:C:H2' | 1:A:646:U:C6 | 2.44 | 0.53 |
| 23:T:61:SER:O | 23:T:65:LYS:HG2 | 2.08 | 0.53 |
| 1:A:1320:C:H5'' | 22:S:3:ARG:NH2 | 2.23 | 0.53 |
| 1:A:1317:C:OP1 | 17:N:16:PHE:HA | 2.09 | 0.53 |
| 9:F:62:TRP:CD1 | 21:R:35:ARG:CZ | 2.92 | 0.53 |
| 1:A:986:A:C4' | 22:S:55:LYS:CG | 2.81 | 0.53 |
| 16:M:88:ARG:HB2 | 16:M:98:VAL:CG1 | 2.39 | 0.53 |
| 2:V:7:U:H5' | 2:V:8:U:P | 2.49 | 0.53 |
| 11:H:112:LEU:HD22 | 11:H:114:THR:HG22 | 1.91 | 0.53 |
| 22:S:39:THR:HA | 22:S:70:LYS:HA | 1.89 | 0.52 |
| 1:A:302:G:N3 | 1:A:556:C:H5'' | 2.24 | 0.52 |
| 7:D:3:ARG:CD | 7:D:118:ARG:NH1 | 2.71 | 0.52 |
| 1:A:1345:U:O2 | 1:A:1375:A:N1 | 2.42 | 0.52 |
| 9:F:50:TYR:OH | 21:R:77:GLY:HA2 | 2.09 | 0.52 |
| 9:F:37:VAL:HA | 9:F:65:VAL:HG12 | 1.91 | 0.52 |
| 1:A:129(A):G:C6 | 1:A:190(D):U:H4' | 2.44 | 0.52 |
| 1:A:501:C:O2 | 1:A:549:C:O2' | 2.22 | 0.52 |
| 1:A:854:G:H3' | 1:A:871:U:O4 | 2.08 | 0.52 |
| 1:A:1220:G:H4' | 22:S:36:ARG:CD | 2.39 | 0.52 |
| 1:A:410:G:P | 7:D:25:ARG:CZ | 2.92 | 0.52 |
| 1:A:818:G:C2' | 1:A:819:A:H5'' | 2.39 | 0.52 |
| 1:A:576:G:C8 | 1:A:881:G:H1' | 2.43 | 0.52 |
| 7:D:11:LEU:C | 7:D:13:ARG:N | 2.63 | 0.52 |
| 15:L:53:ARG:NH1 | 15:L:93:LEU:HD22 | 2.23 | 0.52 |
| 1:A:1080:A:H5' | 8:E:14:ARG:HH22 | 1.74 | 0.52 |
| 5:B:36:ARG:HB2 | 5:B:41:ILE:HD13 | 1.90 | 0.52 |
| 19:P:4:ILE:HG12 | 19:P:21:VAL:CG1 | 2.39 | 0.52 |
| 1:A:11:G:O2' | 1:A:506:G:N2 | 2.42 | 0.52 |
| 1:A:340:U:H2' | 1:A:341:C:H6 | 1.74 | 0.52 |
| 6:C:142:MET:HA | 6:C:146:ALA:HB3 | 1.91 | 0.52 |
| 1:A:1329:A:H5'' | 16:M:26:GLY:HA3 | 1.88 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1297:C:H1' | 1:A:1298:C:H5 | 1.75 | 0.52 |
| 1:A:1298:C:H5'' | 1:A:1299:A:P | 2.49 | 0.52 |
| 15:L:71:PRO:O | 15:L:102:ARG:HD2 | 2.09 | 0.52 |
| 8:E:17:ALA:HA | 8:E:26:PHE:CB | 2.39 | 0.52 |
| 1:A:1201:A:O2' | 1:A:1202:G:OP2 | 2.21 | 0.52 |
| 1:A:1298:C:P | 10:G:114:ARG:HH12 | 2.32 | 0.52 |
| 8:E:79:GLU:OE2 | 11:H:104:ARG:HD3 | 2.09 | 0.52 |
| 1:A:281:G:O2' | 1:A:282:A:H8 | 1.91 | 0.52 |
| 1:A:878:G:O4' | 11:H:3:THR:HG21 | 2.09 | 0.52 |
| 1:A:640:A:H2' | 11:H:115:SER:OG | 2.10 | 0.52 |
| 1:A:823:G:H21 | 11:H:1:MET:H3 | 1.58 | 0.52 |
| 16:M:11:ARG:HH12 | 16:M:46:LYS:HB3 | 1.74 | 0.52 |
| 11:H:34:GLU:HA | 11:H:37:ARG:HB3 | 1.90 | 0.52 |
| 1:A:361(A):C:O2' | 1:A:1362:C:O4' | 2.21 | 0.52 |
| 1:A:791:G:OP2 | 1:A:791:G:H8 | 1.92 | 0.52 |
| 1:A:1405:G:N2 | 1:A:1518:A:C2 | 2.76 | 0.52 |
| 1:A:1101:A:O2' | 1:A:1102:A:P | 2.67 | 0.52 |
| 1:A:590:C:H5'' | 11:H:30:ARG:HD2 | 1.90 | 0.52 |
| 5:B:91:PRO:HG2 | 5:B:155:LEU:HB2 | 1.92 | 0.52 |
| 14:K:108:ILE:HB | 21:R:87:ARG:O | 2.10 | 0.52 |
| 1:A:1058:G:P | 6:C:199:LYS:HE3 | 2.50 | 0.52 |
| 1:A:1297:C:O2' | 10:G:114:ARG:HD3 | 2.10 | 0.52 |
| 2:V:37:G:C2 | 4:X:116:U:C2 | 2.97 | 0.52 |
| 10:G:106:GLN:O | 10:G:110:GLN:HG2 | 2.09 | 0.52 |
| 1:A:1254:C:OP1 | 13:J:45:ARG:HD2 | 2.10 | 0.52 |
| 1:A:20:U:C1' | 1:A:572:A:C2 | 2.93 | 0.52 |
| 3:W:40:C:O2 | 10:G:144:MET:SD | 2.68 | 0.52 |
| 1:A:377:G:OP1 | 19:P:5:ARG:NH1 | 2.40 | 0.52 |
| 9:F:50:TYR:HE1 | 21:R:77:GLY:HA2 | 1.72 | 0.52 |
| 1:A:686:U:O2 | 1:A:686:U:H2' | 2.09 | 0.52 |
| 1:A:578:C:H2' | 1:A:579:G:C8 | 2.45 | 0.52 |
| 6:C:205:GLY:O | 6:C:206:GLU:HB2 | 2.09 | 0.52 |
| 5:B:47:THR:HG23 | 5:B:202:PRO:HD2 | 1.91 | 0.52 |
| 1:A:1014:A:C2 | 22:S:34:TRP:CE2 | 2.98 | 0.52 |
| 1:A:1317:C:C6 | 17:N:16:PHE:CD2 | 2.98 | 0.52 |
| 1:A:1314:C:C4 | 22:S:4:SER:HB2 | 2.45 | 0.52 |
| 4:X:117:U:O2' | 4:X:118:C:H5' | 2.10 | 0.52 |
| 1:A:190(E):U:H3 | 20:Q:63:ARG:HB2 | 1.73 | 0.52 |
| 3:W:41:U:C5' | 3:W:41:U:H6 | 2.13 | 0.52 |
| 3:W:65:G:C3' | 3:W:66:A:H5' | 2.40 | 0.52 |
| 7:D:173:TRP:CG | 7:D:189:PRO:HB3 | 2.44 | 0.52 |
| 1:A:928:G:O2' | 1:A:1533:C:N4 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 6:C:12:LEU:CD1 | 17:N:51:GLY:CA | 2.87 | 0.52 |
| 2:V:48:C:C2' | 2:V:48:C:O2 | 2.55 | 0.52 |
| 2:V:73:A:HO3' | 2:V:74:C:P | 2.27 | 0.52 |
| 1:A:939:G:OP1 | 10:G:102:ARG:NH2 | 2.43 | 0.52 |
| 1:A:1037:C:C4 | 1:A:1038:C:H5 | 2.22 | 0.52 |
| 23:T:60:GLU:HA | 23:T:63:ILE:HD12 | 1.91 | 0.52 |
| 6:C:29:TYR:CE2 | 17:N:54:PRO:HG2 | 2.45 | 0.52 |
| 1:A:1230:C:H2' | 1:A:1231:G:H8 | 1.75 | 0.52 |
| 3:W:25:C:O3' | 3:W:26:G:O5' | 2.28 | 0.52 |
| 2:V:37:G:H2' | 2:V:38:A:H8 | 1.75 | 0.52 |
| 1:A:668:G:C5' | 18:O:48:LYS:O | 2.56 | 0.52 |
| 1:A:660:G:H1 | 1:A:745:C:H42 | 1.57 | 0.52 |
| 1:A:1305:G:N2 | 1:A:1331:G:H2' | 2.24 | 0.52 |
| 11:H:38:ILE:HG13 | 11:H:118:VAL:HB | 1.92 | 0.52 |
| 6:C:5:ILE:HG23 | 13:J:51:ARG:HH22 | 1.75 | 0.51 |
| 1:A:15:G:H2' | 1:A:16:A:C8 | 2.45 | 0.51 |
| 1:A:397:A:C5 | 1:A:548:G:C8 | 2.98 | 0.51 |
| 1:A:1095:U:H5' | 1:A:1109:C:O2 | 2.10 | 0.51 |
| 1:A:450:G:N2 | 19:P:13:HIS:CE1 | 2.78 | 0.51 |
| 6:C:52:LEU:O | 6:C:53:ALA:HB2 | 2.10 | 0.51 |
| 19:P:48:TRP:H | 19:P:48:TRP:HD1 | 1.58 | 0.51 |
| 1:A:436:C:C2' | 1:A:437:U:C6 | 2.92 | 0.51 |
| 1:A:1329:A:O3' | 16:M:25:ILE:N | 2.43 | 0.51 |
| 1:A:880:C:H3' | 15:L:9:GLN:NE2 | 2.25 | 0.51 |
| 1:A:22:G:N3 | 1:A:914:A:N7 | 2.58 | 0.51 |
| 1:A:1347:G:H5'' | 12:I:107:ARG:HA | 1.93 | 0.51 |
| 1:A:1373:G:C5' | 12:I:42:ARG:HH21 | 2.23 | 0.51 |
| 6:C:52:LEU:O | 6:C:53:ALA:CB | 2.58 | 0.51 |
| 1:A:1381:U:H2' | 1:A:1381:U:O2 | 2.10 | 0.51 |
| 1:A:927:G:N2 | 1:A:1391:U:H1' | 2.25 | 0.51 |
| 1:A:1396:A:C2 | 1:A:1398:A:C2 | 2.98 | 0.51 |
| 1:A:397:A:C6 | 1:A:548:G:C6 | 2.98 | 0.51 |
| 1:A:949:A:HO2' | 1:A:971:G:H1 | 1.57 | 0.51 |
| 3:W:25:C:O2 | 3:W:26:G:C2 | 2.59 | 0.51 |
| 1:A:926:G:H22 | 4:X:116:U:P | 2.33 | 0.51 |
| 2:V:36:A:C6 | 4:X:117:U:C2 | 2.99 | 0.51 |
| 1:A:888:G:H21 | 1:A:909:A:H62 | 1.58 | 0.51 |
| 1:A:1251:A:H5' | 12:I:12:GLU:HB2 | 1.90 | 0.51 |
| 10:G:149:ARG:HD2 | 14:K:59:TYR:CE1 | 2.45 | 0.51 |
| 1:A:1514:C:O5' | 1:A:1514:C:H6 | 1.93 | 0.51 |
| 1:A:1127:G:H8 | 1:A:1127:G:O5' | 1.93 | 0.51 |
| 3:W:40:C:H2' | 3:W:41:U:C5' | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 15:L:85:ILE:HG12 | 15:L:98:TYR:HB3 | 1.92 | 0.51 |
| 10:G:153:HIS:CE1 | 14:K:58:PRO:CG | 2.93 | 0.51 |
| 3:W:69:U:H2' | 3:W:70:C:C6 | 2.46 | 0.51 |
| 1:A:1268:A:H2 | 1:A:1327:C:C1' | 2.23 | 0.51 |
| 17:N:37:PHE:HE1 | 17:N:53:LEU:HD13 | 1.75 | 0.51 |
| 1:A:1255:G:N2 | 1:A:1258:G:H21 | 2.04 | 0.51 |
| 1:A:889:A:C4' | 1:A:890:G:H4' | 2.28 | 0.51 |
| 1:A:22:G:N2 | 1:A:913:A:O2' | 2.44 | 0.51 |
| 1:A:717:C:H2' | 1:A:734:G:H5' | 1.92 | 0.51 |
| 14:K:66:LEU:HB3 | 14:K:70:LYS:HE3 | 1.93 | 0.51 |
| 16:M:87:TYR:CD1 | 22:S:73:GLU:O | 2.64 | 0.51 |
| 1:A:1070:U:H5' | 8:E:18:ARG:HH12 | 1.76 | 0.51 |
| 1:A:1206:G:H2' | 1:A:1207:G:O4' | 2.11 | 0.51 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.46 | 0.51 |
| 1:A:897:C:O2 | 1:A:903:G:C2 | 2.64 | 0.51 |
| 1:A:1510:U:H3 | 1:A:1525:G:H1 | 1.56 | 0.51 |
| 11:H:20:TYR:HA | 11:H:65:TYR:OH | 2.10 | 0.51 |
| 1:A:1241:G:H8 | 1:A:1241:G:OP2 | 1.93 | 0.51 |
| 1:A:327:A:H4' | 1:A:328:C:OP1 | 2.11 | 0.51 |
| 7:D:170:VAL:HG12 | 7:D:171:GLY:N | 2.26 | 0.51 |
| 22:S:44:MET:HA | 22:S:47:HIS:HD2 | 1.76 | 0.51 |
| 1:A:730:G:C5 | 1:A:731:G:H1' | 2.46 | 0.51 |
| 1:A:1484:C:H2' | 1:A:1485:U:O4' | 2.11 | 0.51 |
| 10:G:59:LEU:O | 10:G:63:LYS:HG2 | 2.10 | 0.51 |
| 1:A:409:G:OP1 | 7:D:25:ARG:HB3 | 2.11 | 0.51 |
| 6:C:8:ILE:HG21 | 17:N:50:LYS:O | 2.11 | 0.51 |
| 1:A:123:C:C5' | 1:A:311:C:O2' | 2.58 | 0.51 |
| 1:A:571:U:H3' | 1:A:572:A:H5' | 1.90 | 0.51 |
| 1:A:36:C:H4' | 15:L:117:ARG:HH22 | 1.73 | 0.51 |
| 1:A:1150:U:H2' | 1:A:1151:A:C8 | 2.46 | 0.51 |
| 1:A:1306:A:N6 | 1:A:1331:G:H1' | 2.25 | 0.51 |
| 23:T:63:ILE:HG21 | 23:T:81:LYS:HG3 | 1.93 | 0.51 |
| 10:G:33:ASP:HB2 | 10:G:35:LYS:HD3 | 1.91 | 0.51 |
| 7:D:22:LYS:HB2 | 7:D:26:CYS:SG | 2.51 | 0.51 |
| 1:A:1317:C:C2 | 17:N:16:PHE:CE2 | 2.98 | 0.51 |
| 17:N:24:CYS:HB2 | 17:N:39:LEU:CA | 2.41 | 0.51 |
| 7:D:3:ARG:CB | 7:D:118:ARG:HH11 | 2.23 | 0.51 |
| 1:A:113:G:H1' | 1:A:354:G:H5'' | 1.91 | 0.51 |
| 1:A:1270:C:P | 24:U:24:ARG:HH21 | 2.31 | 0.51 |
| 1:A:792:A:C4 | 1:A:794:A:N6 | 2.79 | 0.51 |
| 1:A:1235:U:OP1 | 24:U:3:LYS:HD3 | 2.10 | 0.51 |
| 1:A:501:C:OP1 | 15:L:124:LYS:HD3 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 11:H:113:SER:HB2 | 11:H:134:ILE:HD11 | 1.92 | 0.51 |
| 8:E:126:ARG:HA | 8:E:131:ILE:HG13 | 1.93 | 0.51 |
| 5:B:63:MET:HB3 | 5:B:225:ALA:HB1 | 1.92 | 0.51 |
| 1:A:1014:A:N1 | 22:S:34:TRP:CH2 | 2.79 | 0.51 |
| 7:D:8:VAL:HB | 7:D:115:ARG:NH2 | 2.25 | 0.51 |
| 1:A:1317:C:OP1 | 17:N:16:PHE:HB3 | 2.10 | 0.51 |
| 13:J:48:THR:HG22 | 13:J:60:ARG:HG3 | 1.93 | 0.51 |
| 2:V:36:A:N6 | 4:X:116:U:H3 | 2.09 | 0.51 |
| 1:A:864:A:H2 | 1:A:917:G:N3 | 2.09 | 0.51 |
| 1:A:22:G:C2' | 1:A:913:A:H2 | 2.24 | 0.51 |
| 1:A:22:G:N2 | 1:A:914:A:C8 | 2.79 | 0.51 |
| 1:A:1205:U:C4' | 6:C:195:VAL:HG21 | 2.39 | 0.51 |
| 1:A:118:U:H3' | 1:A:288:A:H61 | 1.75 | 0.51 |
| 1:A:1361:G:HO3' | 1:A:361(A):C:P | 2.29 | 0.51 |
| 3:W:37:YYG:H191 | 10:G:83:ALA:O | 2.11 | 0.51 |
| 1:A:953:G:HO2' | 16:M:124:PRO:C | 2.01 | 0.51 |
| 2:V:33:U:C5 | 12:I:128:ARG:O | 2.64 | 0.51 |
| 1:A:116:A:N1 | 1:A:313:A:C2' | 2.72 | 0.51 |
| 1:A:670:G:O2' | 9:F:77:ARG:NH2 | 2.44 | 0.51 |
| 1:A:949:A:C4' | 1:A:1364:U:H3 | 2.23 | 0.51 |
| 1:A:1117:G:N2 | 1:A:1180:A:H1' | 2.25 | 0.51 |
| 11:H:88:LYS:O | 11:H:90:GLY:N | 2.44 | 0.51 |
| 1:A:739:C:H5'' | 18:O:2:PRO:HD3 | 1.92 | 0.51 |
| 1:A:1074:G:N2 | 1:A:1102:A:C8 | 2.78 | 0.51 |
| 2:V:55:U:C2 | 2:V:57:G:OP2 | 2.65 | 0.51 |
| 12:I:112:LYS:HG3 | 12:I:117:HIS:O | 2.10 | 0.51 |
| 1:A:1441:G:H1' | 1:A:1461:G:N2 | 2.25 | 0.51 |
| 14:K:42:TRP:HZ3 | 14:K:47:VAL:HG21 | 1.76 | 0.51 |
| 1:A:68:G:C4' | 1:A:171:A:H1' | 2.41 | 0.51 |
| 1:A:1060:C:C4' | 13:J:52:GLY:N | 2.72 | 0.50 |
| 7:D:3:ARG:HG3 | 7:D:118:ARG:HH12 | 1.67 | 0.50 |
| 1:A:1302:U:P | 16:M:13:LYS:NZ | 2.84 | 0.50 |
| 15:L:88:GLY:O | 15:L:99:HIS:CE1 | 2.64 | 0.50 |
| 5:B:15:VAL:HG22 | 5:B:209:ARG:HD2 | 1.93 | 0.50 |
| 1:A:986:A:C1' | 22:S:54:GLY:O | 2.59 | 0.50 |
| 5:B:112:VAL:CA | 5:B:113:HIS:N | 2.71 | 0.50 |
| 5:B:115:LEU:HB2 | 5:B:145:LEU:HD12 | 1.93 | 0.50 |
| 1:A:583:A:H2' | 1:A:584:G:O4' | 2.11 | 0.50 |
| 3:W:65:G:O3' | 3:W:66:A:C5' | 2.60 | 0.50 |
| 1:A:452:A:O2' | 19:P:72:ARG:CZ | 2.59 | 0.50 |
| 20:Q:54:GLY:HA2 | 20:Q:85:VAL:HG21 | 1.94 | 0.50 |
| 1:A:975:A:O2' | 17:N:32:SER:HB2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 13:J:51:ARG:CB | 13:J:59:SER:HB3 | 2.11 | 0.50 |
| 1:A:765:G:H21 | 1:A:816:A:H2 | 1.56 | 0.50 |
| 1:A:983:A:H8 | 1:A:1201:A:C2 | 2.27 | 0.50 |
| 1:A:901:A:H8 | 1:A:901:A:O5' | 1.94 | 0.50 |
| 3:W:10:G:C8 | 3:W:45:G:O2' | 2.63 | 0.50 |
| 1:A:942:G:H2' | 1:A:943:U:H6 | 1.77 | 0.50 |
| 7:D:62:GLN:HE22 | 7:D:65:ARG:HD3 | 1.75 | 0.50 |
| 5:B:17:PHE:CD1 | 5:B:18:GLY:N | 2.78 | 0.50 |
| 12:I:74:ILE:HA | 12:I:77:ILE:HD12 | 1.93 | 0.50 |
| 6:C:139:GLN:HA | 6:C:170:GLN:HE22 | 1.77 | 0.50 |
| 10:G:113:GLU:HG3 | 10:G:118:VAL:HB | 1.93 | 0.50 |
| 16:M:22:ILE:HG23 | 16:M:67:GLU:HB2 | 1.94 | 0.50 |
| 1:A:1397:C:H2' | 1:A:1397:C:O2 | 2.11 | 0.50 |
| 1:A:1516:G:H22 | 1:A:1518:A:H3' | 1.76 | 0.50 |
| 11:H:29:SER:CB | 11:H:32:LYS:HZ1 | 2.23 | 0.50 |
| 5:B:174:VAL:HG13 | 5:B:184:VAL:HG11 | 1.94 | 0.50 |
| 1:A:104:G:O3' | 1:A:174:C:H4' | 2.12 | 0.50 |
| 1:A:66:G:N2 | 1:A:172:A:H2 | 2.10 | 0.50 |
| 14:K:12:ARG:HH12 | 14:K:40:ILE:HA | 1.74 | 0.50 |
| 3:W:16:U:O2' | 3:W:17:U:OP2 | 2.21 | 0.50 |
| 6:C:43:LEU:O | 6:C:47:LEU:HB2 | 2.11 | 0.50 |
| 7:D:27:TYR:OH | 7:D:106:TYR:OH | 2.08 | 0.50 |
| 7:D:98:GLU:C | 7:D:100:ARG:H | 2.15 | 0.50 |
| 5:B:167:PRO:HG2 | 5:B:192:SER:HB3 | 1.93 | 0.50 |
| 1:A:1020:U:H2' | 1:A:1021:G:C8 | 2.46 | 0.50 |
| 16:M:87:TYR:HD1 | 22:S:73:GLU:O | 1.94 | 0.50 |
| 1:A:31:G:O4' | 1:A:306:G:C2 | 2.64 | 0.50 |
| 1:A:1127:G:H2' | 1:A:1128:C:H6 | 1.75 | 0.50 |
| 2:V:24:G:H2' | 2:V:25:C:C6 | 2.47 | 0.50 |
| 6:C:141:VAL:HG11 | 6:C:202:ILE:HG12 | 1.93 | 0.50 |
| 1:A:1268:A:C2' | 24:U:20:LYS:CA | 2.70 | 0.50 |
| 1:A:1199:U:H4' | 13:J:54:PHE:CE2 | 2.47 | 0.50 |
| 11:H:12:ARG:HH11 | 11:H:27:PRO:HD3 | 1.76 | 0.50 |
| 20:Q:22:LEU:HD12 | 20:Q:23:VAL:C | 2.32 | 0.50 |
| 1:A:944:G:C8 | 1:A:945:G:C8 | 2.99 | 0.50 |
| 1:A:668:G:H1' | 18:O:46:HIS:CD2 | 2.46 | 0.50 |
| 1:A:946:A:H1' | 1:A:1334:G:O4' | 2.12 | 0.50 |
| 14:K:18:ARG:NH2 | 14:K:37:GLY:HA2 | 2.27 | 0.50 |
| 12:I:111:ARG:HG2 | 12:I:112:LYS:O | 2.12 | 0.50 |
| 1:A:1014:A:C6 | 22:S:34:TRP:CZ3 | 2.99 | 0.50 |
| 1:A:1314:C:C5 | 22:S:4:SER:HB2 | 2.47 | 0.50 |
| 1:A:541:G:H5' | 7:D:42:GLN:HE21 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:453:A:C4' | 19:P:72:ARG:HD2 | 2.42 | 0.50 |
| 1:A:760:G:N1 | 20:Q:104:LYS:O | 2.44 | 0.50 |
| 1:A:162:A:H1' | 1:A:348:G:O2' | 2.12 | 0.50 |
| 6:C:119:ARG:HG2 | 6:C:140:ARG:HH12 | 1.75 | 0.50 |
| 22:S:60:VAL:HG11 | 22:S:74:PHE:HB3 | 1.94 | 0.50 |
| 1:A:1502:A:H2 | 1:A:1505:G:N1 | 2.07 | 0.50 |
| 1:A:1298:C:N4 | 10:G:114:ARG:O | 2.45 | 0.50 |
| 1:A:1230:C:O2' | 16:M:126:LYS:CD | 2.60 | 0.50 |
| 1:A:280:C:O2 | 20:Q:38:ARG:HG3 | 2.12 | 0.50 |
| 5:B:162:ILE:HD13 | 5:B:162:ILE:H | 1.75 | 0.50 |
| 21:R:21:LYS:H | 21:R:55:ARG:HH12 | 1.60 | 0.50 |
| 1:A:1220:G:H5' | 22:S:35:SER:HA | 1.94 | 0.49 |
| 1:A:1307:U:H4' | 16:M:109:THR:CG2 | 2.41 | 0.49 |
| 1:A:1317:C:C4 | 17:N:16:PHE:CZ | 3.00 | 0.49 |
