



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2014 – 11:45 PM EDT

PDB ID : 4L6J
Title : Crystal Structure of Blastcidin S Bound to Thermus Thermophilus 70S Ribosome. This file contains the 50S subunit and blastcidin S molecule from the first 70S ribosome.
Authors : Svidritskiy, E.; Ling, C.; Ermolenko, D.N.; Korostelev, A.A.
Deposited on : 2013-06-12
Resolution : 3.40 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>

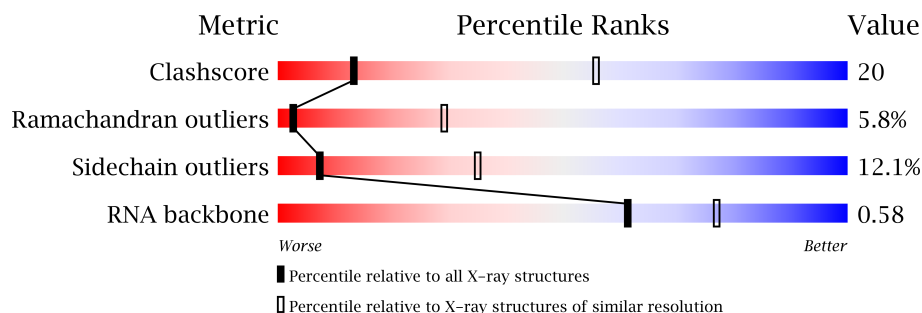
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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 | 1214 (3.50-3.30) |
| Ramachandran outliers | 78287 | 1177 (3.50-3.30) |
| Sidechain outliers | 78261 | 1177 (3.50-3.30) |
| RNA backbone | 1838 | 1002 (4.02-2.76) |





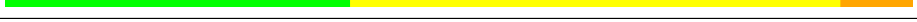

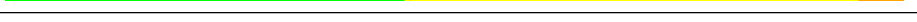

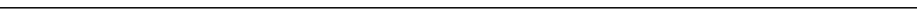





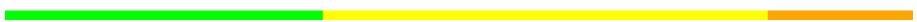

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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 | 2879 | |
| 2 | B | 119 | |
| 3 | D | 271 | |
| 4 | E | 204 | |
| 5 | F | 202 | |
| 6 | G | 181 | |
| 7 | H | 159 | |
| 8 | I | 145 | |
| 9 | J | 137 | |
| 10 | K | 122 | |
| 11 | L | 146 | |
| 12 | M | 134 | |
| 13 | N | 117 | |
| 14 | O | 98 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | P | 137 |  |
| 16 | Q | 117 |  |
| 17 | R | 101 |  |
| 18 | S | 112 |  |
| 19 | T | 92 |  |
| 20 | U | 100 |  |
| 21 | V | 187 |  |
| 22 | W | 76 |  |
| 23 | X | 88 |  |
| 24 | Y | 62 |  |
| 25 | Z | 59 |  |
| 26 | 1 | 30 |  |
| 27 | 2 | 52 |  |
| 28 | 3 | 44 |  |
| 29 | 4 | 48 |  |
| 30 | 5 | 63 |  |

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 93956 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 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | A | 2832 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60991 | 27143 | 11396 | 19620 | 2832 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|---------------|
| A | 276 | C | A | CONFLICT | GB AE017221.1 |
| A | 277 | A | C | CONFLICT | GB AE017221.1 |
| A | 1142 | U | C | CONFLICT | GB AE017221.1 |
| A | 2825 | U | G | CONFLICT | GB AE017221.1 |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | B | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2555 | 1136 | 471 | 829 | 119 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | D | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2105 | 1329 | 416 | 357 | 3 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | E | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1564 | 988 | 299 | 271 | 6 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | F | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1587 | 1011 | 297 | 276 | 3 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | G | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1475 | 943 | 268 | 260 | 4 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | H | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1223 | 773 | 228 | 221 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | I | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 724 | 200 | 208 | 1 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | J | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1097 | 707 | 205 | 182 | 3 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | K | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 587 | 171 | 170 | 4 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | L | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | M | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1065 | 680 | 201 | 179 | 5 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 13 | N | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | | |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 14 | O | 98 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 771 | 486 | 154 | 131 | | | | |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | P | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 713 | 234 | 196 | 1 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | Q | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | R | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | S | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 891 | 560 | 175 | 154 | 2 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19 | T | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 726 | 471 | 131 | 124 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | U | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 776 | 500 | 148 | 124 | 4 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | V | 187 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1483 | 945 | 264 | 272 | 2 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | W | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 605 | 376 | 126 | 102 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 23 | X | 88 | Total | C | N | O | 0 | 0 | 0 |
| | | | 695 | 435 | 141 | 119 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 24 | Y | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 521 | 325 | 102 | 92 | 2 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 25 | Z | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 468 | 298 | 90 | 79 | 1 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | 1 | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 226 | 142 | 36 | 44 | 4 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | 2 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 405 | 255 | 79 | 66 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 3 | 44 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 381 | 235 | 77 | 65 | 4 | | | |

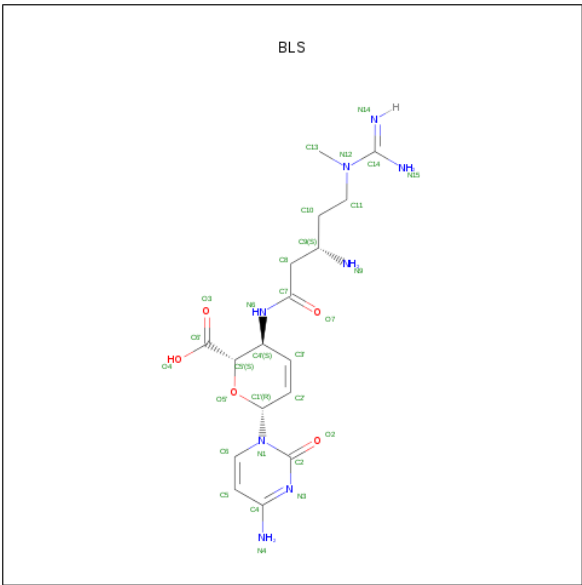
- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29 | 4 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 419 | 257 | 104 | 56 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30 | 5 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 508 | 326 | 101 | 79 | 2 | | | |

- Molecule 31 is BLASTICIDIN S (three-letter code: BLS) (formula: C₁₇H₂₆N₈O₅).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 31 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 30 | 17 | 8 | 5 | | |

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 32 | P | 13 | Total | Mg | 0 | 0 |
| | | | 13 | 13 | | |
| 32 | G | 7 | Total | Mg | 0 | 0 |
| | | | 7 | 7 | | |
| 32 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | D | 20 | Total | Mg | 0 | 0 |
| | | | 20 | 20 | | |
| 32 | K | 15 | Total | Mg | 0 | 0 |
| | | | 15 | 15 | | |
| 32 | E | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 32 | B | 50 | Total | Mg | 0 | 0 |
| | | | 50 | 50 | | |
| 32 | V | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 32 | 3 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 32 | A | 4209 | Total | Mg | 0 | 0 |
| | | | 4209 | 4209 | | |
| 32 | 4 | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |

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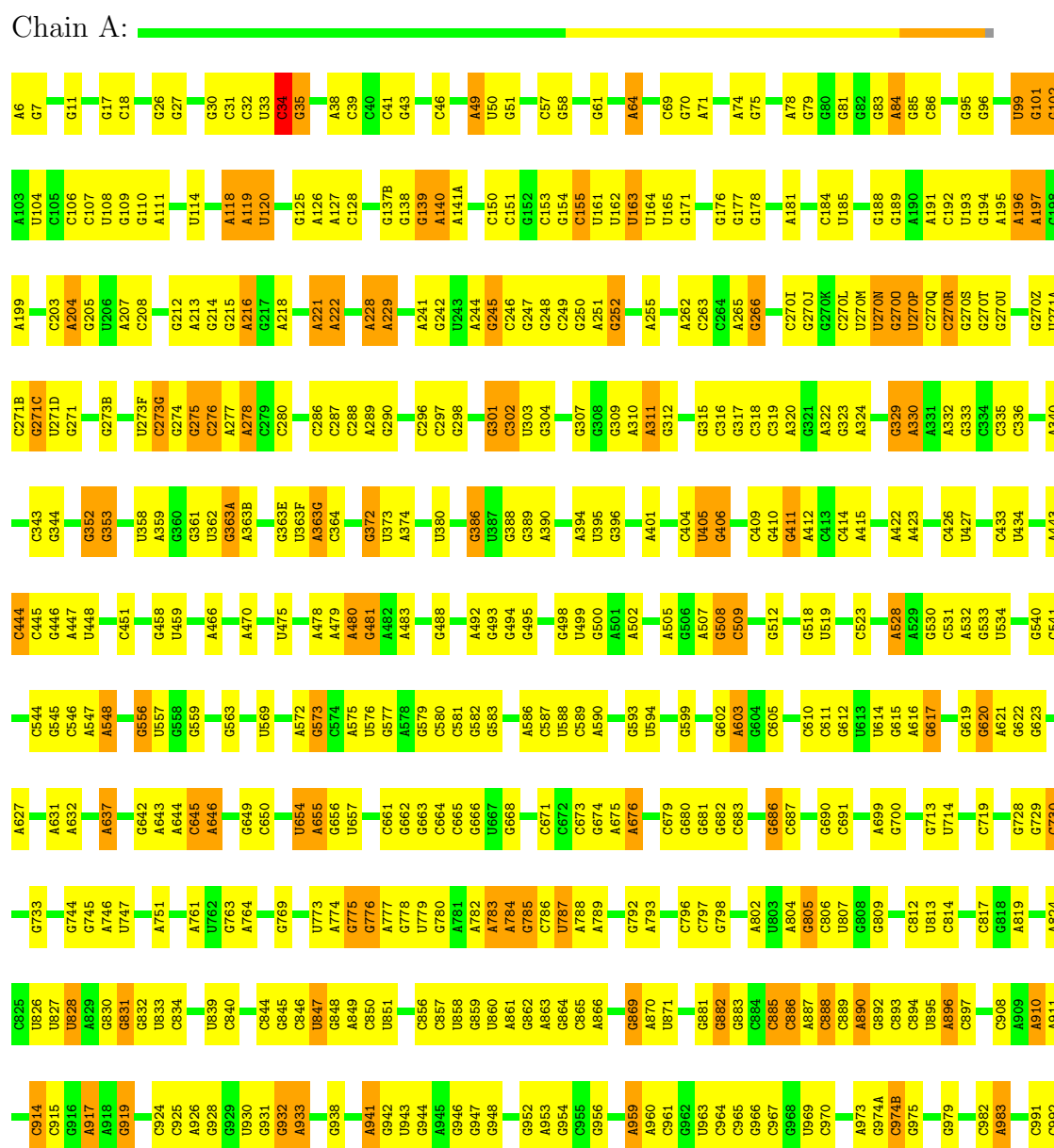
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 32 | N | 4 | Total 4 | Mg 4 | 0 | 0 |
| 32 | X | 7 | Total 7 | Mg 7 | 0 | 0 |
| 32 | O | 1 | Total 1 | Mg 1 | 0 | 0 |
| 32 | R | 5 | Total 5 | Mg 5 | 0 | 0 |
| 32 | Y | 1 | Total 1 | Mg 1 | 0 | 0 |
| 32 | L | 2 | Total 2 | Mg 2 | 0 | 0 |
| 32 | S | 6 | Total 6 | Mg 6 | 0 | 0 |
| 32 | F | 6 | Total 6 | Mg 6 | 0 | 0 |
| 32 | M | 4 | Total 4 | Mg 4 | 0 | 0 |