| 1:A:1084:G:H3' | 1:A:1085:U:H3' | 1.94 | 0.49 |
| 1:A:1286:A:N6 | 1:A:1355:G:P | 2.85 | 0.49 |
| 13:J:11:PHE:CD2 | 17:N:55:GLY:CA | 2.95 | 0.49 |
| 13:J:11:PHE:HE2 | 13:J:65:LEU:HG | 1.75 | 0.49 |
| 1:A:1377:A:P | 10:G:94:ARG:NH2 | 2.85 | 0.49 |
| 2:V:58:A:C6 | 2:V:61:C:C6 | 2.99 | 0.49 |
| 1:A:1418:A:H8 | 1:A:1419:G:C1' | 2.25 | 0.49 |
| 14:K:40:ILE:HG23 | 14:K:75:TYR:CD2 | 2.47 | 0.49 |
| 1:A:1240:U:O4' | 10:G:42:ILE:HD11 | 2.12 | 0.49 |
| 1:A:579:G:O5' | 1:A:728:A:O2' | 2.30 | 0.49 |
| 9:F:80:ARG:HG3 | 9:F:88:VAL:HG21 | 1.95 | 0.49 |
| 8:E:122:GLU:HB3 | 8:E:126:ARG:HG2 | 1.93 | 0.49 |
| 1:A:665:A:C1' | 1:A:733:A:H1' | 2.42 | 0.49 |
| 1:A:1462:G:H2' | 1:A:1463:C:C6 | 2.46 | 0.49 |
| 1:A:687:A:O2' | 1:A:688:G:P | 2.70 | 0.49 |
| 1:A:976:G:P | 17:N:32:SER:HA | 2.52 | 0.49 |
| 3:W:23:A:O2' | 3:W:24:G:H5' | 2.12 | 0.49 |
| 1:A:1065:U:O2 | 1:A:1066:C:H5 | 1.95 | 0.49 |
| 1:A:106:C:H2' | 1:A:107:G:H8 | 1.75 | 0.49 |
| 3:W:14:A:C5 | 3:W:22:G:N2 | 2.80 | 0.49 |
| 1:A:778:G:H2' | 1:A:779:C:H6 | 1.77 | 0.49 |
| 3:W:30:G:O2' | 3:W:31:A:H5' | 2.12 | 0.49 |
| 1:A:416:G:H2' | 1:A:417:C:C6 | 2.48 | 0.49 |
| 22:S:15:LEU:HD22 | 22:S:33:THR:HG21 | 1.94 | 0.49 |
| 1:A:1229:A:H8 | 1:A:1229:A:O5' | 1.95 | 0.49 |
| 1:A:120:A:O5' | 1:A:120:A:C8 | 2.65 | 0.49 |
| 1:A:891:U:C5 | 1:A:906:G:C2 | 3.00 | 0.49 |
| 1:A:1179:A:H2' | 1:A:1180:A:C8 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:281:G:HO2' | 1:A:282:A:H8 | 1.60 | 0.49 |
| 18:O:42:HIS:O | 18:O:45:VAL:O | 2.30 | 0.49 |
| 5:B:71:VAL:HG11 | 5:B:170:GLU:HG2 | 1.94 | 0.49 |
| 1:A:60:A:H62 | 1:A:110:C:H42 | 1.57 | 0.49 |
| 2:V:5:A:H2' | 2:V:6:U:C6 | 2.38 | 0.49 |
| 1:A:1100:C:O2' | 1:A:1101:A:H4' | 2.12 | 0.49 |
| 1:A:92:C:H2' | 1:A:93:G:C8 | 2.47 | 0.49 |
| 7:D:101:LEU:HD22 | 7:D:138:TYR:HB3 | 1.94 | 0.49 |
| 16:M:81:LEU:HA | 16:M:84:ILE:HG12 | 1.94 | 0.49 |
| 13:J:63:PHE:CE2 | 17:N:49:HIS:CE1 | 2.94 | 0.49 |
| 1:A:1521:G:H2' | 1:A:1522:U:H6 | 1.77 | 0.49 |
| 1:A:676:A:H2' | 1:A:677:U:C6 | 2.47 | 0.49 |
| 1:A:375:U:H4' | 19:P:6:LEU:HD23 | 1.94 | 0.49 |
| 1:A:668:G:N3 | 18:O:46:HIS:CE1 | 2.80 | 0.49 |
| 10:G:74:GLU:HG2 | 10:G:75:VAL:N | 2.25 | 0.49 |
| 1:A:741:G:O2' | 18:O:55:GLY:HA3 | 2.13 | 0.49 |
| 2:V:59:U:O2 | 2:V:59:U:H2' | 2.10 | 0.49 |
| 1:A:981:U:O5' | 1:A:981:U:H6 | 1.95 | 0.49 |
| 1:A:1464:G:H2' | 1:A:1465:C:C6 | 2.48 | 0.49 |
| 1:A:989:C:H4' | 1:A:1016:A:C2 | 2.47 | 0.49 |
| 1:A:986:A:H2' | 1:A:987:G:C8 | 2.47 | 0.49 |
| 1:A:406:G:H4' | 7:D:5:ILE:CG2 | 2.26 | 0.49 |
| 1:A:1326:C:H5'' | 24:U:19:GLY:HA3 | 1.88 | 0.49 |
| 5:B:112:VAL:HA | 5:B:115:LEU:HB3 | 1.94 | 0.49 |
| 1:A:1229:A:C2' | 16:M:125:ARG:NH1 | 2.76 | 0.49 |
| 17:N:27:CYS:N | 17:N:43:CYS:HB3 | 2.27 | 0.49 |
| 13:J:11:PHE:CE2 | 13:J:65:LEU:HG | 2.47 | 0.49 |
| 5:B:152:PHE:CD1 | 5:B:152:PHE:C | 2.86 | 0.49 |
| 1:A:404:U:C5 | 7:D:2:GLY:CA | 2.94 | 0.49 |
| 17:N:16:PHE:O | 17:N:18:VAL:N | 2.45 | 0.49 |
| 1:A:1093:A:C2 | 1:A:1109:C:O2 | 2.65 | 0.49 |
| 1:A:20:U:H1' | 1:A:572:A:N3 | 2.28 | 0.49 |
| 1:A:767:A:N6 | 1:A:813:U:N3 | 2.57 | 0.49 |
| 7:D:62:GLN:NE2 | 7:D:65:ARG:HD3 | 2.27 | 0.49 |
| 1:A:144:G:H1 | 1:A:178:C:H42 | 1.60 | 0.49 |
| 1:A:112:G:C5' | 1:A:389:A:H4' | 2.43 | 0.49 |
| 2:V:24:G:H2' | 2:V:25:C:H6 | 1.77 | 0.49 |
| 1:A:291:C:H3' | 1:A:305:G:H22 | 1.78 | 0.49 |
| 3:W:72:C:C3' | 3:W:73:A:H5' | 2.39 | 0.49 |
| 9:F:95:GLU:CB | 9:F:96:PRO:HD3 | 2.29 | 0.49 |
| 1:A:18:C:N3 | 1:A:918:A:N1 | 2.60 | 0.49 |
| 1:A:1370:G:H5'' | 12:I:12:GLU:CD | 2.33 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:106:C:H2' | 1:A:107:G:C8 | 2.47 | 0.49 |
| 22:S:44:MET:HA | 22:S:47:HIS:CD2 | 2.48 | 0.49 |
| 1:A:815:A:C6 | 1:A:1508:G:N2 | 2.80 | 0.49 |
| 7:D:3:ARG:HD2 | 7:D:118:ARG:NH1 | 2.27 | 0.49 |
| 1:A:1370:G:H5'' | 12:I:12:GLU:HG3 | 1.93 | 0.49 |
| 1:A:453:A:H4' | 19:P:72:ARG:HD2 | 1.94 | 0.49 |
| 1:A:484:G:C8 | 1:A:486:U:C2 | 3.00 | 0.49 |
| 1:A:1378:C:O2 | 1:A:1378:C:H2' | 2.13 | 0.49 |
| 1:A:1320:C:H1' | 22:S:73:GLU:CA | 2.43 | 0.49 |
| 7:D:68:TYR:CZ | 7:D:97:LEU:HB3 | 2.48 | 0.49 |
| 1:A:1004:A:C3' | 1:A:1025:U:N3 | 2.75 | 0.49 |
| 1:A:19:C:O2' | 1:A:572:A:N1 | 2.34 | 0.49 |
| 6:C:122:GLU:HA | 6:C:125:GLU:CG | 2.43 | 0.49 |
| 1:A:1374:A:OP1 | 10:G:36:LYS:NZ | 2.44 | 0.49 |
| 1:A:596:C:H2' | 1:A:597:G:H8 | 1.78 | 0.49 |
| 1:A:401:C:H1' | 1:A:622:A:H1' | 1.94 | 0.49 |
| 1:A:1233:G:H2' | 1:A:1234:C:C6 | 2.47 | 0.49 |
| 1:A:130:A:H8 | 1:A:130:A:OP1 | 1.95 | 0.49 |
| 1:A:960:U:H4' | 1:A:961:U:OP2 | 2.11 | 0.49 |
| 1:A:958:A:C2 | 22:S:55:LYS:CB | 2.91 | 0.49 |
| 1:A:1328:C:C3' | 16:M:28:ALA:HB3 | 2.42 | 0.49 |
| 1:A:1250:A:C2 | 1:A:1370:G:O2' | 2.64 | 0.49 |
| 1:A:1270:C:OP2 | 24:U:24:ARG:NH2 | 2.45 | 0.49 |
| 21:R:58:LEU:HD22 | 21:R:62:GLU:HG2 | 1.95 | 0.49 |
| 12:I:115:GLY:O | 12:I:116:LYS:C | 2.52 | 0.49 |
| 1:A:1319:A:H5' | 22:S:5:LEU:CD2 | 2.43 | 0.48 |
| 16:M:77:ASN:O | 16:M:81:LEU:HD13 | 2.13 | 0.48 |
| 16:M:81:LEU:HD21 | 16:M:88:ARG:HE | 1.76 | 0.48 |
| 13:J:47:PHE:HE1 | 13:J:63:PHE:HB2 | 1.78 | 0.48 |
| 17:N:26:ARG:HH12 | 17:N:46:GLU:HB2 | 1.78 | 0.48 |
| 7:D:3:ARG:CB | 7:D:118:ARG:NH1 | 2.76 | 0.48 |
| 1:A:1406:U:H1' | 1:A:1518:A:O4' | 2.13 | 0.48 |
| 7:D:100:ARG:HB2 | 7:D:103:ASN:HB3 | 1.95 | 0.48 |
| 12:I:104:ARG:O | 12:I:105:ASP:HB2 | 2.13 | 0.48 |
| 1:A:1149:C:OP1 | 12:I:9:ARG:HD3 | 2.13 | 0.48 |
| 1:A:585:G:O2' | 1:A:879:C:C5' | 2.56 | 0.48 |
| 1:A:1073:U:C2' | 1:A:1074:G:H5' | 2.42 | 0.48 |
| 7:D:79:PHE:HB2 | 7:D:93:PHE:CZ | 2.48 | 0.48 |
| 7:D:126:ILE:O | 7:D:132:ARG:HB3 | 2.13 | 0.48 |
| 20:Q:90:ILE:HA | 20:Q:93:GLN:HB2 | 1.95 | 0.48 |
| 20:Q:29:HIS:N | 20:Q:33:GLY:O | 2.46 | 0.48 |
| 1:A:1328:C:P | 24:U:20:LYS:HZ3 | 2.36 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 2.09 | 0.48 |
| 6:C:8:ILE:CG2 | 17:N:50:LYS:O | 2.61 | 0.48 |
| 1:A:671:G:C2 | 1:A:672:U:C2 | 3.00 | 0.48 |
| 1:A:1067:A:H3' | 1:A:1093:A:O3' | 2.12 | 0.48 |
| 13:J:8:LEU:HB2 | 13:J:70:ARG:HB2 | 1.94 | 0.48 |
| 1:A:376:G:H5'' | 19:P:5:ARG:HD2 | 1.94 | 0.48 |
| 15:L:54:LYS:CG | 15:L:75:HIS:CE1 | 2.88 | 0.48 |
| 1:A:323:U:H3 | 1:A:327:A:N6 | 2.10 | 0.48 |
| 5:B:73:THR:HG21 | 5:B:97:TRP:H | 1.77 | 0.48 |
| 1:A:686:U:H1' | 14:K:42:TRP:NE1 | 2.27 | 0.48 |
| 1:A:1172:C:H2' | 1:A:1173:G:H8 | 1.78 | 0.48 |
| 1:A:1225:A:OP2 | 1:A:1226:C:C5 | 2.66 | 0.48 |
| 1:A:1395:C:H4' | 1:A:1401:G:O2' | 2.12 | 0.48 |
| 1:A:1107:C:OP1 | 6:C:172:ARG:CA | 2.61 | 0.48 |
| 1:A:945:G:N2 | 1:A:1337:G:C2 | 2.81 | 0.48 |
| 1:A:1279:A:N3 | 1:A:1279:A:H2' | 2.26 | 0.48 |
| 1:A:1305:G:O2' | 1:A:1331:G:N2 | 2.46 | 0.48 |
| 7:D:201:GLN:O | 7:D:205:GLU:CG | 2.61 | 0.48 |
| 1:A:956:U:O2' | 22:S:80:TYR:HA | 2.14 | 0.48 |
| 16:M:77:ASN:HA | 16:M:80:ARG:HB3 | 1.95 | 0.48 |
| 1:A:1317:C:C5 | 17:N:16:PHE:CG | 3.01 | 0.48 |
| 1:A:235:C:H2' | 1:A:236:G:H8 | 1.78 | 0.48 |
| 1:A:17:U:H3 | 1:A:918:A:N6 | 2.10 | 0.48 |
| 6:C:121:ALA:O | 6:C:125:GLU:HG2 | 2.13 | 0.48 |
| 1:A:813:U:OP1 | 1:A:904:C:C5' | 2.60 | 0.48 |
| 20:Q:64:PRO:HB3 | 20:Q:70:ARG:HH11 | 1.77 | 0.48 |
| 1:A:1455:G:O3' | 23:T:28:ALA:HB1 | 2.13 | 0.48 |
| 1:A:834:C:H2' | 1:A:835:U:C6 | 2.48 | 0.48 |
| 1:A:1226:C:H5'' | 16:M:103:THR:O | 2.13 | 0.48 |
| 16:M:92:HIS:CE1 | 16:M:98:VAL:HG23 | 2.46 | 0.48 |
| 1:A:1327:C:OP1 | 24:U:20:LYS:HG2 | 2.13 | 0.48 |
| 13:J:47:PHE:CE1 | 13:J:63:PHE:HB2 | 2.49 | 0.48 |
| 11:H:29:SER:CB | 11:H:32:LYS:NZ | 2.77 | 0.48 |
| 1:A:794:A:O2' | 1:A:1521:G:O3' | 2.31 | 0.48 |
| 5:B:70:PHE:O | 5:B:92:TYR:HA | 2.14 | 0.48 |
| 1:A:526:C:O5' | 1:A:526:C:H6 | 1.96 | 0.48 |
| 18:O:64:ARG:HA | 18:O:67:LEU:HD12 | 1.94 | 0.48 |
| 1:A:1014:A:C2 | 22:S:34:TRP:CH2 | 3.01 | 0.48 |
| 1:A:988:G:H21 | 1:A:1016:A:H1' | 1.76 | 0.48 |
| 16:M:91:ARG:HH12 | 16:M:103:THR:HB | 1.78 | 0.48 |
| 1:A:116:A:H2' | 1:A:117:G:O4' | 2.13 | 0.48 |
| 1:A:1206:G:H4' | 6:C:194:GLY:N | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:878:G:H5'' | 11:H:89:PRO:O | 2.13 | 0.48 |
| 8:E:152:ARG:HA | 11:H:64:LYS:NZ | 2.28 | 0.48 |
| 1:A:67:C:H4' | 1:A:172:A:H4' | 1.95 | 0.48 |
| 1:A:599:C:H4' | 11:H:96:GLY:HA3 | 1.94 | 0.48 |
| 7:D:140:VAL:HG13 | 7:D:144:ASP:HB2 | 1.95 | 0.48 |
| 8:E:87:SER:OG | 8:E:130:ASN:HB3 | 2.13 | 0.48 |
| 12:I:20:ARG:O | 12:I:60:ASP:N | 2.47 | 0.48 |
| 12:I:26:VAL:HB | 12:I:33:PHE:HB2 | 1.96 | 0.48 |
| 1:A:1320:C:C5 | 22:S:70:LYS:HD2 | 2.48 | 0.48 |
| 1:A:405:U:P | 7:D:5:ILE:HD13 | 2.53 | 0.48 |
| 1:A:1340:A:O4' | 2:V:31:A:O2' | 2.15 | 0.48 |
| 1:A:1061:G:H5'' | 13:J:59:SER:H | 1.79 | 0.48 |
| 6:C:12:LEU:HD11 | 17:N:51:GLY:N | 2.28 | 0.48 |
| 1:A:462:G:N2 | 19:P:82:GLN:HE21 | 1.90 | 0.48 |
| 1:A:273:A:H2' | 1:A:274:A:O4' | 2.13 | 0.48 |
| 15:L:117:ARG:HB2 | 15:L:117:ARG:NH1 | 2.28 | 0.48 |
| 11:H:36:LEU:HD13 | 11:H:48:TYR:HB2 | 1.96 | 0.48 |
| 1:A:594:G:H2' | 1:A:595:G:O4' | 2.14 | 0.48 |
| 6:C:182:ILE:HG12 | 6:C:203:PHE:HA | 1.96 | 0.48 |
| 5:B:82:ARG:HB2 | 5:B:94:ASN:HD21 | 1.79 | 0.48 |
| 1:A:671:G:H2' | 1:A:672:U:C6 | 2.49 | 0.48 |
| 1:A:1314:C:H41 | 22:S:4:SER:CA | 2.26 | 0.48 |
| 1:A:950:U:H1' | 1:A:971:G:N3 | 2.29 | 0.48 |
| 2:V:71:G:H2' | 2:V:72:C:H6 | 1.77 | 0.48 |
| 1:A:1259:C:O2' | 1:A:1284:C:H4' | 2.13 | 0.48 |
| 6:C:122:GLU:HA | 6:C:125:GLU:HG3 | 1.96 | 0.48 |
| 1:A:482:A:N3 | 1:A:482:A:H2' | 2.27 | 0.48 |
| 1:A:413:G:H2' | 1:A:413:G:N3 | 2.28 | 0.48 |
| 6:C:106:VAL:O | 6:C:107:GLN:O | 2.23 | 0.48 |
| 2:V:20:G:N3 | 2:V:20:G:C2' | 2.77 | 0.48 |
| 23:T:81:LYS:HA | 23:T:84:LEU:HB3 | 1.95 | 0.48 |
| 21:R:29:PHE:HE1 | 21:R:36:ASN:OD1 | 1.97 | 0.48 |
| 1:A:109:A:N6 | 1:A:326:G:C6 | 2.82 | 0.48 |
| 14:K:67:ASP:HA | 14:K:70:LYS:HD2 | 1.95 | 0.48 |
| 1:A:1060:C:C1' | 13:J:52:GLY:HA3 | 2.44 | 0.48 |
| 13:J:60:ARG:O | 13:J:61:GLU:CB | 2.62 | 0.48 |
| 1:A:296:U:O2 | 1:A:556:C:O2' | 2.32 | 0.48 |
| 2:V:49:C:O2 | 2:V:49:C:H2' | 2.12 | 0.48 |
| 1:A:719:C:H3' | 1:A:720:C:C6 | 2.49 | 0.48 |
| 1:A:1504:G:H3' | 1:A:1504:G:OP1 | 2.14 | 0.48 |
| 1:A:928:G:O3' | 1:A:1533:C:N4 | 2.47 | 0.48 |
| 1:A:1226:C:N4 | 16:M:104:ARG:HG3 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:W:33:U:O2 | 3:W:35:A:H5' | 2.13 | 0.48 |
| 1:A:1517:G:H3' | 1:A:1518:A:C8 | 2.49 | 0.48 |
| 1:A:190(E):U:H3 | 20:Q:63:ARG:CB | 2.26 | 0.48 |
| 5:B:180:LEU:O | 5:B:181:PHE:CB | 2.58 | 0.48 |
| 1:A:429:U:H4' | 1:A:430:A:O5' | 2.13 | 0.48 |
| 7:D:173:TRP:CD1 | 7:D:189:PRO:HB3 | 2.49 | 0.48 |
| 11:H:64:LYS:HG2 | 11:H:79:VAL:HG21 | 1.95 | 0.48 |
| 7:D:30:LYS:O | 7:D:32:ALA:N | 2.39 | 0.48 |
| 1:A:68:G:O4' | 1:A:171:A:H1' | 2.14 | 0.48 |
| 1:A:545:C:H5'' | 7:D:72:GLU:HG2 | 1.95 | 0.48 |
| 11:H:6:ILE:O | 11:H:10:LEU:HG | 2.13 | 0.48 |
| 1:A:1222:G:P | 1:A:1322:C:C5 | 3.07 | 0.47 |
| 7:D:22:LYS:O | 7:D:113:SER:CB | 2.49 | 0.47 |
| 7:D:8:VAL:HG21 | 7:D:115:ARG:HD3 | 1.95 | 0.47 |
| 2:V:7:U:C4 | 2:V:49:C:C4 | 3.02 | 0.47 |
| 11:H:17:THR:HB | 11:H:18:ARG:NH2 | 2.28 | 0.47 |
| 2:V:60:C:OP2 | 2:V:61:C:C5 | 2.68 | 0.47 |
| 15:L:41:ARG:HG2 | 15:L:42:THR:H | 1.78 | 0.47 |
| 7:D:76:ARG:O | 7:D:79:PHE:HB3 | 2.13 | 0.47 |
| 16:M:22:ILE:HD12 | 16:M:25:ILE:HD12 | 1.95 | 0.47 |
| 1:A:1317:C:C2' | 22:S:10:PHE:CD2 | 2.97 | 0.47 |
| 1:A:1406:U:H1' | 1:A:1518:A:C1' | 2.44 | 0.47 |
| 1:A:19:C:C2 | 1:A:917:G:N2 | 2.83 | 0.47 |
| 1:A:1374:A:P | 10:G:36:LYS:HZ3 | 2.37 | 0.47 |
| 2:V:19:G:H1' | 2:V:57:G:N2 | 2.29 | 0.47 |
| 1:A:1540:U:H2' | 1:A:1541:U:O4' | 2.13 | 0.47 |
| 10:G:49:ILE:HA | 10:G:52:GLU:HB2 | 1.96 | 0.47 |
| 1:A:1220:G:C3' | 22:S:36:ARG:HD3 | 2.44 | 0.47 |
| 13:J:51:ARG:HA | 17:N:45:ARG:CZ | 2.45 | 0.47 |
| 17:N:24:CYS:HB3 | 17:N:40:CYS:HB3 | 1.79 | 0.47 |
| 6:C:12:LEU:CD1 | 17:N:51:GLY:HA3 | 2.44 | 0.47 |
| 15:L:23:LYS:N | 15:L:24:VAL:N | 2.60 | 0.47 |
| 1:A:312:C:H2' | 1:A:313:A:H8 | 1.80 | 0.47 |
| 1:A:31:G:H5' | 1:A:306:G:N1 | 2.28 | 0.47 |
| 1:A:820:U:C3' | 1:A:821:G:P | 3.00 | 0.47 |
| 1:A:1085:U:O4' | 1:A:1094:G:C6 | 2.67 | 0.47 |
| 1:A:1068:G:OP2 | 1:A:1094:G:H8 | 1.97 | 0.47 |
| 2:V:56:C:C5 | 2:V:57:G:C5 | 3.02 | 0.47 |
| 1:A:1242:C:O5' | 1:A:1242:C:H6 | 1.97 | 0.47 |
| 12:I:48:GLU:N | 12:I:49:PRO:HD2 | 2.29 | 0.47 |
| 1:A:692:U:H5 | 14:K:26:ASN:HD21 | 1.61 | 0.47 |
| 1:A:1221:G:H5'' | 1:A:1321:C:C2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 7:D:21:LEU:O | 7:D:114:ARG:N | 2.47 | 0.47 |
| 1:A:1060:C:H4' | 13:J:52:GLY:CA | 2.44 | 0.47 |
| 1:A:39:G:C8 | 1:A:498:U:N3 | 2.82 | 0.47 |
| 1:A:952:U:C2 | 16:M:126:LYS:O | 2.59 | 0.47 |
| 1:A:1046:A:C3' | 1:A:1047:G:P | 3.00 | 0.47 |
| 1:A:1286:A:H62 | 1:A:1354:C:C5' | 2.16 | 0.47 |
| 11:H:29:SER:HB2 | 11:H:32:LYS:NZ | 2.28 | 0.47 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.79 | 0.47 |
| 15:L:85:ILE:HA | 15:L:100:ILE:HA | 1.95 | 0.47 |
| 9:F:48:LEU:HD13 | 9:F:52:ILE:HB | 1.97 | 0.47 |
| 1:A:191:G:N2 | 23:T:103:GLY:O | 2.46 | 0.47 |
| 1:A:1328:C:P | 16:M:28:ALA:HB1 | 2.53 | 0.47 |
| 1:A:1060:C:C4' | 13:J:52:GLY:CA | 2.92 | 0.47 |
| 6:C:9:GLY:HA3 | 17:N:49:HIS:O | 2.01 | 0.47 |
| 1:A:765:G:N2 | 1:A:816:A:C2 | 2.74 | 0.47 |
| 11:H:98:LYS:HG2 | 11:H:98:LYS:O | 2.15 | 0.47 |
| 1:A:33:A:H2' | 1:A:34:C:C6 | 2.49 | 0.47 |
| 1:A:1511:G:H2' | 1:A:1512:U:O4' | 2.14 | 0.47 |
| 1:A:1150:U:H1' | 1:A:1280:A:N6 | 2.29 | 0.47 |
| 13:J:24:VAL:O | 13:J:28:ARG:HG3 | 2.14 | 0.47 |
| 1:A:920:U:O4' | 1:A:1080:A:N1 | 2.47 | 0.47 |
| 15:L:12:ARG:HD2 | 15:L:13:LYS:HZ2 | 1.79 | 0.47 |
| 1:A:197:A:O5' | 1:A:197:A:H8 | 1.98 | 0.47 |
| 5:B:19:HIS:CE1 | 5:B:206:ASP:HB2 | 2.50 | 0.47 |
| 16:M:94:ARG:HB2 | 16:M:96:LEU:HD21 | 1.96 | 0.47 |
| 16:M:88:ARG:HB2 | 16:M:98:VAL:HG13 | 1.95 | 0.47 |
| 24:U:16:GLY:O | 24:U:17:THR:C | 2.52 | 0.47 |
| 6:C:8:ILE:O | 6:C:12:LEU:HG | 2.14 | 0.47 |
| 1:A:403:C:OP1 | 7:D:3:ARG:NH1 | 2.47 | 0.47 |
| 1:A:18:C:C4 | 1:A:918:A:N1 | 2.82 | 0.47 |
| 1:A:571:U:C4 | 1:A:865:A:N1 | 2.83 | 0.47 |
| 19:P:6:LEU:HA | 19:P:18:ARG:O | 2.15 | 0.47 |
| 1:A:192:U:H2' | 1:A:193:C:C6 | 2.50 | 0.47 |
| 1:A:252:U:O2' | 1:A:275:G:N2 | 2.48 | 0.47 |
| 1:A:528:C:N4 | 15:L:49:ASN:CG | 2.67 | 0.47 |
| 5:B:160:ASP:O | 5:B:161:ALA:CB | 2.62 | 0.47 |
| 1:A:62:U:OP1 | 1:A:385:C:O2' | 2.29 | 0.47 |
| 1:A:986:A:O4' | 22:S:55:LYS:CA | 2.55 | 0.47 |
| 7:D:19:LEU:CD2 | 7:D:67:ILE:HG12 | 2.45 | 0.47 |
| 1:A:1326:C:C4' | 24:U:19:GLY:HA2 | 2.44 | 0.47 |
| 1:A:1269:A:C5' | 24:U:19:GLY:CA | 2.91 | 0.47 |
| 1:A:1500:A:OP1 | 1:A:1508:G:OP1 | 2.32 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:277:C:OP1 | 20:Q:41:LYS:HD2 | 2.14 | 0.47 |
| 5:B:170:GLU:O | 5:B:174:VAL:HG23 | 2.13 | 0.47 |
| 1:A:737:A:H2' | 1:A:738:C:C6 | 2.50 | 0.47 |
| 7:D:173:TRP:CD2 | 7:D:189:PRO:HB3 | 2.49 | 0.47 |
| 1:A:1491:G:HO2' | 1:A:1492:A:H8 | 1.61 | 0.47 |
| 2:V:18:G:C2' | 2:V:19:G:O5' | 2.63 | 0.47 |
| 1:A:741:G:H5' | 18:O:39:LEU:HD11 | 1.96 | 0.47 |
| 5:B:152:PHE:C | 5:B:152:PHE:HD1 | 2.17 | 0.47 |
| 12:I:115:GLY:HA2 | 13:J:57:LYS:NZ | 2.30 | 0.47 |
| 6:C:36:ASP:HA | 6:C:39:ILE:HD12 | 1.97 | 0.47 |
| 2:V:11:C:H2' | 2:V:12:U:H6 | 1.80 | 0.47 |
| 1:A:1198:G:H2' | 1:A:1199:U:O4' | 2.14 | 0.47 |
| 1:A:826:C:C4' | 11:H:12:ARG:HG2 | 2.41 | 0.47 |
| 1:A:3(A):G:O6 | 1:A:1038:C:C2 | 2.68 | 0.47 |
| 1:A:32:A:C6 | 1:A:33:A:C6 | 3.03 | 0.47 |
| 1:A:60:A:C2 | 1:A:107:G:N3 | 2.83 | 0.47 |
| 21:R:80:PRO:HB2 | 21:R:83:GLU:HB2 | 1.96 | 0.47 |
| 1:A:796:C:OP1 | 14:K:123:LYS:HD3 | 2.13 | 0.47 |
| 15:L:60:LEU:HD23 | 15:L:64:TYR:CB | 2.44 | 0.47 |
| 1:A:1328:C:OP1 | 16:M:28:ALA:HB1 | 2.15 | 0.47 |
| 1:A:817:C:H4' | 1:A:818:G:OP1 | 2.14 | 0.47 |
| 1:A:1254:C:H2' | 1:A:1255:G:H8 | 1.79 | 0.47 |
| 1:A:22:G:N9 | 1:A:914:A:N6 | 2.63 | 0.47 |
| 1:A:392:G:O2' | 1:A:483:C:H1' | 2.15 | 0.47 |
| 3:W:65:G:H2' | 3:W:66:A:H5' | 1.96 | 0.47 |
| 15:L:45:PRO:CD | 15:L:50:SER:HA | 2.44 | 0.47 |
| 13:J:90:LEU:N | 13:J:91:PRO:HD2 | 2.26 | 0.47 |
| 9:F:50:TYR:CZ | 21:R:77:GLY:HA2 | 2.49 | 0.47 |
| 1:A:1305:G:H21 | 1:A:1331:G:H2' | 1.80 | 0.47 |
| 5:B:28:PHE:HZ | 5:B:42:ILE:HD11 | 1.80 | 0.47 |
| 1:A:834:C:H2' | 1:A:835:U:H6 | 1.80 | 0.47 |
| 1:A:1082:G:H2' | 1:A:1083:U:O4' | 2.15 | 0.47 |
| 2:V:13:C:H2' | 2:V:13:C:O2 | 2.14 | 0.47 |
| 1:A:979:C:P | 1:A:1223:C:N4 | 2.82 | 0.47 |
| 1:A:1225:A:H5' | 22:S:78:ARG:NH1 | 2.30 | 0.47 |
| 2:V:31:A:C3' | 12:I:127:LYS:HB2 | 2.45 | 0.47 |
| 1:A:450:G:O2' | 19:P:42:ARG:HD3 | 2.14 | 0.47 |
| 1:A:1180:A:O2' | 1:A:1184:G:H1' | 2.15 | 0.47 |
| 11:H:49:GLU:OE1 | 11:H:60:ARG:HB3 | 2.15 | 0.47 |
| 1:A:1344:C:H4' | 12:I:120:ARG:HB3 | 1.97 | 0.47 |
| 12:I:37:PHE:CZ | 12:I:74:ILE:HG12 | 2.50 | 0.47 |
| 1:A:95:U:H2' | 1:A:96:G:C8 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 12:I:114:TYR:CD1 | 13:J:60:ARG:HB2 | 2.51 | 0.46 |
| 1:A:39:G:C8 | 1:A:547:A:N7 | 2.84 | 0.46 |
| 6:C:48:TYR:HE1 | 6:C:122:GLU:OE2 | 1.98 | 0.46 |
| 1:A:193:C:O2' | 23:T:64:ASP:HB2 | 2.15 | 0.46 |
| 11:H:65:TYR:HA | 11:H:79:VAL:HG23 | 1.96 | 0.46 |
| 7:D:198:VAL:O | 7:D:199:ASN:HB3 | 2.15 | 0.46 |
| 22:S:13:ASP:HA | 22:S:16:LEU:HB3 | 1.96 | 0.46 |
| 1:A:187:C:Cl' | 23:T:85:MET:SD | 3.03 | 0.46 |
| 1:A:1015:A:P | 22:S:14:HIS:HE1 | 2.34 | 0.46 |
| 1:A:1308:U:H2' | 1:A:1309:G:H8 | 1.81 | 0.46 |
| 1:A:1199:U:C4' | 13:J:54:PHE:CE2 | 2.98 | 0.46 |
| 3:W:72:C:H2' | 3:W:73:A:O5' | 2.15 | 0.46 |
| 2:V:7:U:C3' | 2:V:8:U:P | 2.99 | 0.46 |
| 5:B:54:THR:HG22 | 5:B:58:ILE:HD11 | 1.97 | 0.46 |
| 1:A:1279:A:H5'' | 1:A:1280:A:OP1 | 2.15 | 0.46 |
| 1:A:659:U:H2' | 1:A:660:G:C8 | 2.50 | 0.46 |
| 5:B:239:VAL:HG12 | 5:B:240:GLN:N | 2.28 | 0.46 |
| 6:C:82:GLU:HG3 | 6:C:83:ARG:N | 2.30 | 0.46 |
| 1:A:1225:A:P | 16:M:104:ARG:HB2 | 2.56 | 0.46 |
| 16:M:92:HIS:CE1 | 16:M:110:ARG:HH21 | 2.33 | 0.46 |
| 1:A:1325:C:OP1 | 24:U:15:ARG:CG | 2.63 | 0.46 |
| 1:A:983:A:N7 | 1:A:1201:A:N1 | 2.61 | 0.46 |
| 1:A:303:A:H5' | 1:A:556:C:OP1 | 2.14 | 0.46 |
| 1:A:757:U:H2' | 1:A:758:G:O4' | 2.15 | 0.46 |
| 20:Q:21:VAL:CG1 | 20:Q:23:VAL:HG23 | 2.38 | 0.46 |
| 10:G:31:MET:HG2 | 10:G:32:ARG:N | 2.30 | 0.46 |
| 1:A:878:G:OP1 | 11:H:88:LYS:HB3 | 2.15 | 0.46 |
| 1:A:413:G:N1 | 7:D:36:ARG:NH1 | 2.63 | 0.46 |
| 1:A:67:C:H1' | 1:A:172:A:H1' | 1.97 | 0.46 |
| 7:D:59:ARG:CZ | 7:D:59:ARG:HA | 2.46 | 0.46 |
| 1:A:824:C:H1' | 11:H:1:MET:CA | 2.45 | 0.46 |
| 14:K:29:ILE:HG22 | 14:K:44:SER:HB2 | 1.98 | 0.46 |
| 23:T:50:GLU:H | 23:T:99:LEU:HD12 | 1.80 | 0.46 |
| 11:H:9:MET:HG3 | 11:H:26:VAL:HG21 | 1.96 | 0.46 |
| 6:C:10:PHE:CG | 6:C:10:PHE:O | 2.68 | 0.46 |
| 7:D:23:GLY:N | 7:D:113:SER:HB2 | 2.23 | 0.46 |
| 16:M:84:ILE:HG13 | 16:M:85:GLY:H | 1.80 | 0.46 |
| 1:A:1229:A:O3' | 2:V:30:G:C5' | 2.62 | 0.46 |
| 1:A:119:A:H4' | 1:A:120:A:O5' | 2.14 | 0.46 |
| 1:A:1144:G:N2 | 1:A:1146:A:H62 | 2.12 | 0.46 |
| 1:A:1373:G:O2' | 10:G:34:GLY:HA2 | 2.14 | 0.46 |
| 1:A:668:G:O2' | 18:O:46:HIS:CD2 | 2.68 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:761:G:H5'' | 20:Q:102:GLY:HA3 | 1.97 | 0.46 |
| 1:A:1053:G:C8 | 1:A:1053:G:H5'' | 2.47 | 0.46 |
| 5:B:155:LEU:HB2 | 5:B:159:PRO:HG3 | 1.97 | 0.46 |
| 12:I:45:ALA:O | 12:I:78:LYS:HG3 | 2.15 | 0.46 |
| 22:S:66:MET:HB2 | 22:S:74:PHE:CE2 | 2.50 | 0.46 |
| 1:A:1091:U:OP1 | 1:A:1172:C:H4' | 2.15 | 0.46 |
| 1:A:187:C:O4' | 23:T:85:MET:SD | 2.73 | 0.46 |
| 1:A:256:U:H2' | 1:A:257:G:O4' | 2.15 | 0.46 |
| 1:A:979:C:P | 1:A:1222:G:O6 | 2.74 | 0.46 |
| 1:A:1326:C:C5' | 24:U:19:GLY:CA | 2.83 | 0.46 |
| 1:A:1060:C:C5 | 6:C:2:GLY:C | 2.89 | 0.46 |
| 1:A:120:A:C3' | 1:A:120:A:C8 | 2.99 | 0.46 |
| 1:A:1298:C:C4' | 1:A:1299:A:P | 3.04 | 0.46 |
| 1:A:819:A:N1 | 1:A:1529:G:N7 | 2.63 | 0.46 |
| 1:A:757:U:C5' | 1:A:822:C:O2 | 2.61 | 0.46 |
| 7:D:96:LEU:HD23 | 7:D:139:ARG:NH2 | 2.30 | 0.46 |
| 11:H:63:LEU:HD22 | 11:H:63:LEU:H | 1.81 | 0.46 |
| 1:A:324:G:N2 | 1:A:327:A:H8 | 2.13 | 0.46 |
| 19:P:27:LYS:C | 19:P:29:ASP:H | 2.18 | 0.46 |
| 15:L:25:PRO:C | 15:L:27:LEU:H | 2.18 | 0.46 |
| 7:D:128:VAL:O | 7:D:130:GLY:N | 2.49 | 0.46 |
| 1:A:1443:G:H5' | 1:A:1443:G:C8 | 2.50 | 0.46 |
| 1:A:964:A:H5'' | 1:A:1198:G:O3' | 2.16 | 0.46 |
| 1:A:236:G:H5'' | 20:Q:42:TYR:OH | 2.15 | 0.46 |
| 1:A:890:G:N2 | 1:A:907:A:O5' | 2.49 | 0.46 |
| 13:J:12:ASP:O | 13:J:16:LEU:HD23 | 2.16 | 0.46 |
| 1:A:376:G:O3' | 19:P:5:ARG:NH1 | 2.48 | 0.46 |
| 1:A:597:G:O5' | 1:A:597:G:C8 | 2.68 | 0.46 |
| 11:H:35:ILE:O | 11:H:39:LEU:HD23 | 2.16 | 0.46 |
| 1:A:573:A:N3 | 1:A:883:C:C2' | 2.79 | 0.46 |
| 5:B:60:ASP:O | 5:B:64:ARG:HB3 | 2.15 | 0.46 |
| 10:G:70:LYS:HB3 | 10:G:96:GLN:HG2 | 1.96 | 0.46 |
| 5:B:160:ASP:O | 5:B:161:ALA:HB2 | 2.16 | 0.46 |
| 1:A:1429:C:H2' | 1:A:1430:C:H6 | 1.81 | 0.46 |
| 5:B:9:GLU:OE2 | 5:B:12:GLU:HG2 | 2.16 | 0.46 |
| 1:A:780:A:H8 | 1:A:780:A:O5' | 1.98 | 0.46 |
| 1:A:989:C:H4' | 1:A:1016:A:H2 | 1.81 | 0.46 |
| 16:M:23:TYR:O | 16:M:70:LEU:HD13 | 2.16 | 0.46 |
| 12:I:114:TYR:HD1 | 13:J:60:ARG:CB | 2.26 | 0.46 |
| 1:A:949:A:H2' | 1:A:950:U:C6 | 2.51 | 0.46 |
| 1:A:781:A:O3' | 1:A:1522:U:H1' | 2.16 | 0.46 |
| 1:A:1346:A:N6 | 1:A:1374:A:H3' | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1291:G:H5' | 12:I:40:LEU:CD2 | 2.45 | 0.46 |
| 1:A:1062:U:H2' | 1:A:1063:C:C5 | 2.51 | 0.46 |
| 10:G:150:ALA:HA | 14:K:59:TYR:CD2 | 2.50 | 0.46 |
| 1:A:568:G:C2 | 1:A:574:A:H2 | 2.32 | 0.46 |
| 1:A:241:C:H42 | 1:A:285:G:H1 | 1.64 | 0.46 |
| 1:A:118:U:H3' | 1:A:288:A:N6 | 2.31 | 0.46 |
| 1:A:1007:C:C2 | 1:A:1022:G:N2 | 2.83 | 0.46 |
| 1:A:1414:U:H2' | 1:A:1415:G:C8 | 2.51 | 0.46 |
| 1:A:1194:U:H4' | 8:E:22:GLY:C | 2.36 | 0.46 |
| 16:M:27:LYS:O | 16:M:28:ALA:HB2 | 2.16 | 0.46 |
| 1:A:1371:G:H5'' | 12:I:68:GLY:C | 2.35 | 0.46 |
| 7:D:14:ARG:CD | 7:D:66:ARG:NH1 | 2.74 | 0.46 |
| 18:O:32:LEU:HB2 | 18:O:63:ARG:HG2 | 1.97 | 0.46 |
| 20:Q:15:MET:HB2 | 20:Q:18:THR:HB | 1.98 | 0.46 |
| 18:O:33:THR:O | 18:O:36:ILE:HG22 | 2.16 | 0.46 |
| 1:A:690:G:H2' | 1:A:691:G:C8 | 2.50 | 0.46 |
| 22:S:47:HIS:O | 22:S:62:ILE:HG22 | 2.16 | 0.46 |
| 2:V:28:C:H2' | 2:V:29:A:H8 | 1.81 | 0.46 |
| 1:A:909:A:C2 | 1:A:910:C:H1' | 2.51 | 0.46 |
| 1:A:22:G:C2' | 1:A:913:A:N1 | 2.78 | 0.46 |
| 7:D:49:ARG:O | 7:D:51:PRO:CD | 2.56 | 0.46 |
| 1:A:1304:G:H21 | 1:A:1333:A:H62 | 1.62 | 0.46 |
| 10:G:150:ALA:HB1 | 14:K:57:THR:HG21 | 1.98 | 0.46 |
| 8:E:151:LEU:CB | 11:H:79:VAL:HG22 | 2.45 | 0.46 |
| 23:T:66:ALA:HB3 | 23:T:72:LEU:HD12 | 1.98 | 0.46 |
| 1:A:1192:C:C6 | 1:A:1192:C:C3' | 2.99 | 0.46 |
| 1:A:1220:G:C5' | 22:S:36:ARG:HG2 | 2.46 | 0.46 |
| 1:A:361(A):C:H3' | 1:A:1362:C:OP2 | 2.16 | 0.46 |
| 3:W:37:YYG:O2' | 3:W:37:YYG:H31 | 2.15 | 0.46 |
| 1:A:953:G:C4' | 16:M:124:PRO:O | 2.64 | 0.46 |
| 3:W:34:G:OP1 | 3:W:34:G:C8 | 2.64 | 0.46 |
| 1:A:500:G:O2' | 1:A:548:G:N2 | 2.49 | 0.46 |
| 1:A:939:G:H5'' | 10:G:102:ARG:NH1 | 2.30 | 0.46 |
| 1:A:909:A:H3' | 1:A:910:C:C6 | 2.50 | 0.46 |
| 1:A:863:U:H2' | 1:A:865:A:OP2 | 2.16 | 0.46 |
| 1:A:1143:G:H2' | 1:A:1144:G:C8 | 2.51 | 0.46 |
| 5:B:181:PHE:CD1 | 11:H:71:GLY:HA3 | 2.51 | 0.46 |
| 1:A:641:U:C4' | 11:H:115:SER:OG | 2.63 | 0.46 |
| 1:A:721:G:H4' | 1:A:722:A:O4' | 2.16 | 0.46 |
| 5:B:80:ILE:HG23 | 5:B:212:GLN:HG2 | 1.98 | 0.46 |
| 1:A:302:G:H5'' | 1:A:302:G:C8 | 2.50 | 0.45 |
| 1:A:51:A:H61 | 1:A:314:C:H1' | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 12:I:67:GLY:O | 12:I:73:GLN:NE2 | 2.45 | 0.45 |
| 1:A:370:C:HO2' | 1:A:482:A:HO2' | 1.58 | 0.45 |
| 1:A:274:A:O2' | 1:A:275:G:O4' | 2.33 | 0.45 |
| 19:P:20:VAL:HG11 | 19:P:32:TYR:HB3 | 1.97 | 0.45 |
| 3:W:7:U:O2' | 3:W:49:C:OP2 | 2.29 | 0.45 |
| 8:E:102:ALA:O | 8:E:107:ARG:NH2 | 2.49 | 0.45 |
| 6:C:52:LEU:HA | 6:C:70:VAL:HG22 | 1.96 | 0.45 |
| 1:A:948:C:OP1 | 16:M:108:ARG:N | 2.49 | 0.45 |
| 2:V:27:C:H2' | 2:V:28:C:H6 | 1.81 | 0.45 |
| 1:A:246:A:O2' | 1:A:247:G:OP2 | 2.28 | 0.45 |
| 23:T:45:GLN:HG2 | 23:T:91:LEU:HD22 | 1.99 | 0.45 |
| 5:B:69:LEU:HD23 | 5:B:91:PRO:HB2 | 1.98 | 0.45 |
| 16:M:11:ARG:HH12 | 16:M:46:LYS:HD2 | 1.81 | 0.45 |
| 1:A:868:C:H1' | 1:A:873:A:C4 | 2.51 | 0.45 |
| 1:A:687:A:O2' | 1:A:688:G:O5' | 2.32 | 0.45 |
| 1:A:304:U:H2' | 1:A:305:G:H8 | 1.81 | 0.45 |
| 7:D:25:ARG:C | 7:D:27:TYR:N | 2.69 | 0.45 |
| 1:A:953:G:H4' | 16:M:124:PRO:HB2 | 1.97 | 0.45 |
| 1:A:411:A:H2' | 1:A:413:G:H1' | 1.98 | 0.45 |
| 1:A:451:A:H1' | 1:A:452:A:C8 | 2.51 | 0.45 |
| 21:R:62:GLU:HB3 | 21:R:66:LEU:HD23 | 1.98 | 0.45 |
| 1:A:573:A:H2 | 1:A:883:C:O2 | 1.99 | 0.45 |
| 1:A:1409:C:H42 | 1:A:1491:G:H1 | 1.64 | 0.45 |
| 1:A:1490:C:C6 | 1:A:1490:C:H5'' | 2.48 | 0.45 |
| 1:A:686:U:H1' | 14:K:42:TRP:HE1 | 1.79 | 0.45 |
| 1:A:1443:G:H8 | 1:A:1443:G:H5' | 1.81 | 0.45 |
| 13:J:27:ALA:HB2 | 13:J:85:LEU:HD21 | 1.99 | 0.45 |
| 1:A:1034:G:H2' | 1:A:1035:A:C8 | 2.52 | 0.45 |
| 15:L:69:TYR:HB2 | 15:L:90:VAL:HG21 | 1.99 | 0.45 |
| 13:J:40:LEU:HB3 | 13:J:41:PRO:HD2 | 1.97 | 0.45 |
| 7:D:20:TYR:HA | 7:D:31:CYS:SG | 2.56 | 0.45 |
| 16:M:23:TYR:CD2 | 16:M:70:LEU:HB3 | 2.51 | 0.45 |
| 1:A:1406:U:H1' | 1:A:1518:A:C4' | 2.47 | 0.45 |
| 1:A:944:G:C2' | 1:A:945:G:H5' | 2.47 | 0.45 |
| 8:E:151:LEU:HB3 | 11:H:79:VAL:HG22 | 1.99 | 0.45 |
| 1:A:112:G:H4' | 1:A:389:A:O5' | 2.17 | 0.45 |
| 1:A:741:G:C5' | 18:O:39:LEU:HD11 | 2.46 | 0.45 |
| 1:A:228:A:O2' | 19:P:62:VAL:HG21 | 2.16 | 0.45 |
| 23:T:76:ALA:HA | 23:T:79:ARG:NH1 | 2.31 | 0.45 |
| 17:N:39:LEU:HD22 | 17:N:43:CYS:HB2 | 1.99 | 0.45 |
| 1:A:1070:U:OP1 | 8:E:18:ARG:CZ | 2.65 | 0.45 |
| 1:A:1255:G:H21 | 1:A:1258:G:H22 | 1.57 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 9:F:62:TRP:HB3 | 21:R:35:ARG:HH12 | 1.80 | 0.45 |
| 1:A:1236:A:H5' | 1:A:1304:G:H5'' | 1.98 | 0.45 |
| 1:A:1525:G:H2' | 1:A:1526:G:O4' | 2.16 | 0.45 |
| 1:A:323:U:O4 | 1:A:327:A:N7 | 2.49 | 0.45 |
| 15:L:32:PHE:HB3 | 15:L:84:LEU:HD21 | 1.98 | 0.45 |
| 1:A:531:U:H4' | 1:A:532:A:C5' | 2.46 | 0.45 |
| 17:N:12:ARG:O | 17:N:13:THR:C | 2.54 | 0.45 |
| 1:A:935:A:H2' | 1:A:936:C:C6 | 2.51 | 0.45 |
| 1:A:1329:A:C5' | 16:M:25:ILE:C | 2.74 | 0.45 |
| 1:A:1329:A:C5' | 16:M:26:GLY:CA | 2.79 | 0.45 |
| 1:A:1229:A:H4' | 2:V:29:A:O3' | 2.16 | 0.45 |
| 6:C:5:ILE:HG21 | 13:J:61:GLU:OE2 | 2.17 | 0.45 |
| 1:A:923:A:OP1 | 8:E:21:ALA:HB2 | 2.16 | 0.45 |
| 7:D:3:ARG:HD2 | 7:D:118:ARG:HH12 | 1.82 | 0.45 |
| 1:A:1070:U:C5 | 1:A:1085:U:C4 | 3.05 | 0.45 |
| 1:A:426:G:O2' | 7:D:42:GLN:HG3 | 2.16 | 0.45 |
| 1:A:413:G:H1 | 7:D:36:ARG:NH1 | 2.15 | 0.45 |
| 1:A:267:C:OP2 | 20:Q:67:LYS:HD3 | 2.17 | 0.45 |
| 1:A:1089:G:O2' | 1:A:1169:A:H2 | 2.00 | 0.45 |
| 1:A:340:U:H2' | 1:A:341:C:C6 | 2.52 | 0.45 |
| 5:B:153:ARG:HH22 | 5:B:156:LYS:HB2 | 1.82 | 0.45 |
| 23:T:30:LYS:HA | 23:T:33:ILE:HD12 | 1.99 | 0.45 |
| 1:A:1496:C:H2' | 1:A:1497:G:O4' | 2.15 | 0.45 |
| 1:A:1220:G:O2' | 22:S:36:ARG:CD | 2.58 | 0.45 |
| 1:A:1060:C:C5 | 6:C:2:GLY:CA | 3.00 | 0.45 |
| 1:A:1395:C:O2' | 1:A:1398:A:H4' | 2.17 | 0.45 |
| 7:D:70:ILE:CD1 | 7:D:100:ARG:NH2 | 2.80 | 0.45 |
| 11:H:11:THR:HA | 11:H:14:ARG:HD2 | 1.99 | 0.45 |
| 1:A:1189:C:H5'' | 1:A:1190:G:P | 2.56 | 0.45 |
| 1:A:280:C:H1' | 20:Q:38:ARG:NE | 2.32 | 0.45 |
| 1:A:673:G:N2 | 1:A:734:G:H1' | 2.31 | 0.45 |
| 1:A:501:C:H6 | 1:A:501:C:H3' | 1.82 | 0.45 |
| 1:A:828:A:H2' | 1:A:829:G:O4' | 2.15 | 0.45 |
| 1:A:160:A:H1' | 1:A:344:A:H62 | 1.82 | 0.45 |
| 1:A:1219:U:O2' | 22:S:35:SER:N | 2.50 | 0.45 |
| 1:A:1320:C:H4' | 22:S:73:GLU:CD | 2.37 | 0.45 |
| 1:A:1396:A:O2' | 1:A:1397:C:OP2 | 2.31 | 0.45 |
| 1:A:450:G:N7 | 1:A:481:G:C6 | 2.85 | 0.45 |
| 12:I:9:ARG:HB3 | 12:I:104:ARG:HE | 1.81 | 0.45 |
| 1:A:942:G:H2' | 1:A:943:U:C6 | 2.52 | 0.45 |
| 1:A:768:A:H2 | 1:A:1512:U:H4' | 1.82 | 0.45 |
| 10:G:153:HIS:ND1 | 14:K:58:PRO:HG2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 14:K:103:LEU:O | 14:K:104:GLN:C | 2.55 | 0.45 |
| 1:A:579:G:C4' | 1:A:728:A:H1' | 2.47 | 0.45 |
| 14:K:24:SER:C | 14:K:26:ASN:H | 2.19 | 0.45 |
| 1:A:1438:G:OP1 | 23:T:34:LYS:HE3 | 2.17 | 0.45 |
| 24:U:20:LYS:HG3 | 24:U:21:TYR:N | 2.32 | 0.45 |
| 1:A:1197:G:P | 1:A:1197:G:C8 | 3.10 | 0.45 |
| 8:E:20:GLN:OE1 | 8:E:21:ALA:N | 2.49 | 0.45 |
| 17:N:27:CYS:H | 17:N:43:CYS:HB3 | 1.81 | 0.45 |
| 1:A:950:U:H5'' | 16:M:102:ARG:HH22 | 1.82 | 0.45 |
| 1:A:1517:G:H3' | 1:A:1518:A:H8 | 1.80 | 0.45 |
| 1:A:427:U:H1' | 1:A:541:G:OP1 | 2.17 | 0.45 |
| 1:A:3(A):G:C2 | 1:A:1038:C:H1' | 2.52 | 0.45 |
| 19:P:7:ALA:N | 19:P:18:ARG:H | 2.14 | 0.45 |
| 1:A:574:A:O5' | 1:A:574:A:H8 | 2.00 | 0.45 |
| 6:C:156:ARG:HD3 | 6:C:193:TYR:O | 2.16 | 0.45 |
| 11:H:87:SER:HB3 | 11:H:92:ARG:HA | 1.99 | 0.45 |
| 1:A:190(I):G:H2' | 1:A:190(J):U:C6 | 2.51 | 0.45 |
| 18:O:3:ILE:H | 18:O:3:ILE:HG13 | 1.58 | 0.45 |
| 1:A:544:G:C6 | 1:A:545:C:C4 | 3.05 | 0.45 |
| 7:D:191:ARG:NH2 | 7:D:196:LEU:O | 2.47 | 0.45 |
| 1:A:1411:C:H2' | 1:A:1412:C:H6 | 1.81 | 0.45 |
| 7:D:24:GLU:CA | 7:D:112:VAL:HG12 | 2.47 | 0.45 |
| 16:M:84:ILE:HG13 | 16:M:85:GLY:N | 2.31 | 0.45 |
| 1:A:786:G:C2 | 1:A:787:A:H1' | 2.51 | 0.45 |
| 9:F:95:GLU:HB2 | 9:F:96:PRO:HD2 | 1.90 | 0.45 |
| 1:A:1156:G:C3' | 1:A:1157:A:P | 3.05 | 0.45 |
| 1:A:390:C:O3' | 19:P:28:ARG:NH2 | 2.50 | 0.45 |
| 1:A:279:A:OP1 | 1:A:281:G:H5' | 2.17 | 0.45 |
| 5:B:69:LEU:HB3 | 5:B:162:ILE:HG22 | 1.99 | 0.45 |
| 7:D:58:LEU:HD13 | 7:D:59:ARG:NH1 | 2.32 | 0.45 |
| 1:A:474:G:H5' | 19:P:81:ARG:HG3 | 1.99 | 0.45 |
| 1:A:52:G:H8 | 1:A:52:G:H5'' | 1.81 | 0.45 |
| 1:A:1320:C:H4' | 22:S:3:ARG:HH22 | 1.78 | 0.44 |
| 16:M:94:ARG:CA | 16:M:95:GLY:N | 2.80 | 0.44 |
| 1:A:405:U:OP1 | 7:D:5:ILE:HD13 | 2.18 | 0.44 |
| 1:A:407:G:N2 | 1:A:436:C:H1' | 2.32 | 0.44 |
| 7:D:8:VAL:HG11 | 7:D:115:ARG:NE | 2.32 | 0.44 |
| 1:A:1308:U:H3' | 16:M:99:ARG:HH12 | 1.82 | 0.44 |
| 1:A:557:G:H5'' | 1:A:558:G:OP2 | 2.17 | 0.44 |
| 1:A:881:G:OP2 | 15:L:9:GLN:CG | 2.64 | 0.44 |
| 3:W:23:A:H2' | 3:W:24:G:C8 | 2.52 | 0.44 |
| 1:A:1181:G:H4' | 1:A:1184:G:O4' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:944:G:H2' | 1:A:945:G:H5' | 1.99 | 0.44 |
| 1:A:1240:U:N3 | 10:G:30:ILE:O | 2.44 | 0.44 |
| 14:K:111:ASP:O | 14:K:112:THR:C | 2.55 | 0.44 |
| 1:A:475:G:H2' | 1:A:476:G:H8 | 1.81 | 0.44 |
| 10:G:64:GLN:HE21 | 10:G:68:ASN:HD21 | 1.64 | 0.44 |
| 1:A:962:C:C2 | 1:A:963:G:C8 | 3.05 | 0.44 |
| 1:A:976:G:C6 | 1:A:361(A):C:C5 | 3.06 | 0.44 |
| 7:D:12:CYS:HB3 | 7:D:31:CYS:HB3 | 1.76 | 0.44 |
| 1:A:1367:C:OP1 | 12:I:114:TYR:HA | 2.18 | 0.44 |
| 1:A:983:A:H3' | 1:A:983:A:N3 | 2.33 | 0.44 |
| 8:E:76:ILE:CG2 | 8:E:142:LEU:HD22 | 2.47 | 0.44 |
| 1:A:1004:A:C2' | 1:A:1025:U:N3 | 2.80 | 0.44 |
| 1:A:1249:C:C2 | 12:I:70:LYS:NZ | 2.83 | 0.44 |
| 1:A:1206:G:H4' | 6:C:194:GLY:H | 1.82 | 0.44 |
| 1:A:501:C:P | 15:L:124:LYS:HD3 | 2.57 | 0.44 |
| 11:H:25:ASP:OD1 | 11:H:60:ARG:HD3 | 2.17 | 0.44 |
| 1:A:528:C:N4 | 15:L:49:ASN:ND2 | 2.66 | 0.44 |
| 1:A:67:C:C1' | 1:A:172:A:H1' | 2.46 | 0.44 |
| 1:A:111:G:H3' | 1:A:112:G:H8 | 1.82 | 0.44 |
| 1:A:263:A:OP1 | 23:T:75:ASN:HB2 | 2.16 | 0.44 |
| 5:B:88:ALA:HA | 5:B:222:ILE:HD11 | 2.00 | 0.44 |
| 20:Q:46:ASP:HA | 20:Q:47:PRO:HD3 | 1.80 | 0.44 |
| 1:A:977:A:N3 | 1:A:1223:C:C5 | 2.85 | 0.44 |
| 1:A:1319:A:C4' | 22:S:70:LYS:HE2 | 2.43 | 0.44 |
| 1:A:959:A:N6 | 22:S:78:ARG:HA | 2.32 | 0.44 |
| 1:A:1269:A:H4' | 24:U:19:GLY:HA2 | 1.97 | 0.44 |
| 1:A:497:A:HO2' | 1:A:498:U:P | 2.40 | 0.44 |
| 3:W:25:C:H41 | 3:W:44:A:N6 | 2.16 | 0.44 |
| 1:A:889:A:H62 | 1:A:908:A:H62 | 1.64 | 0.44 |
| 6:C:91:LEU:HD21 | 6:C:99:VAL:N | 2.23 | 0.44 |
| 1:A:667:G:H2' | 1:A:668:G:C8 | 2.53 | 0.44 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.52 | 0.44 |
| 2:V:5:A:O2' | 2:V:6:U:H5' | 2.17 | 0.44 |
| 1:A:774:G:C4 | 1:A:775:G:C8 | 3.05 | 0.44 |
| 5:B:100:GLY:O | 5:B:104:ASN:HB3 | 2.16 | 0.44 |
| 1:A:1169:A:O5' | 1:A:1169:A:H8 | 2.01 | 0.44 |
| 1:A:1496:C:H2' | 1:A:1497:G:C1' | 2.47 | 0.44 |
| 1:A:475:G:H2' | 1:A:476:G:C8 | 2.52 | 0.44 |
| 14:K:45:GLY:O | 14:K:50:TYR:HB2 | 2.17 | 0.44 |
| 16:M:40:ASN:HA | 16:M:41:PRO:HD3 | 1.88 | 0.44 |
| 7:D:31:CYS:C | 7:D:33:MET:N | 2.60 | 0.44 |
| 1:A:1058:G:OP1 | 6:C:199:LYS:CE | 2.58 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:303:A:H4' | 1:A:555:C:O3' | 2.17 | 0.44 |
| 2:V:68:U:H2' | 2:V:69:U:C6 | 2.52 | 0.44 |
| 1:A:1181:G:H4' | 1:A:1184:G:C4' | 2.48 | 0.44 |
| 1:A:60:A:C2 | 1:A:107:G:N2 | 2.85 | 0.44 |
| 1:A:36:C:O2' | 1:A:501:C:H5'' | 2.18 | 0.44 |
| 1:A:451:A:N6 | 1:A:480:U:H2' | 2.28 | 0.44 |
| 1:A:509:A:H8 | 7:D:54:TYR:CE2 | 2.25 | 0.44 |
| 11:H:46:LYS:HE3 | 11:H:64:LYS:HG3 | 1.99 | 0.44 |
| 1:A:1411:C:H42 | 1:A:1489:G:H1 | 1.65 | 0.44 |
| 1:A:986:A:H1' | 22:S:54:GLY:C | 2.37 | 0.44 |
| 1:A:302:G:C2' | 1:A:556:C:H5'' | 2.34 | 0.44 |
| 1:A:394:G:H3' | 1:A:395:C:P | 2.57 | 0.44 |
| 1:A:1347:G:O2' | 1:A:1348:U:OP2 | 2.32 | 0.44 |
| 1:A:1375:A:H5' | 10:G:28:ASN:HB3 | 1.99 | 0.44 |
| 1:A:193:C:H2' | 1:A:194:C:C6 | 2.53 | 0.44 |
| 5:B:54:THR:O | 5:B:58:ILE:HG13 | 2.17 | 0.44 |
| 1:A:453:A:H4' | 19:P:72:ARG:CD | 2.46 | 0.44 |
| 1:A:1150:U:H1' | 1:A:1280:A:C6 | 2.53 | 0.44 |
| 1:A:728:A:N7 | 18:O:54:ARG:HD2 | 2.32 | 0.44 |
| 1:A:1429:C:H2' | 1:A:1430:C:C6 | 2.51 | 0.44 |
| 1:A:1316:G:N7 | 22:S:6:LYS:HE2 | 2.33 | 0.44 |
| 1:A:1329:A:HO2' | 16:M:24:GLY:HA2 | 1.77 | 0.44 |
| 1:A:121:C:H1' | 1:A:123:C:H41 | 1.83 | 0.44 |
| 1:A:129(A):G:C2' | 1:A:190(E):U:H5'' | 2.46 | 0.44 |
| 1:A:1205:U:C4' | 6:C:195:VAL:HG23 | 2.47 | 0.44 |
| 5:B:164:VAL:HG22 | 5:B:165:VAL:N | 2.32 | 0.44 |
| 11:H:13:ILE:O | 11:H:17:THR:OG1 | 2.30 | 0.44 |
| 1:A:761:G:C5' | 20:Q:102:GLY:HA3 | 2.47 | 0.44 |
| 1:A:1239:A:H1' | 1:A:1241:G:C4 | 2.53 | 0.44 |
| 16:M:9:ILE:N | 16:M:10:PRO:CD | 2.80 | 0.44 |
| 1:A:458:C:H42 | 1:A:474:G:H1 | 1.65 | 0.44 |
| 7:D:133:VAL:C | 7:D:135:LEU:H | 2.21 | 0.44 |
| 1:A:1534:A:H3' | 1:A:1534:A:N3 | 2.32 | 0.44 |
| 23:T:82:SER:O | 23:T:86:ARG:HB3 | 2.17 | 0.44 |
| 1:A:979:C:O5' | 1:A:1222:G:O6 | 2.34 | 0.44 |
| 7:D:120:LEU:HG | 7:D:125:HIS:HB2 | 1.99 | 0.44 |
| 1:A:1325:C:C5' | 24:U:17:THR:OG1 | 2.66 | 0.44 |
| 1:A:1317:C:C5 | 17:N:16:PHE:CD1 | 3.06 | 0.44 |
| 13:J:49:VAL:O | 13:J:60:ARG:HA | 2.17 | 0.44 |
| 3:W:34:G:H3' | 3:W:35:A:H5'' | 2.00 | 0.44 |
| 1:A:1399:C:C2 | 1:A:1502:A:N6 | 2.85 | 0.44 |
| 17:N:37:PHE:HB3 | 17:N:39:LEU:HD12 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:E:76:ILE:O | 8:E:93:PRO:HB3 | 2.17 | 0.44 |
| 1:A:1259:C:HO2' | 1:A:1283:G:H2' | 1.82 | 0.44 |
| 1:A:571:U:H3' | 1:A:572:A:H5'' | 1.95 | 0.44 |
| 13:J:16:LEU:HD12 | 13:J:70:ARG:HG2 | 1.99 | 0.44 |
| 1:A:1236:A:H4' | 1:A:1304:G:C4' | 2.46 | 0.44 |
| 7:D:101:LEU:HB2 | 7:D:138:TYR:HB3 | 2.00 | 0.44 |
| 1:A:1541:U:H2' | 1:A:1542:U:O3' | 2.16 | 0.44 |
| 6:C:64:VAL:HG12 | 6:C:66:VAL:HG23 | 2.00 | 0.44 |
| 1:A:922:G:C2 | 1:A:1398:A:C2 | 3.04 | 0.44 |
| 6:C:18:TRP:CD1 | 17:N:53:LEU:C | 2.91 | 0.44 |
| 1:A:296:U:H1' | 1:A:556:C:H1' | 2.00 | 0.44 |
| 1:A:116:A:C2 | 1:A:314:C:O4' | 2.70 | 0.44 |
| 1:A:1277:C:H4' | 1:A:1282:C:C1' | 2.48 | 0.44 |
| 1:A:600:C:OP1 | 11:H:97:VAL:CB | 2.50 | 0.44 |
| 1:A:22:G:C2 | 1:A:914:A:C8 | 3.05 | 0.44 |
| 1:A:1128:C:H42 | 1:A:1143:G:H1 | 1.63 | 0.44 |
| 1:A:1115:C:C1' | 17:N:61:TRP:O | 2.56 | 0.44 |
| 1:A:1073:U:H2' | 1:A:1074:G:C5' | 2.48 | 0.44 |
| 5:B:95:GLN:O | 5:B:96:ARG:C | 2.56 | 0.44 |
| 2:V:11:C:H2' | 2:V:12:U:C6 | 2.53 | 0.44 |
| 1:A:531:U:H4' | 1:A:532:A:O5' | 2.17 | 0.44 |
| 5:B:79:ASP:O | 5:B:83:MET:HG2 | 2.18 | 0.44 |
| 20:Q:58:GLU:HB2 | 20:Q:74:LEU:HB3 | 1.99 | 0.44 |
| 15:L:78:GLN:H | 15:L:81:SER:HB2 | 1.83 | 0.44 |
| 11:H:120:THR:O | 11:H:121:ASP:C | 2.56 | 0.44 |
| 1:A:1396:A:O2' | 1:A:1397:C:P | 2.76 | 0.44 |
| 1:A:924:C:H2' | 1:A:925:G:C8 | 2.53 | 0.44 |
| 2:V:36:A:H61 | 4:X:116:U:H3 | 1.58 | 0.44 |
| 1:A:918:A:H2' | 1:A:919:A:O4' | 2.18 | 0.44 |
| 6:C:121:ALA:HA | 6:C:124:ILE:HD12 | 1.99 | 0.44 |
| 1:A:370:C:H42 | 1:A:391:G:H1 | 1.66 | 0.44 |
| 1:A:401:C:OP2 | 7:D:73:ARG:NH2 | 2.51 | 0.44 |
| 7:D:79:PHE:HE1 | 7:D:204:ILE:HG13 | 1.82 | 0.44 |
| 1:A:962:C:H2' | 1:A:963:G:O4' | 2.18 | 0.44 |
| 23:T:73:HIS:C | 23:T:74:LYS:HG2 | 2.38 | 0.44 |
| 2:V:45:G:H2' | 2:V:46:G:OP2 | 2.18 | 0.44 |
| 1:A:1319:A:C4' | 22:S:70:LYS:HZ1 | 2.18 | 0.43 |
| 1:A:986:A:H1' | 22:S:54:GLY:O | 2.17 | 0.43 |
| 1:A:1309:G:OP2 | 16:M:99:ARG:NH1 | 2.50 | 0.43 |
| 1:A:1328:C:O2' | 16:M:29:ARG:HG3 | 2.18 | 0.43 |
| 1:A:25:C:O2' | 1:A:524:G:N2 | 2.51 | 0.43 |
| 8:E:76:ILE:HG21 | 8:E:142:LEU:HD22 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:996:A:N1 | 1:A:1046:A:H4' | 2.32 | 0.43 |
| 1:A:695:A:H2' | 1:A:696:A:O4' | 2.17 | 0.43 |
| 1:A:1288:A:H2 | 1:A:1352:C:O2 | 2.01 | 0.43 |
| 1:A:20:U:C1' | 1:A:572:A:C4 | 3.01 | 0.43 |
| 21:R:46:GLU:CB | 21:R:85:LEU:HD13 | 2.47 | 0.43 |
| 8:E:95:ALA:CB | 8:E:96:PRO:HD3 | 2.44 | 0.43 |
| 1:A:1343:G:H2' | 1:A:1344:C:C6 | 2.53 | 0.43 |
| 5:B:93:VAL:HG11 | 5:B:97:TRP:HA | 2.00 | 0.43 |
| 5:B:205:ASP:O | 5:B:211:ILE:HD11 | 2.18 | 0.43 |
| 1:A:1358:U:OP1 | 17:N:35:ARG:N | 2.51 | 0.43 |
| 1:A:1317:C:O2 | 22:S:10:PHE:CE2 | 2.71 | 0.43 |
| 1:A:953:G:H4' | 16:M:124:PRO:O | 2.18 | 0.43 |
| 17:N:26:ARG:HB3 | 17:N:43:CYS:HB2 | 2.01 | 0.43 |
| 1:A:500:G:N2 | 1:A:546:G:H1' | 2.32 | 0.43 |
| 1:A:908:A:H2' | 1:A:909:A:C8 | 2.52 | 0.43 |
| 1:A:1511:G:C6 | 1:A:1512:U:N3 | 2.85 | 0.43 |
| 21:R:31:LEU:HD11 | 21:R:62:GLU:HG3 | 2.00 | 0.43 |
| 13:J:90:LEU:H | 13:J:91:PRO:CD | 2.27 | 0.43 |
| 2:V:58:A:C5 | 2:V:61:C:C4 | 3.06 | 0.43 |
| 1:A:665:A:H2' | 1:A:725:G:N2 | 2.33 | 0.43 |
| 1:A:980:C:H2' | 1:A:981:U:O4' | 2.18 | 0.43 |
| 1:A:517:G:N2 | 1:A:533:A:OP2 | 2.51 | 0.43 |
| 16:M:33:ALA:HA | 16:M:59:TYR:HE2 | 1.83 | 0.43 |
| 1:A:752:G:H1' | 1:A:754:C:N4 | 2.33 | 0.43 |
| 1:A:1221:G:H1' | 22:S:53:ASN:O | 2.17 | 0.43 |
| 1:A:1320:C:H2' | 1:A:1321:C:C6 | 2.53 | 0.43 |
| 1:A:1325:C:H5' | 24:U:17:THR:OG1 | 2.18 | 0.43 |
| 2:V:32:C:OP2 | 12:I:128:ARG:N | 2.52 | 0.43 |
| 2:V:32:C:OP2 | 12:I:127:LYS:HB2 | 2.18 | 0.43 |
| 1:A:769:G:H22 | 1:A:811:C:H1' | 1.84 | 0.43 |
| 3:W:43:G:H2' | 3:W:44:A:C8 | 2.53 | 0.43 |
| 2:V:35:A:C6 | 4:X:118:C:N4 | 2.82 | 0.43 |
| 1:A:1004:A:O4' | 1:A:1025:U:C4 | 2.71 | 0.43 |
| 1:A:426:G:C3' | 7:D:42:GLN:HA | 2.47 | 0.43 |
| 1:A:21:G:H2' | 1:A:22:G:C8 | 2.54 | 0.43 |
| 1:A:585:G:C2' | 1:A:879:C:H5'' | 2.48 | 0.43 |
| 1:A:253:U:H4' | 1:A:276:G:O2' | 2.18 | 0.43 |
| 3:W:14:A:C6 | 3:W:22:G:C4 | 3.06 | 0.43 |
| 1:A:1057:G:H5'' | 6:C:154:SER:HB2 | 2.00 | 0.43 |
| 10:G:93:PRO:HA | 10:G:96:GLN:HB2 | 1.98 | 0.43 |
| 1:A:112:G:OP1 | 19:P:27:LYS:HD3 | 2.18 | 0.43 |
| 3:W:50:U:O2' | 3:W:51:G:H5' | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:770:C:C4 | 1:A:771:G:N7 | 2.85 | 0.43 |
| 5:B:112:VAL:C | 5:B:113:HIS:CA | 2.77 | 0.43 |
| 1:A:564:C:H2' | 1:A:565:U:O4' | 2.17 | 0.43 |
| 7:D:96:LEU:CD2 | 7:D:139:ARG:NH1 | 2.81 | 0.43 |
| 1:A:1255:G:N2 | 1:A:1258:G:H22 | 2.14 | 0.43 |
| 1:A:944:G:H3' | 1:A:945:G:H5' | 2.00 | 0.43 |
| 1:A:659:U:H2' | 1:A:660:G:H8 | 1.83 | 0.43 |
| 1:A:1343:G:H4' | 12:I:122:ALA:HB3 | 2.00 | 0.43 |
| 1:A:686:U:O2 | 14:K:42:TRP:HZ2 | 2.01 | 0.43 |
| 1:A:99:C:H2' | 1:A:101:A:C8 | 2.53 | 0.43 |
| 11:H:38:ILE:O | 11:H:38:ILE:HG22 | 2.19 | 0.43 |
| 1:A:1078:U:H4' | 8:E:84:PHE:CZ | 2.53 | 0.43 |
| 6:C:135:LYS:HZ1 | 8:E:50:GLU:HB3 | 1.83 | 0.43 |
| 1:A:1449:C:H42 | 1:A:1454:G:H1 | 1.67 | 0.43 |
| 1:A:15:G:C6 | 1:A:1396:A:N1 | 2.86 | 0.43 |
| 1:A:558:G:H2' | 1:A:559:A:H2 | 1.83 | 0.43 |
| 1:A:123:C:H5'' | 1:A:311:C:C2' | 2.47 | 0.43 |
| 1:A:1377:A:P | 10:G:94:ARG:HH21 | 2.42 | 0.43 |
| 6:C:178:LEU:O | 6:C:179:ARG:HB2 | 2.18 | 0.43 |
| 12:I:27:THR:HB | 12:I:62:TYR:HD1 | 1.83 | 0.43 |
| 1:A:1006:C:H2' | 1:A:1006:C:O2 | 2.18 | 0.43 |
| 16:M:24:GLY:CA | 16:M:70:LEU:HD11 | 2.48 | 0.43 |
| 1:A:815:A:N3 | 1:A:1527:C:O2' | 2.42 | 0.43 |
| 1:A:39:G:H1' | 1:A:498:U:C5 | 2.52 | 0.43 |
| 1:A:1250:A:OP1 | 12:I:66:ARG:NE | 2.51 | 0.43 |
| 1:A:1506:U:O2' | 1:A:1507:A:H5' | 2.19 | 0.43 |
| 1:A:878:G:C5' | 11:H:89:PRO:O | 2.67 | 0.43 |
| 1:A:54:C:H41 | 1:A:352:C:C2' | 2.32 | 0.43 |
| 3:W:14:A:N6 | 3:W:22:G:C4 | 2.87 | 0.43 |
| 14:K:120:ARG:HA | 14:K:121:PRO:HD3 | 1.87 | 0.43 |
| 3:W:16:U:C2' | 3:W:17:U:OP2 | 2.65 | 0.43 |
| 1:A:1417:G:N2 | 1:A:1484:C:C4 | 2.87 | 0.43 |
| 1:A:1163:C:H42 | 1:A:1173:G:H1 | 1.67 | 0.43 |
| 1:A:1194:U:H4' | 8:E:22:GLY:O | 2.17 | 0.43 |
| 1:A:531:U:H4' | 1:A:532:A:H5'' | 2.01 | 0.43 |
| 1:A:819:A:C2 | 1:A:1529:G:O6 | 2.71 | 0.43 |
| 7:D:70:ILE:HD11 | 7:D:100:ARG:NH2 | 2.33 | 0.43 |
| 1:A:462:G:N2 | 19:P:82:GLN:NE2 | 2.51 | 0.43 |
| 1:A:17:U:N3 | 1:A:919:A:C2 | 2.86 | 0.43 |
| 1:A:104:G:C6 | 1:A:105:G:N7 | 2.87 | 0.43 |
| 1:A:738:C:OP1 | 9:F:2:ARG:NH1 | 2.51 | 0.43 |
| 15:L:87:GLY:O | 15:L:99:HIS:CE1 | 2.70 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 21:R:21:LYS:H | 21:R:55:ARG:NH1 | 2.16 | 0.43 |
| 1:A:834:C:C2 | 1:A:853:G:C2 | 3.06 | 0.43 |
| 1:A:833:U:H3 | 1:A:853:G:H1 | 1.65 | 0.43 |
| 20:Q:11:VAL:HB | 20:Q:88:TYR:CE2 | 2.53 | 0.43 |
| 7:D:15:GLU:OE2 | 7:D:63:LYS:CA | 2.66 | 0.43 |
| 16:M:24:GLY:HA2 | 16:M:70:LEU:CD1 | 2.48 | 0.43 |
| 1:A:303:A:C4' | 1:A:556:C:OP1 | 2.67 | 0.43 |
| 1:A:562:C:C1' | 15:L:15:ARG:HD2 | 2.39 | 0.43 |
| 1:A:819:A:N6 | 1:A:1529:G:C8 | 2.86 | 0.43 |
| 1:A:1047:G:H5'' | 17:N:4:LYS:HD2 | 2.01 | 0.43 |
| 1:A:909:A:H3' | 1:A:910:C:H6 | 1.84 | 0.43 |
| 1:A:1278:U:H5'' | 1:A:1279:A:O4' | 2.19 | 0.43 |
| 11:H:44:PHE:O | 11:H:64:LYS:HD3 | 2.19 | 0.43 |
| 8:E:81:GLU:HB3 | 8:E:90:VAL:HG22 | 2.00 | 0.43 |
| 1:A:1240:U:N3 | 10:G:30:ILE:HG22 | 2.34 | 0.43 |
| 3:W:50:U:C2' | 3:W:51:G:H5' | 2.48 | 0.43 |
| 5:B:136:VAL:HA | 5:B:139:LYS:HE3 | 2.01 | 0.43 |
| 1:A:146:G:H1 | 1:A:176:C:H42 | 1.65 | 0.43 |
| 1:A:409:G:O5' | 7:D:25:ARG:HB3 | 2.18 | 0.43 |
| 1:A:1197:G:C2' | 1:A:1198:G:H5' | 2.47 | 0.43 |
| 1:A:297:G:N2 | 1:A:300:A:OP2 | 2.48 | 0.43 |
| 1:A:25:C:H5' | 1:A:524:G:H1' | 2.01 | 0.43 |
| 1:A:563:A:C2 | 1:A:567:G:C4 | 3.07 | 0.43 |
| 1:A:123:C:H2' | 1:A:124:G:H8 | 1.84 | 0.43 |
| 1:A:1095:U:C5' | 1:A:1109:C:O2 | 2.66 | 0.43 |
| 13:J:64:GLU:HG2 | 17:N:59:ALA:CA | 2.39 | 0.43 |
| 1:A:1259:C:O2' | 1:A:1284:C:C1' | 2.67 | 0.43 |
| 1:A:1250:A:OP1 | 12:I:66:ARG:CG | 2.65 | 0.43 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.54 | 0.43 |
| 15:L:102:ARG:HE | 15:L:109:GLY:C | 2.21 | 0.43 |
| 1:A:551:U:H6 | 1:A:551:U:O5' | 2.02 | 0.43 |
| 3:W:14:A:N6 | 3:W:22:G:C5 | 2.86 | 0.43 |
| 1:A:69:G:H1 | 1:A:99:C:H42 | 1.65 | 0.43 |
| 1:A:1015:A:O2' | 1:A:1218:C:H4' | 2.18 | 0.43 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.53 | 0.43 |
| 1:A:409:G:H5'' | 7:D:25:ARG:HB2 | 0.49 | 0.43 |
| 2:V:40:C:H2' | 2:V:41:U:C5' | 2.26 | 0.43 |
| 1:A:880:C:OP2 | 15:L:6:THR:OG1 | 2.31 | 0.43 |
| 1:A:541:G:H5' | 7:D:42:GLN:NE2 | 2.34 | 0.43 |
| 1:A:570:G:H2' | 1:A:571:U:C6 | 2.54 | 0.43 |
| 1:A:1346:A:H61 | 1:A:1374:A:H3' | 1.84 | 0.43 |
| 1:A:522:C:H5'' | 15:L:120:TYR:OH | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:685:G:H2' | 1:A:686:U:H6 | 1.83 | 0.43 |
| 1:A:1269:A:C4 | 1:A:1326:C:H1' | 2.45 | 0.42 |
| 1:A:965:A:P | 1:A:1198:G:H5'' | 2.59 | 0.42 |
| 13:J:51:ARG:HG3 | 13:J:60:ARG:O | 2.19 | 0.42 |
| 1:A:116:A:N6 | 1:A:313:A:N3 | 2.67 | 0.42 |
| 1:A:949:A:H4' | 1:A:1364:U:N3 | 2.31 | 0.42 |
| 3:W:44:A:C2' | 3:W:45:G:C5' | 2.96 | 0.42 |
| 1:A:1287:A:N6 | 1:A:1371:G:O4' | 2.48 | 0.42 |
| 1:A:1147:C:O2 | 12:I:16:ARG:NH2 | 2.52 | 0.42 |
| 20:Q:97:SER:HB2 | 20:Q:102:GLY:C | 2.39 | 0.42 |
| 6:C:38:ARG:CB | 6:C:94:LEU:HD21 | 2.46 | 0.42 |
| 20:Q:76:LEU:HD11 | 20:Q:79:SER:HB3 | 2.01 | 0.42 |
| 1:A:367:U:H4' | 1:A:368:U:OP1 | 2.18 | 0.42 |
| 1:A:1483:A:OP2 | 1:A:1484:C:C5 | 2.72 | 0.42 |
| 1:A:14:U:O5' | 1:A:14:U:H6 | 2.02 | 0.42 |
| 1:A:1220:G:H5' | 22:S:36:ARG:N | 2.25 | 0.42 |
| 1:A:1317:C:H2' | 22:S:10:PHE:CD2 | 2.54 | 0.42 |
| 1:A:546:G:O3' | 1:A:548:G:H4' | 2.19 | 0.42 |
| 1:A:1298:C:P | 10:G:114:ARG:NH1 | 2.92 | 0.42 |
| 3:W:25:C:N1 | 3:W:26:G:C6 | 2.79 | 0.42 |
| 1:A:1515:C:H2' | 1:A:1516:G:H8 | 1.84 | 0.42 |
| 11:H:39:LEU:HB3 | 11:H:45:ILE:HG12 | 2.01 | 0.42 |
| 2:V:19:G:H1' | 2:V:57:G:H21 | 1.84 | 0.42 |
| 1:A:520:A:N6 | 1:A:529:G:C2 | 2.87 | 0.42 |
| 1:A:66:G:H4' | 1:A:173:U:O4 | 2.19 | 0.42 |
| 1:A:512:U:H2' | 1:A:513:C:C6 | 2.54 | 0.42 |
| 1:A:406:G:O3' | 7:D:5:ILE:HG23 | 2.20 | 0.42 |
| 1:A:914:A:H2' | 1:A:915:A:C8 | 2.53 | 0.42 |
| 1:A:1250:A:P | 12:I:66:ARG:HG2 | 2.58 | 0.42 |
| 11:H:16:ALA:HB1 | 11:H:21:LYS:HB2 | 2.01 | 0.42 |
| 1:A:1289:A:C2 | 1:A:1372:U:C4' | 3.01 | 0.42 |
| 10:G:150:ALA:CA | 14:K:59:TYR:HB3 | 2.47 | 0.42 |
| 2:V:58:A:C5 | 2:V:61:C:C5 | 3.08 | 0.42 |
| 1:A:823:G:H21 | 11:H:1:MET:N | 2.17 | 0.42 |
| 5:B:15:VAL:HG21 | 5:B:209:ARG:HB3 | 2.01 | 0.42 |
| 15:L:26:ALA:O | 15:L:33:ARG:HD2 | 2.19 | 0.42 |
| 19:P:36:ILE:HD12 | 19:P:56:ALA:HB2 | 2.02 | 0.42 |
| 1:A:1532:U:H3' | 1:A:1532:U:C6 | 2.55 | 0.42 |
| 7:D:15:GLU:OE2 | 7:D:63:LYS:HA | 2.19 | 0.42 |
| 1:A:953:G:O2' | 16:M:125:ARG:N | 2.51 | 0.42 |
| 2:V:31:A:O3' | 12:I:127:LYS:CB | 2.68 | 0.42 |
| 2:V:36:A:N6 | 4:X:116:U:N3 | 2.62 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:426:G:O2' | 7:D:42:GLN:CG | 2.67 | 0.42 |
| 1:A:573:A:N3 | 1:A:883:C:H2' | 2.34 | 0.42 |
| 16:M:108:ARG:HA | 16:M:108:ARG:HD2 | 1.86 | 0.42 |
| 7:D:102:ASP:O | 7:D:117:ALA:HB1 | 2.19 | 0.42 |
| 1:A:505:G:H4' | 1:A:534:U:C4 | 2.55 | 0.42 |
| 1:A:578:C:H2' | 1:A:579:G:H8 | 1.82 | 0.42 |
| 1:A:929:G:H5' | 1:A:1533:C:H42 | 1.84 | 0.42 |
| 1:A:616:G:H1 | 1:A:624:C:H42 | 1.67 | 0.42 |
| 17:N:29:ARG:HG3 | 17:N:31:ARG:H | 1.83 | 0.42 |
| 1:A:1224:G:C5 | 1:A:1322:C:H5' | 2.54 | 0.42 |
| 1:A:819:A:C6 | 1:A:1529:G:N7 | 2.88 | 0.42 |
| 1:A:1260:C:O5' | 1:A:1285:A:OP2 | 2.38 | 0.42 |
| 1:A:1115:C:H2' | 1:A:1116:C:O4' | 2.20 | 0.42 |
| 1:A:948:C:O5' | 1:A:948:C:C6 | 2.67 | 0.42 |
| 7:D:34:GLU:O | 7:D:35:ARG:HB2 | 2.19 | 0.42 |
| 1:A:191:G:O2' | 23:T:102:GLY:HA2 | 2.18 | 0.42 |
| 8:E:135:THR:O | 8:E:139:LEU:HG | 2.20 | 0.42 |
| 7:D:175:SER:O | 7:D:183:GLY:HA2 | 2.20 | 0.42 |
| 13:J:66:ARG:NH1 | 17:N:57:ARG:NH1 | 2.68 | 0.42 |
| 1:A:1249:C:O2' | 12:I:73:GLN:NE2 | 2.53 | 0.42 |
| 1:A:1189:C:C5' | 1:A:1190:G:OP2 | 2.65 | 0.42 |
| 9:F:62:TRP:CG | 21:R:35:ARG:NH2 | 2.84 | 0.42 |
| 1:A:1506:U:O4 | 1:A:1521:G:H5'' | 2.20 | 0.42 |
| 1:A:946:A:O2' | 1:A:1333:A:C1' | 2.68 | 0.42 |
| 1:A:1242:C:O2' | 1:A:1303:C:C5' | 2.67 | 0.42 |
| 1:A:1164:G:H1 | 1:A:1172:C:H42 | 1.67 | 0.42 |
| 1:A:835:U:OP1 | 21:R:61:LYS:HD2 | 2.20 | 0.42 |
| 1:A:973:G:H3' | 1:A:974:A:H5'' | 2.01 | 0.42 |
| 5:B:51:LEU:O | 5:B:55:PHE:HD1 | 2.02 | 0.42 |
| 1:A:1223:C:H5'' | 1:A:1224:G:H5'' | 2.00 | 0.42 |
| 1:A:1319:A:C5' | 22:S:70:LYS:HE2 | 2.50 | 0.42 |
| 1:A:1221:G:OP1 | 1:A:1321:C:N4 | 2.53 | 0.42 |
| 6:C:12:LEU:HD22 | 17:N:51:GLY:HA3 | 1.91 | 0.42 |
| 1:A:39:G:N9 | 1:A:498:U:C4 | 2.86 | 0.42 |
| 1:A:236:G:H2' | 1:A:237:C:C6 | 2.55 | 0.42 |
| 1:A:1260:C:H4' | 1:A:1284:C:C5' | 2.50 | 0.42 |
| 1:A:1370:G:H5'' | 12:I:12:GLU:CG | 2.50 | 0.42 |
| 1:A:1143:G:H2' | 1:A:1144:G:H8 | 1.84 | 0.42 |
| 20:Q:25:ARG:HB3 | 20:Q:38:ARG:HB3 | 2.01 | 0.42 |
| 1:A:574:A:O2' | 1:A:882:C:H1' | 2.19 | 0.42 |
| 6:C:53:ALA:HB2 | 6:C:115:LEU:HD11 | 2.02 | 0.42 |
| 5:B:162:ILE:HD13 | 5:B:162:ILE:N | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 6:C:153:VAL:HB | 6:C:166:GLU:HB3 | 2.01 | 0.42 |
| 24:U:5:ASP:O | 24:U:11:GLY:HA3 | 2.19 | 0.42 |
| 1:A:361(A):C:HO3' | 1:A:1362:C:H5'' | 1.84 | 0.42 |
| 3:W:37:YYG:H32 | 3:W:38:A:O4' | 2.20 | 0.42 |
| 24:U:6:ARG:HH11 | 24:U:15:ARG:HH22 | 1.66 | 0.42 |
| 1:A:1268:A:HO2' | 24:U:20:LYS:N | 2.09 | 0.42 |
| 1:A:765:G:N1 | 1:A:812:C:H1' | 2.34 | 0.42 |
| 15:L:97:ARG:HG2 | 15:L:97:ARG:O | 2.20 | 0.42 |
| 1:A:881:G:OP2 | 15:L:9:GLN:HG2 | 2.20 | 0.42 |
| 1:A:1004:A:H8 | 1:A:1036:G:O6 | 2.03 | 0.42 |
| 1:A:891:U:H5 | 1:A:906:G:C2 | 2.38 | 0.42 |
| 1:A:450:G:O6 | 1:A:481:G:H2' | 2.20 | 0.42 |
| 1:A:946:A:O2' | 1:A:1333:A:H1' | 2.20 | 0.42 |
| 8:E:151:LEU:O | 11:H:64:LYS:HE3 | 2.20 | 0.42 |
| 1:A:1123:A:O2' | 13:J:38:ILE:HG22 | 2.20 | 0.42 |
| 1:A:948:C:H5' | 1:A:1306:A:O2' | 2.20 | 0.42 |
| 1:A:1114:C:O2' | 17:N:60:SER:C | 2.58 | 0.42 |
| 5:B:80:ILE:CG2 | 5:B:212:GLN:HG2 | 2.49 | 0.42 |
| 1:A:832:C:H1' | 1:A:855:G:N2 | 2.35 | 0.42 |
| 5:B:82:ARG:HD2 | 5:B:92:TYR:HE1 | 1.84 | 0.42 |
| 1:A:870:U:O5' | 1:A:870:U:H6 | 2.02 | 0.42 |
| 1:A:922:G:O2' | 1:A:1398:A:N1 | 2.41 | 0.42 |
| 1:A:427:U:C5' | 7:D:41:GLY:HA2 | 2.30 | 0.42 |
| 1:A:21:G:N2 | 1:A:915:A:H62 | 2.16 | 0.42 |
| 15:L:75:HIS:HB3 | 15:L:102:ARG:HH12 | 1.83 | 0.42 |
| 8:E:26:PHE:HB2 | 8:E:27:ARG:H | 1.74 | 0.42 |
| 1:A:328:C:H4' | 1:A:329:A:H5' | 2.01 | 0.42 |
| 19:P:55:ARG:O | 19:P:59:TRP:HD1 | 2.03 | 0.42 |
| 1:A:1451:A:C8 | 1:A:1451:A:C3' | 3.03 | 0.42 |
| 1:A:1164:G:H1 | 1:A:1172:C:N4 | 2.18 | 0.42 |
| 1:A:1002:G:H2' | 1:A:1003:G:O4' | 2.20 | 0.42 |
| 5:B:182:ILE:HA | 5:B:183:PRO:HD3 | 1.91 | 0.42 |
| 22:S:64:GLU:HG3 | 22:S:65:ASN:N | 2.35 | 0.42 |
| 1:A:1226:C:OP2 | 16:M:103:THR:CB | 2.67 | 0.42 |
| 3:W:37:YYG:H192 | 10:G:83:ALA:O | 2.17 | 0.42 |
| 1:A:967:C:H4' | 12:I:128:ARG:NH2 | 2.35 | 0.42 |
| 1:A:791:G:H22 | 1:A:1498:U:P | 2.43 | 0.42 |
| 1:A:1202:G:H21 | 17:N:27:CYS:HB2 | 1.84 | 0.42 |
| 7:D:68:TYR:CE2 | 7:D:97:LEU:HB3 | 2.54 | 0.42 |
| 1:A:1288:A:C2 | 1:A:1371:G:N3 | 2.88 | 0.42 |
| 1:A:1286:A:C6 | 1:A:1354:C:H5'' | 2.51 | 0.42 |
| 1:A:571:U:H3 | 1:A:865:A:H2 | 1.66 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:991:U:OP1 | 1:A:1018:C:OP1 | 2.37 | 0.42 |
| 19:P:7:ALA:HB3 | 19:P:18:ARG:HB2 | 2.01 | 0.42 |
| 1:A:766:A:H61 | 1:A:1511:G:H1' | 1.84 | 0.42 |
| 1:A:1278:U:H5'' | 1:A:1279:A:C4' | 2.49 | 0.42 |
| 1:A:509:A:O2' | 1:A:510:A:H5' | 2.20 | 0.42 |
| 5:B:28:PHE:CD2 | 5:B:194:PRO:HG3 | 2.55 | 0.42 |
| 1:A:1114:C:H1' | 17:N:60:SER:HB3 | 2.02 | 0.42 |
| 1:A:357:G:H1' | 1:A:368:U:O2 | 2.19 | 0.42 |
| 7:D:63:LYS:O | 7:D:67:ILE:HG13 | 2.20 | 0.41 |
| 1:A:925:G:H1 | 1:A:1391:U:H3 | 1.68 | 0.41 |
| 1:A:1398:A:H3' | 1:A:1398:A:C8 | 2.55 | 0.41 |
| 1:A:120:A:H2' | 1:A:122:G:N7 | 2.35 | 0.41 |
| 1:A:1205:U:C2' | 6:C:195:VAL:HG23 | 2.49 | 0.41 |
| 19:P:9:PHE:HB2 | 19:P:16:HIS:O | 2.20 | 0.41 |
| 7:D:104:VAL:HG12 | 7:D:104:VAL:O | 2.20 | 0.41 |
| 1:A:1268:A:O3' | 24:U:20:LYS:HA | 2.20 | 0.41 |
| 1:A:1060:C:H4' | 13:J:52:GLY:HA3 | 2.01 | 0.41 |
| 1:A:585:G:H1' | 1:A:879:C:H5'' | 2.01 | 0.41 |
| 12:I:35:GLU:O | 12:I:38:GLN:HG2 | 2.21 | 0.41 |
| 1:A:947:G:C4' | 1:A:1332:A:C2 | 2.98 | 0.41 |
| 10:G:12:LEU:CD2 | 10:G:28:ASN:ND2 | 2.83 | 0.41 |
| 1:A:250:A:H5' | 1:A:252:U:O4' | 2.19 | 0.41 |
| 15:L:44:THR:HA | 15:L:45:PRO:HD3 | 1.83 | 0.41 |
| 12:I:55:ALA:HB3 | 12:I:58:ARG:HE | 1.85 | 0.41 |
| 1:A:227:G:H21 | 19:P:62:VAL:HB | 1.85 | 0.41 |
| 1:A:439:A:OP2 | 1:A:494:G:N1 | 2.43 | 0.41 |
| 1:A:489:C:H2' | 1:A:490:G:H8 | 1.85 | 0.41 |
| 1:A:1222:G:O5' | 1:A:1222:G:H8 | 2.04 | 0.41 |
| 1:A:975:A:H8 | 1:A:1365:G:H22 | 1.67 | 0.41 |
| 1:A:1325:C:P | 24:U:15:ARG:NE | 2.93 | 0.41 |
| 1:A:1317:C:N3 | 17:N:16:PHE:CZ | 2.89 | 0.41 |
| 1:A:563:A:N1 | 1:A:567:G:N3 | 2.69 | 0.41 |
| 1:A:695:A:H2' | 1:A:696:A:H8 | 1.84 | 0.41 |
| 1:A:890:G:O2' | 1:A:891:U:H6 | 1.98 | 0.41 |
| 1:A:892:A:C2 | 1:A:893:C:C2 | 3.09 | 0.41 |
| 1:A:1117:G:OP1 | 12:I:104:ARG:NH1 | 2.53 | 0.41 |
| 1:A:279:A:N7 | 20:Q:95:TYR:CE2 | 2.89 | 0.41 |
| 1:A:1377:A:OP1 | 10:G:94:ARG:CZ | 2.68 | 0.41 |
| 11:H:49:GLU:OE1 | 11:H:51:VAL:HG23 | 2.20 | 0.41 |
| 5:B:28:PHE:HE2 | 5:B:189:ASP:O | 2.04 | 0.41 |
| 6:C:139:GLN:HE21 | 6:C:170:GLN:HE22 | 1.68 | 0.41 |
| 5:B:152:PHE:O | 5:B:154:LEU:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-------------------|-------------|----------|
| 5:B:82:ARG:HB2 | 5:B:94:ASN:ND2 | 2.35 | 0.41 |
| 1:A:79:G:H2' | 1:A:80:G:H8 | 1.85 | 0.41 |
| 1:A:1268:A:O2' | 24:U:20:LYS:HB3 | 2.19 | 0.41 |
| 1:A:565:U:H3' | 1:A:566:G:H8 | 1.83 | 0.41 |
| 1:A:31:G:O2' | 1:A:46:G:C4' | 2.67 | 0.41 |
| 1:A:757:U:OP1 | 1:A:822:C:C2' | 2.68 | 0.41 |
| 12:I:102:LEU:O | 12:I:103:THR:CB | 2.68 | 0.41 |
| 6:C:14:ILE:HG22 | 6:C:15:THR:HG23 | 2.02 | 0.41 |
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.56 | 0.41 |
| 19:P:27:LYS:C | 19:P:29:ASP:N | 2.73 | 0.41 |
| 1:A:1428:A:H2' | 1:A:1429:C:C6 | 2.55 | 0.41 |
| 1:A:330:C:C2 | 1:A:331:G:C8 | 3.09 | 0.41 |
| 16:M:94:ARG:C | 16:M:95:GLY:CA | 2.88 | 0.41 |
| 1:A:1307:U:C4' | 16:M:109:THR:HG21 | 2.49 | 0.41 |
| 1:A:1317:C:O2 | 22:S:10:PHE:HE2 | 2.03 | 0.41 |
| 1:A:119:A:H4' | 1:A:120:A:C8 | 2.56 | 0.41 |
| 1:A:937:A:C3' | 1:A:938:A:P | 3.06 | 0.41 |
| 11:H:29:SER:HB3 | 11:H:32:LYS:HG2 | 2.03 | 0.41 |
| 1:A:1127:G:H21 | 1:A:1147:C:H42 | 1.68 | 0.41 |
| 1:A:1148:U:OP1 | 12:I:5:TYR:OH | 2.23 | 0.41 |
| 1:A:246:A:H62 | 1:A:281:G:H21 | 1.69 | 0.41 |
| 1:A:1511:G:C6 | 1:A:1512:U:C2 | 3.08 | 0.41 |
| 7:D:13:ARG:HB3 | 7:D:40:PRO:HD3 | 2.03 | 0.41 |
| 14:K:58:PRO:CA | 14:K:90:GLY:HA3 | 2.48 | 0.41 |
| 9:F:10:LEU:HD11 | 9:F:26:ILE:HD11 | 2.02 | 0.41 |
| 5:B:68:ILE:O | 5:B:91:PRO:HD2 | 2.20 | 0.41 |
| 10:G:27:ILE:HA | 10:G:30:ILE:HD12 | 2.02 | 0.41 |
| 1:A:1021:G:C2 | 1:A:1022:G:H1' | 2.56 | 0.41 |
| 8:E:42:GLY:HA3 | 8:E:66:MET:SD | 2.60 | 0.41 |
| 1:A:807:A:C6 | 1:A:808:C:N3 | 2.88 | 0.41 |
| 9:F:79:LEU:O | 9:F:85:VAL:HG21 | 2.21 | 0.41 |
| 17:N:21:TYR:CD1 | 17:N:21:TYR:N | 2.89 | 0.41 |
| 16:M:66:LEU:HA | 16:M:70:LEU:CD1 | 2.29 | 0.41 |
| 1:A:1229:A:O2' | 16:M:125:ARG:CZ | 2.68 | 0.41 |
| 1:A:1401:G:H2' | 1:A:1402:C:O4' | 2.20 | 0.41 |
| 1:A:1067:A:H2' | 1:A:1093:A:O2' | 2.20 | 0.41 |
| 24:U:22:ARG:HA | 24:U:23:PRO:HD3 | 1.92 | 0.41 |
| 1:A:19:C:H1' | 1:A:917:G:N2 | 2.35 | 0.41 |
| 19:P:3:LYS:HE2 | 19:P:24:ALA:HB2 | 2.03 | 0.41 |
| 10:G:34:GLY:O | 10:G:36:LYS:N | 2.53 | 0.41 |
| 1:A:1377:A:OP1 | 10:G:94:ARG:NE | 2.54 | 0.41 |
| 1:A:528:C:H41 | 15:L:49:ASN:CG | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:190(J):U:H2' | 1:A:190(K):G:H8 | 1.86 | 0.41 |
| 2:V:50:U:C2 | 2:V:51:G:C8 | 3.08 | 0.41 |
| 13:J:38:ILE:HG13 | 13:J:71:LEU:HB3 | 2.01 | 0.41 |
| 1:A:454:C:H3' | 1:A:455:C:C6 | 2.49 | 0.41 |
| 1:A:867:G:N3 | 1:A:873:A:C2 | 2.89 | 0.41 |
| 8:E:36:ASP:OD1 | 8:E:40:ARG:HB2 | 2.20 | 0.41 |
| 13:J:39:PRO:O | 13:J:40:LEU:HB2 | 2.20 | 0.41 |
| 1:A:859:A:H2' | 1:A:860:A:C8 | 2.56 | 0.41 |
| 1:A:1132:C:H42 | 1:A:1142:G:H1 | 1.67 | 0.41 |
| 5:B:50:GLU:HB3 | 5:B:200:ILE:O | 2.20 | 0.41 |
| 1:A:405:U:OP1 | 7:D:5:ILE:HD11 | 2.20 | 0.41 |
| 1:A:407:G:C8 | 1:A:407:G:O5' | 2.65 | 0.41 |
| 16:M:81:LEU:HD21 | 16:M:88:ARG:NE | 2.35 | 0.41 |
| 1:A:983:A:H1' | 1:A:1201:A:C6 | 2.55 | 0.41 |
| 1:A:19:C:H2' | 1:A:20:U:C6 | 2.56 | 0.41 |
| 1:A:392:G:O5' | 19:P:12:LYS:HE2 | 2.20 | 0.41 |
| 1:A:1127:G:H21 | 1:A:1147:C:N4 | 2.19 | 0.41 |
| 1:A:878:G:H8 | 1:A:878:G:O5' | 2.02 | 0.41 |
| 8:E:102:ALA:HB1 | 8:E:106:PRO:HB2 | 2.02 | 0.41 |
| 1:A:948:C:C5 | 16:M:106:ASN:OD1 | 2.73 | 0.41 |
| 1:A:687:A:HO2' | 1:A:688:G:C5' | 2.32 | 0.41 |
| 1:A:1328:C:OP1 | 24:U:20:LYS:NZ | 2.51 | 0.41 |
| 1:A:1340:A:OP2 | 3:W:34:G:O2' | 2.37 | 0.41 |
| 1:A:123:C:H2' | 1:A:124:G:C8 | 2.56 | 0.41 |
| 3:W:9:A:C6 | 3:W:45:G:C6 | 3.09 | 0.41 |
| 1:A:426:G:O2' | 7:D:42:GLN:HB2 | 2.17 | 0.41 |
| 1:A:1250:A:H4' | 12:I:67:GLY:HA2 | 2.00 | 0.41 |
| 6:C:91:LEU:CD1 | 6:C:99:VAL:HG22 | 2.32 | 0.41 |
| 1:A:40:C:H2' | 1:A:41:G:O4' | 2.20 | 0.41 |
| 1:A:668:G:H4' | 18:O:48:LYS:O | 2.20 | 0.41 |
| 1:A:106:C:OP2 | 1:A:106:C:H6 | 2.04 | 0.41 |
| 1:A:522:C:H41 | 15:L:53:ARG:HH21 | 1.68 | 0.41 |
| 5:B:69:LEU:CD2 | 5:B:91:PRO:HB2 | 2.51 | 0.41 |
| 1:A:1097:C:C4' | 1:A:1169:A:H4' | 2.50 | 0.41 |
| 5:B:85:ALA:HA | 5:B:88:ALA:HB3 | 2.02 | 0.41 |
| 2:V:45:G:C2' | 2:V:46:G:OP2 | 2.65 | 0.41 |
| 1:A:362:G:O5' | 15:L:34:ARG:NH2 | 2.54 | 0.41 |
| 1:A:658:G:O2' | 18:O:22:THR:HB | 2.21 | 0.41 |
| 1:A:1388:C:H2' | 1:A:1389:C:C6 | 2.56 | 0.41 |
| 14:K:23:ALA:HB2 | 14:K:28:THR:HG23 | 2.03 | 0.41 |
| 1:A:1320:C:C5' | 22:S:73:GLU:OE2 | 2.69 | 0.41 |
| 1:A:975:A:N9 | 1:A:1357:A:C2 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:975:A:C5 | 1:A:1357:A:C2 | 3.02 | 0.41 |
| 1:A:1320:C:H6 | 22:S:70:LYS:HD2 | 1.82 | 0.41 |
| 6:C:5:ILE:HG23 | 13:J:51:ARG:NH2 | 2.36 | 0.41 |
| 1:A:1367:C:H5' | 13:J:60:ARG:NH2 | 2.36 | 0.41 |
| 1:A:1197:G:OP1 | 1:A:1197:G:H3' | 2.20 | 0.41 |
| 17:N:24:CYS:HB3 | 17:N:40:CYS:N | 2.13 | 0.41 |
| 1:A:672:U:H2' | 1:A:672:U:O2 | 2.21 | 0.41 |
| 2:V:72:C:H2' | 2:V:73:A:O4' | 2.20 | 0.41 |
| 1:A:1095:U:P | 1:A:1108:G:N2 | 2.87 | 0.41 |
| 13:J:46:ARG:NH1 | 17:N:59:ALA:CB | 2.71 | 0.41 |
| 1:A:511:C:H42 | 1:A:541:G:N2 | 2.19 | 0.41 |
| 11:H:27:PRO:HB2 | 11:H:32:LYS:NZ | 2.30 | 0.41 |
| 12:I:13:ALA:HA | 12:I:67:GLY:HA3 | 2.02 | 0.41 |
| 1:A:376:G:OP1 | 19:P:6:LEU:HD22 | 2.21 | 0.41 |
| 7:D:14:ARG:HG2 | 7:D:66:ARG:CZ | 2.51 | 0.41 |
| 1:A:1347:G:N2 | 1:A:1373:G:C4 | 2.89 | 0.41 |
| 1:A:549:C:C4 | 1:A:550:G:N7 | 2.89 | 0.41 |
| 1:A:1074:G:C2 | 1:A:1102:A:C4 | 3.09 | 0.41 |
| 8:E:152:ARG:HA | 11:H:64:LYS:CE | 2.51 | 0.41 |
| 20:Q:97:SER:CB | 20:Q:103:GLY:CA | 2.99 | 0.41 |
| 2:V:16:U:H4' | 2:V:18:G:C5' | 2.51 | 0.41 |
| 2:V:50:U:H2' | 2:V:51:G:C8 | 2.56 | 0.41 |
| 1:A:224:C:H2' | 1:A:225:C:C6 | 2.55 | 0.41 |
| 1:A:599:C:H5'' | 11:H:96:GLY:N | 2.36 | 0.41 |
| 1:A:1114:C:O2' | 17:N:60:SER:HB2 | 2.20 | 0.41 |
| 1:A:512:U:H2' | 1:A:513:C:H6 | 1.86 | 0.41 |
| 1:A:588:G:O3' | 11:H:5:PRO:HG2 | 2.20 | 0.41 |
| 14:K:48:ILE:HD13 | 14:K:63:LEU:HB3 | 2.03 | 0.41 |
| 1:A:1268:A:C4' | 24:U:20:LYS:HB2 | 2.51 | 0.41 |
| 1:A:1329:A:P | 16:M:28:ALA:HB3 | 2.60 | 0.41 |
| 16:M:23:TYR:C | 16:M:70:LEU:HD13 | 2.41 | 0.41 |
| 1:A:950:U:C2 | 1:A:951:G:C8 | 3.08 | 0.41 |
| 2:V:67:A:O2' | 2:V:68:U:H5' | 2.21 | 0.41 |
| 1:A:1067:A:H3' | 1:A:1093:A:H4' | 2.03 | 0.41 |
| 1:A:508:C:H4' | 1:A:509:A:O5' | 2.21 | 0.41 |
| 1:A:54:C:C5 | 1:A:352:C:H2' | 2.56 | 0.41 |
| 21:R:47:THR:O | 21:R:82:THR:HA | 2.21 | 0.41 |
| 5:B:15:VAL:CG2 | 5:B:209:ARG:HD2 | 2.50 | 0.41 |
| 7:D:121:VAL:HG22 | 7:D:126:ILE:HG13 | 2.03 | 0.41 |
| 1:A:95:U:H2' | 1:A:96:G:H8 | 1.85 | 0.41 |
| 1:A:150:C:H2' | 1:A:151:A:O4' | 2.20 | 0.41 |
| 6:C:88:ARG:CZ | 6:C:101:LEU:H | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:D:119:GLN:HG2 | 7:D:123:HIS:CD2 | 2.56 | 0.40 |
| 1:A:409:G:P | 7:D:25:ARG:HB3 | 2.61 | 0.40 |
| 7:D:21:LEU:CD1 | 7:D:67:ILE:HA | 2.50 | 0.40 |
| 6:C:18:TRP:O | 6:C:21:ARG:HG2 | 2.21 | 0.40 |
| 1:A:31:G:C5 | 1:A:306:G:C1' | 2.95 | 0.40 |
| 1:A:908:A:H8 | 1:A:908:A:O5' | 2.04 | 0.40 |
| 1:A:673:G:C2 | 1:A:734:G:C4 | 3.09 | 0.40 |
| 2:V:58:A:N7 | 2:V:61:C:C4 | 2.89 | 0.40 |
| 12:I:58:ARG:HB3 | 12:I:59:PHE:HD1 | 1.86 | 0.40 |
| 1:A:1080:A:H5' | 8:E:14:ARG:NH2 | 2.36 | 0.40 |
| 18:O:39:LEU:HB3 | 18:O:56:LEU:HD13 | 2.03 | 0.40 |
| 15:L:60:LEU:HD23 | 15:L:64:TYR:HB3 | 2.02 | 0.40 |
| 1:A:187:C:H1' | 23:T:85:MET:SD | 2.61 | 0.40 |
| 3:W:52:U:O2' | 3:W:53:G:H5' | 2.20 | 0.40 |
| 1:A:157:G:C2 | 1:A:165:C:N3 | 2.89 | 0.40 |
| 18:O:35:ARG:HH12 | 18:O:59:MET:HG3 | 1.86 | 0.40 |
| 1:A:1320:C:C5' | 22:S:3:ARG:NH2 | 2.83 | 0.40 |
| 1:A:1327:C:H5' | 24:U:20:LYS:CB | 2.44 | 0.40 |
| 1:A:978:A:O2' | 22:S:37:ARG:NH2 | 2.46 | 0.40 |
| 1:A:1339:A:C2 | 2:V:31:A:O4' | 2.74 | 0.40 |
| 1:A:1392:G:N2 | 1:A:1502:A:C8 | 2.87 | 0.40 |
| 1:A:1526:G:H8 | 1:A:1526:G:OP2 | 2.05 | 0.40 |
| 1:A:1182:G:H4' | 1:A:1183:A:H5'' | 2.03 | 0.40 |
| 1:A:1123:A:O2' | 13:J:38:ILE:CG2 | 2.69 | 0.40 |
| 1:A:823:G:N2 | 11:H:1:MET:N | 2.70 | 0.40 |
| 14:K:42:TRP:CZ3 | 14:K:47:VAL:HG21 | 2.55 | 0.40 |
| 9:F:41:GLU:O | 9:F:42:GLU:HB3 | 2.21 | 0.40 |
| 1:A:862:C:H1' | 1:A:874:G:H5'' | 2.02 | 0.40 |
| 10:G:5:ARG:HB3 | 10:G:6:ARG:H | 1.60 | 0.40 |
| 1:A:1220:G:C2' | 22:S:36:ARG:HD3 | 2.49 | 0.40 |
| 1:A:1327:C:H5 | 24:U:6:ARG:HH21 | 1.69 | 0.40 |
| 7:D:187:ARG:O | 7:D:188:LEU:C | 2.60 | 0.40 |
| 1:A:1199:U:O4' | 13:J:54:PHE:CE2 | 2.74 | 0.40 |
| 3:W:72:C:C2 | 3:W:73:A:C8 | 3.10 | 0.40 |
| 7:D:94:LEU:HA | 7:D:97:LEU:HD12 | 2.02 | 0.40 |
| 1:A:1128:C:H1' | 1:A:1146:A:H61 | 1.85 | 0.40 |
| 1:A:376:G:O4' | 19:P:28:ARG:HB2 | 2.21 | 0.40 |
| 1:A:198:G:H2' | 1:A:199:G:H8 | 1.87 | 0.40 |
| 1:A:1368:G:C8 | 12:I:112:LYS:HD2 | 2.56 | 0.40 |
| 1:A:628:G:H2' | 1:A:629:G:C8 | 2.56 | 0.40 |
| 7:D:57:ARG:HB3 | 7:D:206:PHE:HB2 | 2.02 | 0.40 |
| 7:D:58:LEU:HD23 | 7:D:206:PHE:CE1 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:D:79:PHE:CE1 | 7:D:204:ILE:HG13 | 2.56 | 0.40 |
| 5:B:19:HIS:CD2 | 5:B:20:GLU:HG2 | 2.56 | 0.40 |
| 15:L:60:LEU:HD23 | 15:L:64:TYR:HB2 | 2.02 | 0.40 |
| 1:A:204:U:O2 | 1:A:204:U:H2' | 2.21 | 0.40 |
| 1:A:988:G:O2' | 1:A:1014:A:N6 | 2.54 | 0.40 |
| 7:D:21:LEU:HD23 | 7:D:114:ARG:HG3 | 1.96 | 0.40 |
| 16:M:77:ASN:HA | 16:M:80:ARG:HD3 | 2.04 | 0.40 |
| 1:A:39:G:N7 | 1:A:498:U:O4 | 2.54 | 0.40 |
| 1:A:570:G:H2' | 1:A:571:U:H5 | 1.82 | 0.40 |
| 1:A:1118:C:P | 12:I:104:ARG:HB2 | 2.61 | 0.40 |
| 1:A:1206:G:C4' | 6:C:194:GLY:N | 2.85 | 0.40 |
| 10:G:75:VAL:HG23 | 10:G:145:ALA:HA | 2.04 | 0.40 |
| 1:A:1182:G:O2' | 1:A:1183:A:P | 2.79 | 0.40 |
| 16:M:108:ARG:NH2 | 16:M:114:ARG:HA | 2.36 | 0.40 |
| 10:G:26:PHE:CE2 | 10:G:30:ILE:HD11 | 2.56 | 0.40 |
| 1:A:400:C:O5' | 7:D:73:ARG:NH2 | 2.54 | 0.40 |
| 15:L:33:ARG:HG2 | 15:L:60:LEU:HG | 2.03 | 0.40 |
| 1:A:620:C:C4 | 7:D:135:LEU:HD13 | 2.56 | 0.40 |
| 5:B:55:PHE:HD2 | 5:B:221:LEU:HG | 1.86 | 0.40 |
| 12:I:28:VAL:N | 12:I:31:GLN:O | 2.51 | 0.40 |
| 1:A:987:G:HO2' | 22:S:34:TRP:HH2 | 1.64 | 0.40 |
| 13:J:66:ARG:HD3 | 13:J:68:HIS:NE2 | 2.37 | 0.40 |
| 7:D:68:TYR:HB3 | 7:D:70:ILE:HG12 | 2.03 | 0.40 |
| 11:H:63:LEU:HD13 | 11:H:63:LEU:H | 1.84 | 0.40 |
| 13:J:11:PHE:CG | 17:N:55:GLY:HA3 | 2.56 | 0.40 |
| 1:A:130:A:H5'' | 1:A:190(F):G:H2' | 2.03 | 0.40 |
| 23:T:73:HIS:HB3 | 23:T:74:LYS:HE2 | 2.04 | 0.40 |
| 23:T:88:VAL:O | 23:T:92:LEU:HG | 2.22 | 0.40 |
| 1:A:443:C:H42 | 1:A:491:G:H1 | 1.70 | 0.40 |
| 6:C:19:GLU:HA | 6:C:54:ARG:HH21 | 1.86 | 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 | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 5 | B | 232/256 (91%) | 183 (79%) | 34 (15%) | 15 (6%) | 2 | 35 |
| 6 | C | 204/239 (85%) | 165 (81%) | 23 (11%) | 16 (8%) | 1 | 28 |
| 7 | D | 206/209 (99%) | 156 (76%) | 33 (16%) | 17 (8%) | 1 | 26 |
| 8 | E | 148/162 (91%) | 115 (78%) | 29 (20%) | 4 (3%) | 8 | 60 |
| 9 | F | 99/101 (98%) | 85 (86%) | 10 (10%) | 4 (4%) | 5 | 49 |
| 10 | G | 153/156 (98%) | 131 (86%) | 18 (12%) | 4 (3%) | 8 | 60 |
| 11 | H | 136/138 (99%) | 101 (74%) | 25 (18%) | 10 (7%) | 2 | 30 |
| 12 | I | 125/128 (98%) | 87 (70%) | 30 (24%) | 8 (6%) | 2 | 35 |
| 13 | J | 96/105 (91%) | 73 (76%) | 14 (15%) | 9 (9%) | 1 | 23 |
| 14 | K | 117/129 (91%) | 88 (75%) | 22 (19%) | 7 (6%) | 2 | 37 |
| 15 | L | 122/135 (90%) | 92 (75%) | 13 (11%) | 17 (14%) | 0 | 11 |
| 16 | M | 119/126 (94%) | 95 (80%) | 19 (16%) | 5 (4%) | 4 | 47 |
| 17 | N | 58/61 (95%) | 42 (72%) | 12 (21%) | 4 (7%) | 2 | 32 |
| 18 | O | 86/89 (97%) | 76 (88%) | 9 (10%) | 1 (1%) | 19 | 77 |
| 19 | P | 81/88 (92%) | 64 (79%) | 10 (12%) | 7 (9%) | 1 | 25 |
| 20 | Q | 102/105 (97%) | 78 (76%) | 18 (18%) | 6 (6%) | 2 | 38 |
| 21 | R | 71/88 (81%) | 54 (76%) | 11 (16%) | 6 (8%) | 1 | 26 |
| 22 | S | 78/93 (84%) | 60 (77%) | 15 (19%) | 3 (4%) | 5 | 51 |
| 23 | T | 97/106 (92%) | 79 (81%) | 12 (12%) | 6 (6%) | 2 | 36 |
| 24 | U | 22/27 (82%) | 17 (77%) | 3 (14%) | 2 (9%) | 1 | 24 |
| All | All | 2352/2541 (93%) | 1841 (78%) | 360 (15%) | 151 (6%) | 2 | 35 |

All (151) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | B | 24 | TRP |
| 5 | B | 104 | ASN |
| 5 | B | 153 | ARG |
| 5 | B | 154 | LEU |
| 5 | B | 161 | ALA |
| 6 | C | 18 | TRP |
| 6 | C | 19 | GLU |
| 6 | C | 52 | LEU |
| 6 | C | 53 | ALA |
| 7 | D | 5 | ILE |
| 7 | D | 20 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | D | 21 | LEU |
| 7 | D | 29 | PRO |
| 7 | D | 32 | ALA |
| 7 | D | 129 | ASN |
| 7 | D | 170 | VAL |
| 9 | F | 95 | GLU |
| 10 | G | 35 | LYS |
| 11 | H | 44 | PHE |
| 11 | H | 74 | PRO |
| 11 | H | 97 | VAL |
| 11 | H | 121 | ASP |
| 11 | H | 134 | ILE |
| 12 | I | 12 | GLU |
| 12 | I | 70 | LYS |
| 13 | J | 61 | GLU |
| 14 | K | 104 | GLN |
| 15 | L | 12 | ARG |
| 15 | L | 27 | LEU |
| 15 | L | 46 | LYS |
| 15 | L | 48 | PRO |
| 15 | L | 127 | GLU |
| 16 | M | 28 | ALA |
| 18 | O | 88 | ARG |
| 20 | Q | 34 | LYS |
| 20 | Q | 99 | SER |
| 20 | Q | 104 | LYS |
| 21 | R | 81 | PHE |
| 21 | R | 82 | THR |
| 21 | R | 84 | LYS |
| 23 | T | 71 | THR |
| 5 | B | 15 | VAL |
| 5 | B | 17 | PHE |
| 5 | B | 181 | PHE |
| 5 | B | 232 | PRO |
| 6 | C | 4 | LYS |
| 6 | C | 25 | GLY |
| 6 | C | 98 | ASN |
| 6 | C | 179 | ARG |
| 6 | C | 206 | GLU |
| 7 | D | 12 | CYS |
| 7 | D | 30 | LYS |
| 7 | D | 99 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | E | 11 | ILE |
| 8 | E | 37 | ARG |
| 8 | E | 95 | ALA |
| 9 | F | 69 | GLU |
| 11 | H | 89 | PRO |
| 12 | I | 68 | GLY |
| 12 | I | 103 | THR |
| 12 | I | 116 | LYS |
| 13 | J | 34 | VAL |
| 13 | J | 52 | GLY |
| 13 | J | 72 | VAL |
| 14 | K | 126 | ARG |
| 15 | L | 77 | LEU |
| 15 | L | 105 | TYR |
| 15 | L | 116 | SER |
| 15 | L | 121 | GLY |
| 16 | M | 7 | VAL |
| 17 | N | 17 | LYS |
| 20 | Q | 68 | ARG |
| 21 | R | 37 | VAL |
| 22 | S | 64 | GLU |
| 23 | T | 68 | LYS |
| 24 | U | 17 | THR |
| 24 | U | 21 | TYR |
| 5 | B | 96 | ARG |
| 5 | B | 152 | PHE |
| 6 | C | 28 | GLN |
| 6 | C | 64 | VAL |
| 7 | D | 179 | GLU |
| 8 | E | 145 | LYS |
| 11 | H | 75 | ARG |
| 12 | I | 55 | ALA |
| 13 | J | 54 | PHE |
| 14 | K | 103 | LEU |
| 14 | K | 112 | THR |
| 15 | L | 17 | LYS |
| 15 | L | 83 | VAL |
| 16 | M | 15 | VAL |
| 17 | N | 31 | ARG |
| 19 | P | 43 | LYS |
| 19 | P | 81 | ARG |
| 5 | B | 158 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | C | 16 | ARG |
| 6 | C | 66 | VAL |
| 7 | D | 4 | TYR |
| 7 | D | 196 | LEU |
| 10 | G | 90 | GLU |
| 11 | H | 65 | TYR |
| 11 | H | 73 | ASP |
| 11 | H | 77 | GLU |
| 14 | K | 13 | GLN |
| 14 | K | 113 | PRO |
| 14 | K | 128 | ALA |
| 15 | L | 76 | ASN |
| 15 | L | 96 | VAL |
| 15 | L | 126 | LYS |
| 16 | M | 117 | VAL |
| 19 | P | 13 | HIS |
| 19 | P | 44 | THR |
| 21 | R | 21 | LYS |
| 21 | R | 87 | ARG |
| 23 | T | 69 | GLY |
| 23 | T | 97 | ALA |
| 23 | T | 98 | PRO |
| 5 | B | 191 | ASP |
| 7 | D | 131 | ARG |
| 7 | D | 134 | ASP |
| 7 | D | 143 | GLY |
| 9 | F | 15 | ASP |
| 12 | I | 105 | ASP |
| 13 | J | 32 | ALA |
| 13 | J | 58 | ASP |
| 13 | J | 90 | LEU |
| 15 | L | 22 | SER |
| 19 | P | 15 | PRO |
| 5 | B | 130 | ARG |
| 10 | G | 81 | GLY |
| 15 | L | 19 | ARG |
| 16 | M | 68 | GLY |
| 20 | Q | 4 | LYS |
| 20 | Q | 66 | SER |
| 6 | C | 5 | ILE |
| 7 | D | 109 | GLY |
| 17 | N | 7 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | C | 81 | GLY |
| 12 | I | 100 | GLY |
| 17 | N | 56 | VAL |
| 19 | P | 19 | ILE |
| 22 | S | 8 | GLY |
| 22 | S | 45 | VAL |
| 5 | B | 124 | SER |
| 10 | G | 71 | PRO |
| 15 | L | 31 | PRO |
| 23 | T | 96 | GLY |
| 6 | C | 14 | ILE |
| 9 | F | 68 | PRO |
| 13 | J | 82 | ILE |
| 19 | P | 63 | GLY |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5 | B | 202/220 (92%) | 173 (86%) | 29 (14%) | 5 | 31 |
| 6 | C | 160/188 (85%) | 146 (91%) | 14 (9%) | 14 | 57 |
| 7 | D | 180/181 (99%) | 162 (90%) | 18 (10%) | 11 | 50 |
| 8 | E | 115/123 (94%) | 94 (82%) | 21 (18%) | 2 | 17 |
| 9 | F | 90/90 (100%) | 83 (92%) | 7 (8%) | 18 | 63 |
| 10 | G | 126/127 (99%) | 116 (92%) | 10 (8%) | 18 | 62 |
| 11 | H | 119/119 (100%) | 91 (76%) | 28 (24%) | 1 | 9 |
| 12 | I | 98/99 (99%) | 90 (92%) | 8 (8%) | 17 | 60 |
| 13 | J | 88/92 (96%) | 77 (88%) | 11 (12%) | 7 | 38 |
| 14 | K | 90/99 (91%) | 85 (94%) | 5 (6%) | 30 | 75 |
| 15 | L | 104/111 (94%) | 93 (89%) | 11 (11%) | 10 | 47 |
| 16 | M | 100/101 (99%) | 87 (87%) | 13 (13%) | 6 | 36 |
| 17 | N | 49/50 (98%) | 43 (88%) | 6 (12%) | 7 | 39 |
| 18 | O | 79/80 (99%) | 70 (89%) | 9 (11%) | 8 | 42 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 19 | P | 72/74 (97%) | 62 (86%) | 10 (14%) | 5 | 33 |
| 20 | Q | 96/97 (99%) | 87 (91%) | 9 (9%) | 13 | 53 |
| 21 | R | 64/77 (83%) | 57 (89%) | 7 (11%) | 9 | 46 |
| 22 | S | 71/80 (89%) | 64 (90%) | 7 (10%) | 11 | 50 |
| 23 | T | 76/82 (93%) | 68 (90%) | 8 (10%) | 10 | 47 |
| 24 | U | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |
| All | All | 1998/2112 (95%) | 1767 (88%) | 231 (12%) | 8 | 42 |

All (231) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | B | 10 | LEU |
| 5 | B | 11 | LEU |
| 5 | B | 15 | VAL |
| 5 | B | 17 | PHE |
| 5 | B | 21 | ARG |
| 5 | B | 23 | ARG |
| 5 | B | 28 | PHE |
| 5 | B | 30 | ARG |
| 5 | B | 36 | ARG |
| 5 | B | 42 | ILE |
| 5 | B | 48 | MET |
| 5 | B | 64 | ARG |
| 5 | B | 68 | ILE |
| 5 | B | 96 | ARG |
| 5 | B | 103 | THR |
| 5 | B | 135 | GLN |
| 5 | B | 147 | LYS |
| 5 | B | 152 | PHE |
| 5 | B | 154 | LEU |
| 5 | B | 158 | LEU |
| 5 | B | 162 | ILE |
| 5 | B | 169 | LYS |
| 5 | B | 198 | ASP |
| 5 | B | 204 | ASN |
| 5 | B | 205 | ASP |
| 5 | B | 209 | ARG |
| 5 | B | 212 | GLN |
| 5 | B | 215 | LEU |
| 5 | B | 238 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | C | 3 | ASN |
| 6 | C | 23 | TYR |
| 6 | C | 28 | GLN |
| 6 | C | 52 | LEU |
| 6 | C | 82 | GLU |
| 6 | C | 91 | LEU |
| 6 | C | 98 | ASN |
| 6 | C | 99 | VAL |
| 6 | C | 156 | ARG |
| 6 | C | 176 | HIS |
| 6 | C | 177 | THR |
| 6 | C | 188 | LEU |
| 6 | C | 192 | THR |
| 6 | C | 196 | LEU |
| 7 | D | 9 | CYS |
| 7 | D | 20 | TYR |
| 7 | D | 31 | CYS |
| 7 | D | 33 | MET |
| 7 | D | 53 | ASP |
| 7 | D | 60 | GLU |
| 7 | D | 61 | LYS |
| 7 | D | 71 | SER |
| 7 | D | 78 | LEU |
| 7 | D | 79 | PHE |
| 7 | D | 103 | ASN |
| 7 | D | 107 | ARG |
| 7 | D | 122 | ARG |
| 7 | D | 131 | ARG |
| 7 | D | 182 | LYS |
| 7 | D | 191 | ARG |
| 7 | D | 193 | ASP |
| 7 | D | 194 | LEU |
| 8 | E | 5 | ASP |
| 8 | E | 12 | LEU |
| 8 | E | 13 | ILE |
| 8 | E | 14 | ARG |
| 8 | E | 15 | ARG |
| 8 | E | 20 | GLN |
| 8 | E | 27 | ARG |
| 8 | E | 28 | PHE |
| 8 | E | 38 | GLN |
| 8 | E | 41 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | E | 47 | LYS |
| 8 | E | 56 | GLN |
| 8 | E | 63 | ARG |
| 8 | E | 64 | ARG |
| 8 | E | 68 | GLU |
| 8 | E | 80 | ILE |
| 8 | E | 81 | GLU |
| 8 | E | 89 | ILE |
| 8 | E | 112 | LEU |
| 8 | E | 135 | THR |
| 8 | E | 150 | ARG |
| 9 | F | 15 | ASP |
| 9 | F | 48 | LEU |
| 9 | F | 57 | GLN |
| 9 | F | 86 | ARG |
| 9 | F | 94 | GLN |
| 9 | F | 95 | GLU |
| 9 | F | 98 | LEU |
| 10 | G | 3 | ARG |
| 10 | G | 8 | GLU |
| 10 | G | 31 | MET |
| 10 | G | 36 | LYS |
| 10 | G | 37 | ASN |
| 10 | G | 103 | TRP |
| 10 | G | 104 | LEU |
| 10 | G | 106 | GLN |
| 10 | G | 125 | MET |
| 10 | G | 155 | ARG |
| 11 | H | 3 | THR |
| 11 | H | 6 | ILE |
| 11 | H | 8 | ASP |
| 11 | H | 14 | ARG |
| 11 | H | 17 | THR |
| 11 | H | 18 | ARG |
| 11 | H | 25 | ASP |
| 11 | H | 26 | VAL |
| 11 | H | 37 | ARG |
| 11 | H | 41 | ARG |
| 11 | H | 49 | GLU |
| 11 | H | 50 | ARG |
| 11 | H | 56 | LYS |
| 11 | H | 58 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | H | 59 | LEU |
| 11 | H | 63 | LEU |
| 11 | H | 65 | TYR |
| 11 | H | 77 | GLU |
| 11 | H | 84 | ARG |
| 11 | H | 98 | LYS |
| 11 | H | 100 | ILE |
| 11 | H | 101 | PRO |
| 11 | H | 107 | LEU |
| 11 | H | 112 | LEU |
| 11 | H | 122 | ARG |
| 11 | H | 126 | LYS |
| 11 | H | 127 | LEU |
| 11 | H | 136 | GLU |
| 12 | I | 3 | GLN |
| 12 | I | 37 | PHE |
| 12 | I | 47 | LEU |
| 12 | I | 50 | LEU |
| 12 | I | 51 | ARG |
| 12 | I | 102 | LEU |
| 12 | I | 114 | TYR |
| 12 | I | 116 | LYS |
| 13 | J | 13 | HIS |
| 13 | J | 45 | ARG |
| 13 | J | 47 | PHE |
| 13 | J | 60 | ARG |
| 13 | J | 62 | HIS |
| 13 | J | 63 | PHE |
| 13 | J | 71 | LEU |
| 13 | J | 73 | ASP |
| 13 | J | 82 | ILE |
| 13 | J | 87 | THR |
| 13 | J | 94 | VAL |
| 14 | K | 18 | ARG |
| 14 | K | 41 | THR |
| 14 | K | 62 | GLN |
| 14 | K | 103 | LEU |
| 14 | K | 116 | HIS |
| 15 | L | 7 | ILE |
| 15 | L | 22 | SER |
| 15 | L | 23 | LYS |
| 15 | L | 50 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | L | 85 | ILE |
| 15 | L | 99 | HIS |
| 15 | L | 100 | ILE |
| 15 | L | 101 | VAL |
| 15 | L | 113 | ARG |
| 15 | L | 126 | LYS |
| 15 | L | 127 | GLU |
| 16 | M | 32 | GLU |
| 16 | M | 44 | ARG |
| 16 | M | 48 | LEU |
| 16 | M | 64 | TRP |
| 16 | M | 66 | LEU |
| 16 | M | 77 | ASN |
| 16 | M | 80 | ARG |
| 16 | M | 81 | LEU |
| 16 | M | 86 | CYS |
| 16 | M | 88 | ARG |
| 16 | M | 96 | LEU |
| 16 | M | 108 | ARG |
| 16 | M | 110 | ARG |
| 17 | N | 16 | PHE |
| 17 | N | 21 | TYR |
| 17 | N | 22 | THR |
| 17 | N | 24 | CYS |
| 17 | N | 42 | ILE |
| 17 | N | 58 | LYS |
| 18 | O | 3 | ILE |
| 18 | O | 4 | THR |
| 18 | O | 10 | LYS |
| 18 | O | 34 | LEU |
| 18 | O | 36 | ILE |
| 18 | O | 38 | ARG |
| 18 | O | 44 | LYS |
| 18 | O | 46 | HIS |
| 18 | O | 54 | ARG |
| 19 | P | 3 | LYS |
| 19 | P | 6 | LEU |
| 19 | P | 12 | LYS |
| 19 | P | 21 | VAL |
| 19 | P | 27 | LYS |
| 19 | P | 28 | ARG |
| 19 | P | 29 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | P | 34 | GLU |
| 19 | P | 43 | LYS |
| 19 | P | 48 | TRP |
| 20 | Q | 20 | THR |
| 20 | Q | 36 | ILE |
| 20 | Q | 38 | ARG |
| 20 | Q | 48 | GLU |
| 20 | Q | 60 | ILE |
| 20 | Q | 78 | GLU |
| 20 | Q | 93 | GLN |
| 20 | Q | 96 | GLN |
| 20 | Q | 101 | ARG |
| 21 | R | 28 | GLU |
| 21 | R | 36 | ASN |
| 21 | R | 47 | THR |
| 21 | R | 49 | LYS |
| 21 | R | 54 | ARG |
| 21 | R | 79 | LEU |
| 21 | R | 88 | LYS |
| 22 | S | 15 | LEU |
| 22 | S | 18 | LYS |
| 22 | S | 25 | LYS |
| 22 | S | 30 | LEU |
| 22 | S | 34 | TRP |
| 22 | S | 43 | GLU |
| 22 | S | 61 | TYR |
| 23 | T | 26 | ASN |
| 23 | T | 30 | LYS |
| 23 | T | 48 | LYS |
| 23 | T | 71 | THR |
| 23 | T | 73 | HIS |
| 23 | T | 75 | ASN |
| 23 | T | 90 | GLN |
| 23 | T | 100 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | B | 94 | ASN |
| 5 | B | 204 | ASN |
| 5 | B | 212 | GLN |
| 5 | B | 240 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | C | 3 | ASN |
| 6 | C | 136 | GLN |
| 6 | C | 139 | GLN |
| 6 | C | 170 | GLN |
| 6 | C | 176 | HIS |
| 7 | D | 42 | GLN |
| 7 | D | 45 | GLN |
| 7 | D | 62 | GLN |
| 7 | D | 103 | ASN |
| 7 | D | 119 | GLN |
| 7 | D | 123 | HIS |
| 7 | D | 154 | ASN |
| 8 | E | 56 | GLN |
| 9 | F | 7 | ASN |
| 9 | F | 13 | ASN |
| 9 | F | 18 | GLN |
| 9 | F | 32 | ASN |
| 9 | F | 57 | GLN |
| 9 | F | 94 | GLN |
| 10 | G | 64 | GLN |
| 10 | G | 68 | ASN |
| 10 | G | 106 | GLN |
| 11 | H | 82 | HIS |
| 12 | I | 3 | GLN |
| 12 | I | 87 | GLN |
| 13 | J | 56 | HIS |
| 14 | K | 38 | ASN |
| 15 | L | 49 | ASN |
| 15 | L | 75 | HIS |
| 15 | L | 99 | HIS |
| 16 | M | 92 | HIS |
| 17 | N | 49 | HIS |
| 18 | O | 28 | GLN |
| 18 | O | 37 | ASN |
| 18 | O | 42 | HIS |
| 19 | P | 13 | HIS |
| 19 | P | 16 | HIS |
| 19 | P | 82 | GLN |
| 20 | Q | 16 | GLN |
| 22 | S | 14 | HIS |
| 22 | S | 47 | HIS |
| 22 | S | 56 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | T | 18 | GLN |
| 23 | T | 26 | ASN |
| 23 | T | 73 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1496/1522 (98%) | 518 (34%) | 159 (10%) |
| 2 | V | 75/76 (98%) | 17 (22%) | 2 (2%) |
| 3 | W | 68/76 (89%) | 13 (19%) | 4 (5%) |
| 4 | X | 5/18 (27%) | 0 | 0 |
| All | All | 1644/1692 (97%) | 548 (33%) | 165 (10%) |

All (548) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | G |
| 1 | A | 7 | G |
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 12 | U |
| 1 | A | 13 | U |
| 1 | A | 14 | U |
| 1 | A | 17 | U |
| 1 | A | 25 | C |
| 1 | A | 31 | G |
| 1 | A | 32 | A |
| 1 | A | 33 | A |
| 1 | A | 38 | G |
| 1 | A | 39 | G |
| 1 | A | 41 | G |
| 1 | A | 48 | C |
| 1 | A | 49 | U |
| 1 | A | 50 | A |
| 1 | A | 51 | A |
| 1 | A | 52 | G |
| 1 | A | 54 | C |
| 1 | A | 60 | A |
| 1 | A | 61 | G |
| 1 | A | 62 | U |
| 1 | A | 65 | U |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 66 | G |
| 1 | A | 68 | G |
| 1 | A | 69 | G |
| 1 | A | 70 | G |
| 1 | A | 81 | U |
| 1 | A | 83 | U |
| 1 | A | 89 | C |
| 1 | A | 97 | G |
| 1 | A | 106 | C |
| 1 | A | 108 | G |
| 1 | A | 113 | G |
| 1 | A | 114 | U |
| 1 | A | 116 | A |
| 1 | A | 120 | A |
| 1 | A | 121 | C |
| 1 | A | 122 | G |
| 1 | A | 123 | C |
| 1 | A | 129(A) | G |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 137 | C |
| 1 | A | 144 | G |
| 1 | A | 151 | A |
| 1 | A | 152 | A |
| 1 | A | 153 | C |
| 1 | A | 161 | A |
| 1 | A | 163 | C |
| 1 | A | 181 | G |
| 1 | A | 182 | U |
| 1 | A | 190(E) | U |
| 1 | A | 190(F) | G |
| 1 | A | 190(G) | G |
| 1 | A | 193 | C |
| 1 | A | 195 | A |
| 1 | A | 196 | A |
| 1 | A | 197 | A |
| 1 | A | 198 | G |
| 1 | A | 203 | U |
| 1 | A | 204 | U |
| 1 | A | 218 | C |
| 1 | A | 219 | C |
| 1 | A | 231 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 236 | G |
| 1 | A | 244 | U |
| 1 | A | 245 | C |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 252 | U |
| 1 | A | 253 | U |
| 1 | A | 259 | G |
| 1 | A | 263 | A |
| 1 | A | 264 | U |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 275 | G |
| 1 | A | 279 | A |
| 1 | A | 280 | C |
| 1 | A | 281 | G |
| 1 | A | 287 | U |
| 1 | A | 289 | G |
| 1 | A | 291 | C |
| 1 | A | 299 | G |
| 1 | A | 301 | G |
| 1 | A | 306 | G |
| 1 | A | 308 | C |
| 1 | A | 316 | G |
| 1 | A | 317 | G |
| 1 | A | 319 | G |
| 1 | A | 321 | A |
| 1 | A | 323 | U |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 330 | C |
| 1 | A | 332 | G |
| 1 | A | 345 | C |
| 1 | A | 346 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 355 | C |
| 1 | A | 363 | A |
| 1 | A | 366 | C |
| 1 | A | 367 | U |
| 1 | A | 368 | U |
| 1 | A | 373 | A |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 374 | A |
| 1 | A | 388 | G |
| 1 | A | 389 | A |
| 1 | A | 390 | C |
| 1 | A | 392 | G |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 406 | G |
| 1 | A | 410 | G |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 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 |
| 1 | A | 432 | A |
| 1 | A | 433 | C |
| 1 | A | 438 | G |
| 1 | A | 439 | A |
| 1 | A | 445 | G |
| 1 | A | 450 | G |
| 1 | A | 460 | A |
| 1 | A | 461 | C |
| 1 | A | 462 | G |
| 1 | A | 480 | U |
| 1 | A | 481 | G |
| 1 | A | 482 | A |
| 1 | A | 483 | C |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 486 | U |
| 1 | A | 488 | C |
| 1 | A | 496 | A |
| 1 | A | 497 | A |
| 1 | A | 498 | U |
| 1 | A | 500 | G |
| 1 | A | 505 | G |
| 1 | A | 508 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 512 | U |
| 1 | A | 517 | G |
| 1 | A | 518 | C |
| 1 | A | 519 | C |
| 1 | A | 520 | A |
| 1 | A | 521 | G |
| 1 | A | 523 | A |
| 1 | A | 524 | G |
| 1 | A | 527 | G |
| 1 | A | 530 | G |
| 1 | A | 531 | U |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 536 | C |
| 1 | A | 538 | G |
| 1 | A | 546 | G |
| 1 | A | 547 | A |
| 1 | A | 551 | U |
| 1 | A | 552 | U |
| 1 | A | 553 | A |
| 1 | A | 555 | C |
| 1 | A | 557 | G |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 562 | C |
| 1 | A | 563 | A |
| 1 | A | 566 | G |
| 1 | A | 567 | G |
| 1 | A | 568 | G |
| 1 | A | 569 | C |
| 1 | A | 570 | G |
| 1 | A | 571 | U |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 574 | A |
| 1 | A | 575 | G |
| 1 | A | 576 | G |
| 1 | A | 577 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 579 | G |
| 1 | A | 582 | U |
| 1 | A | 589 | C |
| 1 | A | 591 | U |
| 1 | A | 594 | G |
| 1 | A | 595 | G |
| 1 | A | 596 | C |
| 1 | A | 607 | A |
| 1 | A | 609 | A |
| 1 | A | 618 | C |
| 1 | A | 619 | U |
| 1 | A | 623 | C |
| 1 | A | 627 | G |
| 1 | A | 632 | A |
| 1 | A | 637 | G |
| 1 | A | 642 | A |
| 1 | A | 643 | C |
| 1 | A | 650 | G |
| 1 | A | 653 | A |
| 1 | A | 654 | G |
| 1 | A | 661 | G |
| 1 | A | 665 | A |
| 1 | A | 666 | G |
| 1 | A | 667 | G |
| 1 | A | 671 | G |
| 1 | A | 672 | U |
| 1 | A | 673 | G |
| 1 | A | 674 | G |
| 1 | A | 687 | A |
| 1 | A | 688 | G |
| 1 | A | 694 | A |
| 1 | A | 695 | A |
| 1 | A | 702 | A |
| 1 | A | 703 | G |
| 1 | A | 704 | A |
| 1 | A | 714 | G |
| 1 | A | 716 | A |
| 1 | A | 718 | G |
| 1 | A | 719 | C |
| 1 | A | 721 | G |
| 1 | A | 723 | U |
| 1 | A | 724 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 731 | G |
| 1 | A | 733 | A |
| 1 | A | 745 | C |
| 1 | A | 749 | C |
| 1 | A | 751 | U |
| 1 | A | 753 | A |
| 1 | A | 754 | C |
| 1 | A | 755 | G |
| 1 | A | 757 | U |
| 1 | A | 759 | A |
| 1 | A | 760 | G |
| 1 | A | 761 | G |
| 1 | A | 765 | G |
| 1 | A | 774 | G |
| 1 | A | 775 | G |
| 1 | A | 777 | A |
| 1 | A | 781 | A |
| 1 | A | 782 | A |
| 1 | A | 785 | G |
| 1 | A | 787 | A |
| 1 | A | 790 | A |
| 1 | A | 791 | G |
| 1 | A | 792 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 801 | U |
| 1 | A | 811 | C |
| 1 | A | 812 | C |
| 1 | A | 813 | U |
| 1 | A | 814 | A |
| 1 | A | 815 | A |
| 1 | A | 817 | C |
| 1 | A | 818 | G |
| 1 | A | 820 | U |
| 1 | A | 821 | G |
| 1 | A | 828 | A |
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |
| 1 | A | 864 | A |
| 1 | A | 866 | C |
| 1 | A | 870 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 872 | A |
| 1 | A | 873 | A |
| 1 | A | 874 | G |
| 1 | A | 883 | C |
| 1 | A | 884 | U |
| 1 | A | 885 | G |
| 1 | A | 889 | A |
| 1 | A | 890 | G |
| 1 | A | 891 | U |
| 1 | A | 898 | G |
| 1 | A | 902 | G |
| 1 | A | 913 | A |
| 1 | A | 914 | A |
| 1 | A | 916 | G |
| 1 | A | 917 | G |
| 1 | A | 919 | A |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 929 | G |
| 1 | A | 931 | C |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 940 | C |
| 1 | A | 945 | G |
| 1 | A | 948 | C |
| 1 | A | 949 | A |
| 1 | A | 950 | U |
| 1 | A | 956 | U |
| 1 | A | 958 | A |
| 1 | A | 959 | A |
| 1 | A | 960 | U |
| 1 | A | 961 | U |
| 1 | A | 965 | A |
| 1 | A | 966 | G |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 972 | C |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 980 | C |
| 1 | A | 982 | U |
| 1 | A | 983 | A |
| 1 | A | 989 | C |
| 1 | A | 991 | U |
| 1 | A | 993 | G |
| 1 | A | 994 | A |
| 1 | A | 1005 | A |
| 1 | A | 1006 | C |
| 1 | A | 1007 | C |
| 1 | A | 1013 | G |
| 1 | A | 1022 | G |
| 1 | A | 1023 | G |
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1038 | C |
| 1 | A | 1042 | G |
| 1 | A | 1045 | C |
| 1 | A | 1046 | A |
| 1 | A | 1050 | G |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1056 | U |
| 1 | A | 1062 | U |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1067 | A |
| 1 | A | 1078 | U |
| 1 | A | 1079 | G |
| 1 | A | 1084 | G |
| 1 | A | 1085 | U |
| 1 | A | 1086 | U |
| 1 | A | 1089 | G |
| 1 | A | 1095 | U |
| 1 | A | 1096 | C |
| 1 | A | 1099 | G |
| 1 | A | 1101 | A |
| 1 | A | 1102 | A |
| 1 | A | 1104 | G |
| 1 | A | 1107 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1117 | G |
| 1 | A | 1118 | C |
| 1 | A | 1120 | G |
| 1 | A | 1122 | U |
| 1 | A | 1124 | G |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1128 | C |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1140 | C |
| 1 | A | 1143 | G |
| 1 | A | 1144 | G |
| 1 | A | 1145 | C |
| 1 | A | 1146 | A |
| 1 | A | 1147 | C |
| 1 | A | 1148 | U |
| 1 | A | 1151 | A |
| 1 | A | 1152 | A |
| 1 | A | 1154 | G |
| 1 | A | 1158 | C |
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1161 | C |
| 1 | A | 1169 | A |
| 1 | A | 1177 | G |
| 1 | A | 1180 | A |
| 1 | A | 1183 | A |
| 1 | A | 1184 | G |
| 1 | A | 1185 | G |
| 1 | A | 1186 | G |
| 1 | A | 1188 | A |
| 1 | A | 1191 | A |
| 1 | A | 1192 | C |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1199 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1211 | U |
| 1 | A | 1212 | U |
| 1 | A | 1214 | C |
| 1 | A | 1215 | G |
| 1 | A | 1220 | G |
| 1 | A | 1224 | G |
| 1 | A | 1225 | A |
| 1 | A | 1226 | C |
| 1 | A | 1227 | A |
| 1 | A | 1228 | C |
| 1 | A | 1236 | A |
| 1 | A | 1237 | C |
| 1 | A | 1240 | U |
| 1 | A | 1241 | G |
| 1 | A | 1249 | C |
| 1 | A | 1250 | A |
| 1 | A | 1251 | A |
| 1 | A | 1252 | A |
| 1 | A | 1253 | G |
| 1 | A | 1256 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1260 | C |
| 1 | A | 1263 | C |
| 1 | A | 1268 | A |
| 1 | A | 1270 | C |
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1282 | C |
| 1 | A | 1285 | A |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1289 | A |
| 1 | A | 1292 | U |
| 1 | A | 1293 | G |
| 1 | A | 1297 | C |
| 1 | A | 1298 | C |
| 1 | A | 1299 | A |
| 1 | A | 1300 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1303 | C |
| 1 | A | 1305 | G |
| 1 | A | 1312 | G |
| 1 | A | 1318 | A |
| 1 | A | 1320 | C |
| 1 | A | 1322 | C |
| 1 | A | 1323 | G |
| 1 | A | 1329 | A |
| 1 | A | 1331 | G |
| 1 | A | 1332 | A |
| 1 | A | 1336 | C |
| 1 | A | 1340 | A |
| 1 | A | 1345 | U |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |
| 1 | A | 1348 | U |
| 1 | A | 1354 | C |
| 1 | A | 1361 | G |
| 1 | A | 1363 | A |
| 1 | A | 1364 | U |
| 1 | A | 1365 | G |
| 1 | A | 1381 | U |
| 1 | A | 1386 | G |
| 1 | A | 1394 | A |
| 1 | A | 1395 | C |
| 1 | A | 1397 | C |
| 1 | A | 1398 | A |
| 1 | A | 1399 | C |
| 1 | A | 1400 | C |
| 1 | A | 1401 | G |
| 1 | A | 1402 | C |
| 1 | A | 1419 | G |
| 1 | A | 1432 | G |
| 1 | A | 1436 | U |
| 1 | A | 1437 | C |
| 1 | A | 1440 | C |
| 1 | A | 1442 | G |
| 1 | A | 1443 | G |
| 1 | A | 1449 | C |
| 1 | A | 1452 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1454 | G |
| 1 | A | 1468 | A |
| 1 | A | 1475 | G |
| 1 | A | 1482 | G |
| 1 | A | 1488 | G |
| 1 | A | 1490 | C |
| 1 | A | 1497 | G |
| 1 | A | 1498 | U |
| 1 | A | 1499 | A |
| 1 | A | 1500 | A |
| 1 | A | 1502 | A |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1507 | A |
| 1 | A | 1517 | G |
| 1 | A | 1519 | A |
| 1 | A | 1520 | G |
| 1 | A | 1526 | G |
| 1 | A | 1528 | U |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1531 | A |
| 1 | A | 1532 | U |
| 1 | A | 1533 | C |
| 1 | A | 1534 | A |
| 1 | A | 1535 | C |
| 1 | A | 1540 | U |
| 1 | A | 1541 | U |
| 1 | A | 1542 | U |
| 2 | V | 8 | U |
| 2 | V | 10 | G |
| 2 | V | 16 | U |
| 2 | V | 17 | U |
| 2 | V | 18 | G |
| 2 | V | 20 | G |
| 2 | V | 35 | A |
| 2 | V | 41 | U |
| 2 | V | 46 | G |
| 2 | V | 47 | U |
| 2 | V | 48 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | V | 49 | C |
| 2 | V | 58 | A |
| 2 | V | 59 | U |
| 2 | V | 61 | C |
| 2 | V | 73 | A |
| 2 | V | 75 | C |
| 3 | W | 2 | C |
| 3 | W | 3 | G |
| 3 | W | 17 | U |
| 3 | W | 18 | G |
| 3 | W | 19 | G |
| 3 | W | 21 | A |
| 3 | W | 34 | G |
| 3 | W | 35 | A |
| 3 | W | 36 | A |
| 3 | W | 37 | YYG |
| 3 | W | 41 | U |
| 3 | W | 75 | C |
| 3 | W | 76 | A |

All (165) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 5 | U |
| 1 | A | 7 | G |
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 13 | U |
| 1 | A | 25 | C |
| 1 | A | 30 | U |
| 1 | A | 38 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 49 | U |
| 1 | A | 50 | A |
| 1 | A | 51 | A |
| 1 | A | 60 | A |
| 1 | A | 119 | A |
| 1 | A | 121 | C |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 190(F) | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 202 | U |
| 1 | A | 203 | U |
| 1 | A | 231 | G |
| 1 | A | 243 | A |
| 1 | A | 244 | U |
| 1 | A | 246 | A |
| 1 | A | 250 | A |
| 1 | A | 251 | G |
| 1 | A | 262 | A |
| 1 | A | 266 | G |
| 1 | A | 274 | A |
| 1 | A | 279 | A |
| 1 | A | 280 | C |
| 1 | A | 305 | G |
| 1 | A | 327 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 337 | C |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 366 | C |
| 1 | A | 367 | U |
| 1 | A | 372 | C |
| 1 | A | 388 | G |
| 1 | A | 421 | U |
| 1 | A | 422 | C |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 481 | G |
| 1 | A | 484 | G |
| 1 | A | 496 | A |
| 1 | A | 497 | A |
| 1 | A | 499 | A |
| 1 | A | 508 | C |
| 1 | A | 509 | A |
| 1 | A | 511 | C |
| 1 | A | 517 | G |
| 1 | A | 518 | C |
| 1 | A | 531 | U |
| 1 | A | 533 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 535 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 562 | C |
| 1 | A | 563 | A |
| 1 | A | 566 | G |
| 1 | A | 575 | G |
| 1 | A | 587 | G |
| 1 | A | 595 | G |
| 1 | A | 641 | U |
| 1 | A | 652 | U |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 718 | G |
| 1 | A | 721 | G |
| 1 | A | 727 | G |
| 1 | A | 748 | C |
| 1 | A | 753 | A |
| 1 | A | 759 | A |
| 1 | A | 774 | G |
| 1 | A | 792 | A |
| 1 | A | 793 | U |
| 1 | A | 812 | C |
| 1 | A | 815 | A |
| 1 | A | 817 | C |
| 1 | A | 818 | G |
| 1 | A | 819 | A |
| 1 | A | 851 | G |
| 1 | A | 871 | U |
| 1 | A | 872 | A |
| 1 | A | 873 | A |
| 1 | A | 883 | C |
| 1 | A | 889 | A |
| 1 | A | 903 | G |
| 1 | A | 913 | A |
| 1 | A | 914 | A |
| 1 | A | 960 | U |
| 1 | A | 965 | A |
| 1 | A | 968 | A |
| 1 | A | 975 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 982 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 1037 | C |
| 1 | A | 1049 | U |
| 1 | A | 1053 | G |
| 1 | A | 1065 | U |
| 1 | A | 1085 | U |
| 1 | A | 1101 | A |
| 1 | A | 1108 | G |
| 1 | A | 1117 | G |
| 1 | A | 1124 | G |
| 1 | A | 1125 | U |
| 1 | A | 1145 | C |
| 1 | A | 1151 | A |
| 1 | A | 1157 | A |
| 1 | A | 1159 | U |
| 1 | A | 1182 | G |
| 1 | A | 1190 | G |
| 1 | A | 1196 | U |
| 1 | A | 1201 | A |
| 1 | A | 1214 | C |
| 1 | A | 1225 | A |
| 1 | A | 1226 | C |
| 1 | A | 1240 | U |
| 1 | A | 1256 | A |
| 1 | A | 1257 | U |
| 1 | A | 1279 | A |
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1285 | A |
| 1 | A | 1297 | C |
| 1 | A | 1298 | C |
| 1 | A | 1302 | U |
| 1 | A | 1305 | G |
| 1 | A | 1322 | C |
| 1 | A | 1336 | C |
| 1 | A | 1345 | U |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |
| 1 | A | 1363 | A |
| 1 | A | 1380 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1394 | A |
| 1 | A | 1399 | C |
| 1 | A | 1400 | C |
| 1 | A | 1446 | A |
| 1 | A | 1467 | G |
| 1 | A | 1490 | C |
| 1 | A | 1498 | U |
| 1 | A | 1502 | A |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1529 | G |
| 1 | A | 1532 | U |
| 2 | V | 7 | U |
| 2 | V | 19 | G |
| 3 | W | 16 | U |
| 3 | W | 18 | G |
| 3 | W | 21 | A |
| 3 | W | 35 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|-------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 3 | YYG | W | 37 | 10,3 | 40,42,43 | 1.11 | 4 (10%) | 50,62,65 | 11.14 | 11 (22%) |
| 3 | PSU | W | 39 | 3 | 19,21,22 | 0.92 | 1 (5%) | 23,30,33 | 0.88 | 1 (4%) |
| 3 | PSU | W | 55 | 3 | 19,21,22 | 1.15 | 4 (21%) | 23,30,33 | 1.06 | 2 (8%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | YYG | W | 37 | 10,3 | 1/1/8/9 | 0/25/42/43 | 0/1/4/4 |
| 3 | PSU | W | 39 | 3 | - | 0/8/25/26 | 0/2/2/2 |
| 3 | PSU | W | 55 | 3 | - | 0/8/25/26 | 0/2/2/2 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | W | 37 | YYG | C6-N1 | 2.76 | 1.42 | 1.35 |
| 3 | W | 39 | PSU | C6-C5 | -2.73 | 1.33 | 1.38 |
| 3 | W | 37 | YYG | C2-N1 | -2.40 | 1.36 | 1.39 |
| 3 | W | 37 | YYG | P-OP1 | 2.38 | 1.49 | 1.46 |
| 3 | W | 55 | PSU | C6-C5 | -2.32 | 1.34 | 1.38 |
| 3 | W | 55 | PSU | P-OP1 | 2.21 | 1.49 | 1.46 |
| 3 | W | 37 | YYG | C6-C5 | 2.16 | 1.44 | 1.41 |
| 3 | W | 55 | PSU | C6-N1 | 2.10 | 1.34 | 1.32 |
| 3 | W | 55 | PSU | C4-N3 | 2.01 | 1.40 | 1.37 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3 | W | 37 | YYG | C6-C5-N7 | -75.59 | 130.22 | 134.24 |
| 3 | W | 37 | YYG | C11-C12-N1 | 18.56 | 111.39 | 104.24 |
| 3 | W | 37 | YYG | C24-O23-C21 | 5.81 | 123.15 | 115.66 |
| 3 | W | 37 | YYG | C13-C12-C11 | -5.33 | 123.54 | 131.05 |
| 3 | W | 37 | YYG | O23-C21-N20 | 4.02 | 118.46 | 110.72 |
| 3 | W | 37 | YYG | O23-C21-O22 | -3.85 | 119.70 | 124.64 |
| 3 | W | 37 | YYG | C19-O18-C16 | 2.71 | 122.47 | 116.02 |
| 3 | W | 37 | YYG | C12-C11-N2 | -2.28 | 106.53 | 110.31 |
| 3 | W | 37 | YYG | C5-C6-N1 | -2.28 | 111.77 | 117.68 |
| 3 | W | 37 | YYG | C13-C14-C15 | 2.27 | 116.19 | 112.52 |
| 3 | W | 37 | YYG | O18-C16-C15 | 2.19 | 117.58 | 111.59 |
| 3 | W | 39 | PSU | C5-C4-N3 | -2.17 | 114.91 | 118.86 |
| 3 | W | 55 | PSU | O2'-C2'-C1' | -2.07 | 107.19 | 111.93 |
| 3 | W | 55 | PSU | C4-C5-C1' | -2.07 | 116.87 | 120.95 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3 | W | 37 | YYG | C15 |

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.