3 Residue-property plots

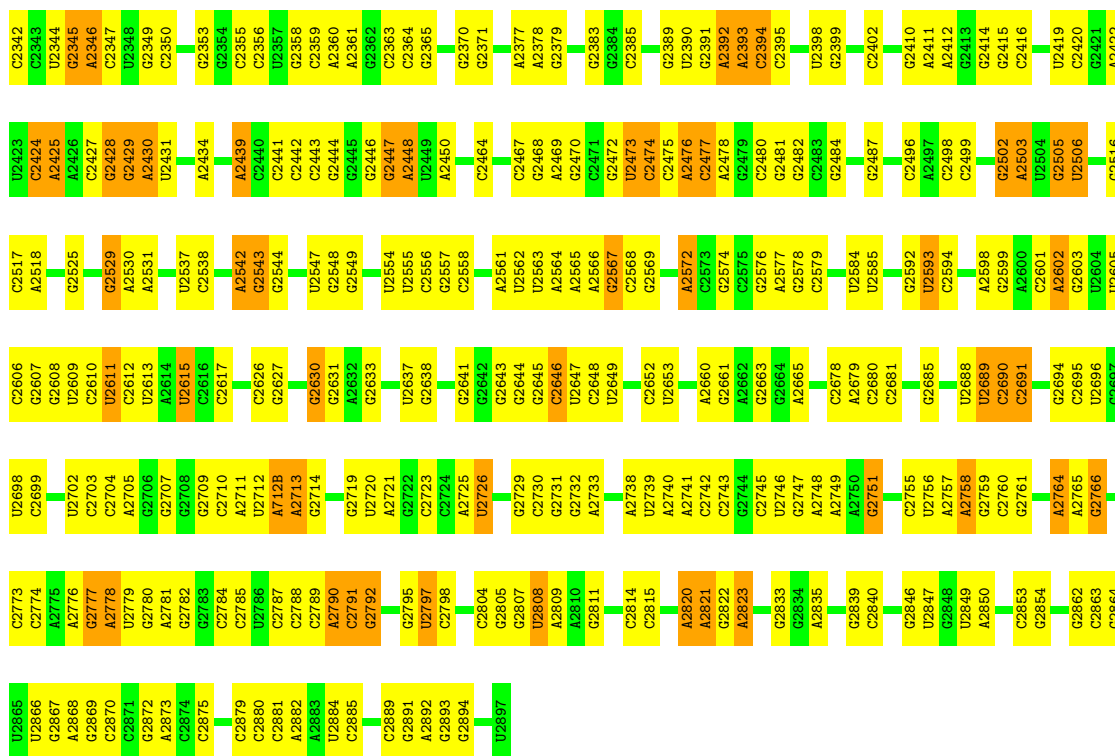
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 23S ribosomal RNA

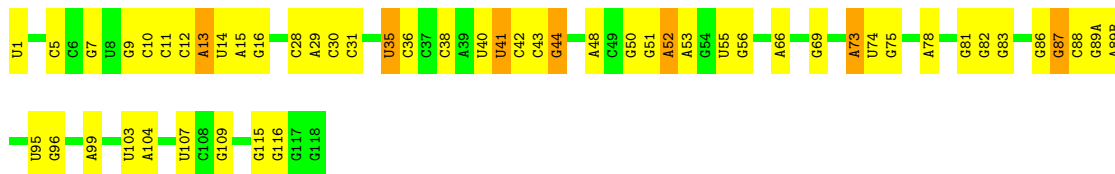






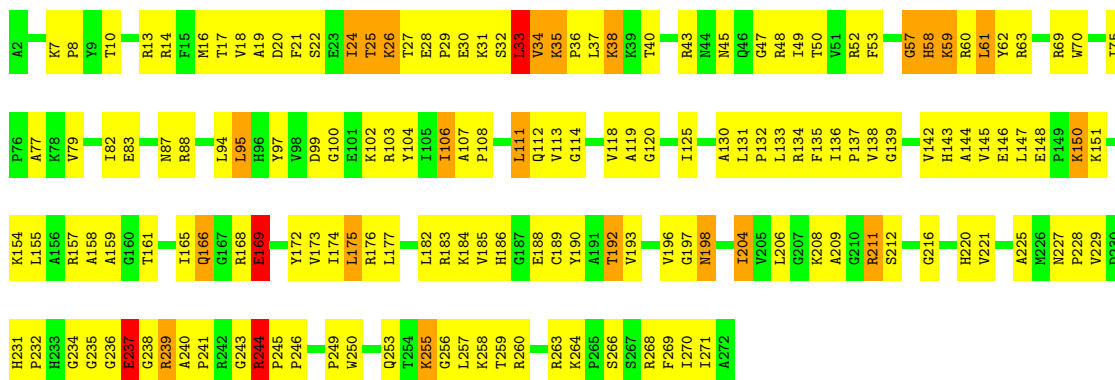
- Molecule 2: 5S ribosomal RNA

Chain B:



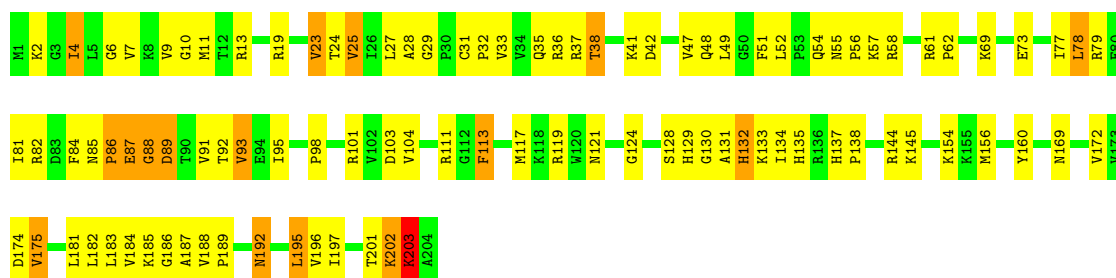
- Molecule 3: 50S ribosomal protein L2

Chain D:



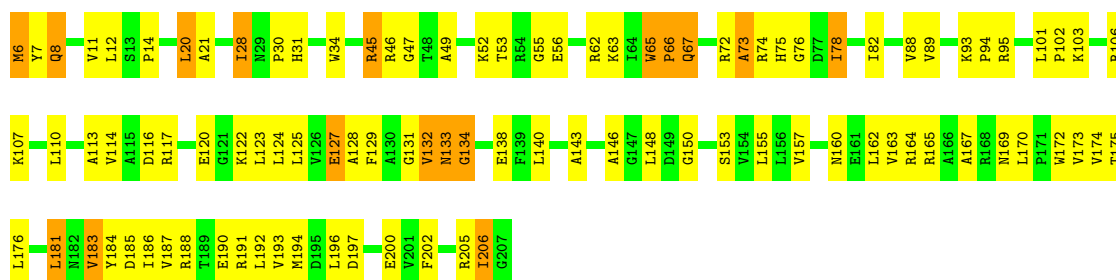
- Molecule 4: 50S ribosomal protein L3

Chain E:



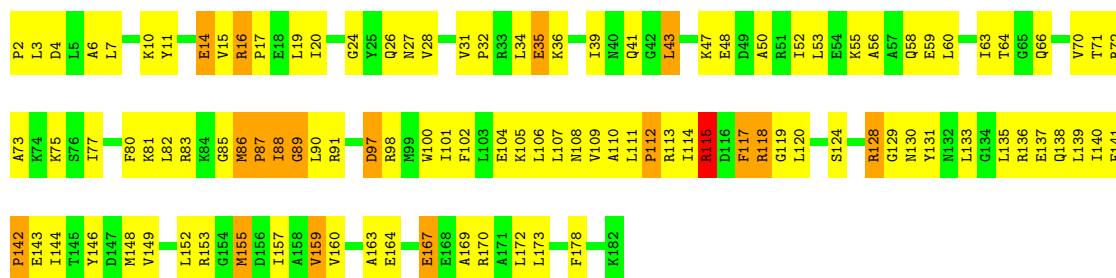
• Molecule 5: 50S ribosomal protein L4

Chain F:



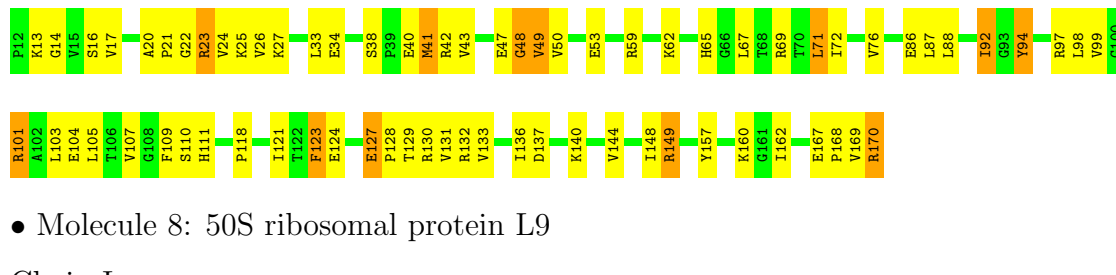
• Molecule 6: 50S ribosomal protein L5

Chain G:



• Molecule 7: 50S ribosomal protein L6

Chain H:

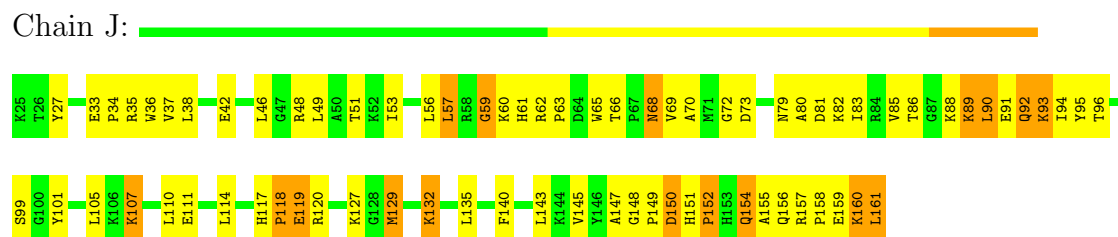


• Molecule 8: 50S ribosomal protein L9

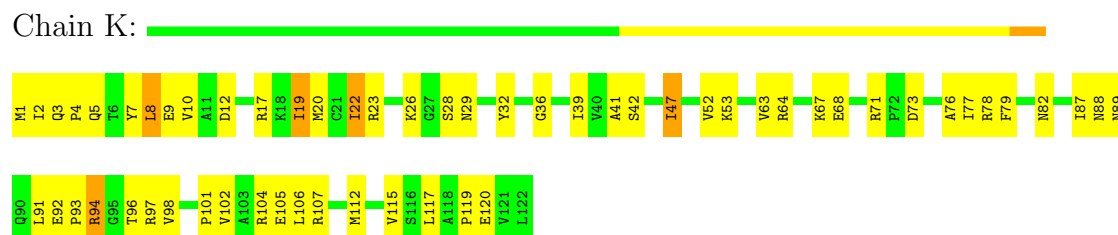
Chain I:



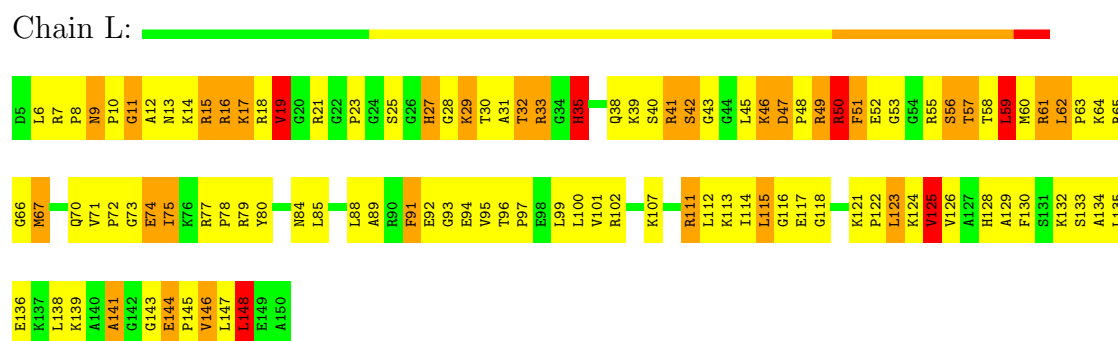
- Molecule 9: 50S ribosomal protein L13



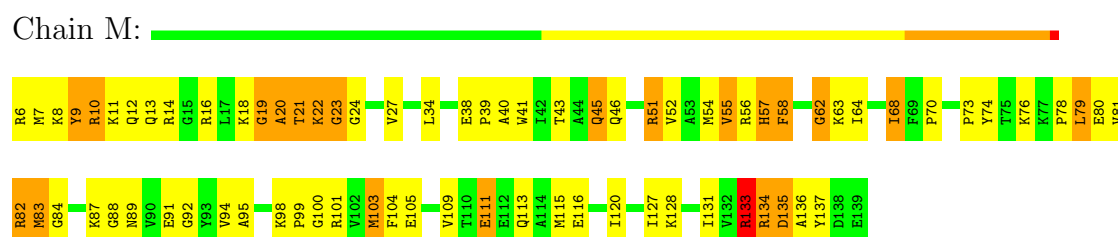
- Molecule 10: 50S ribosomal protein L14



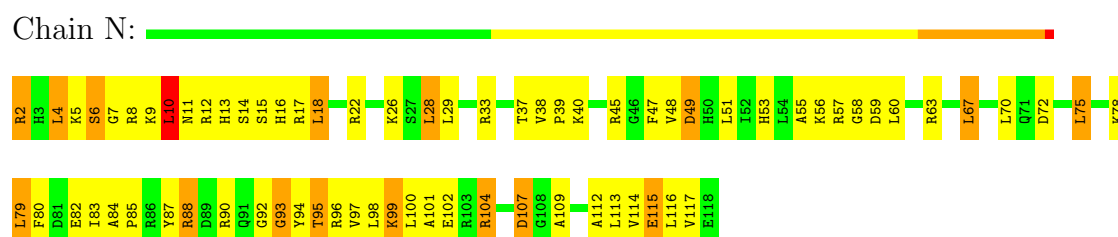
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16

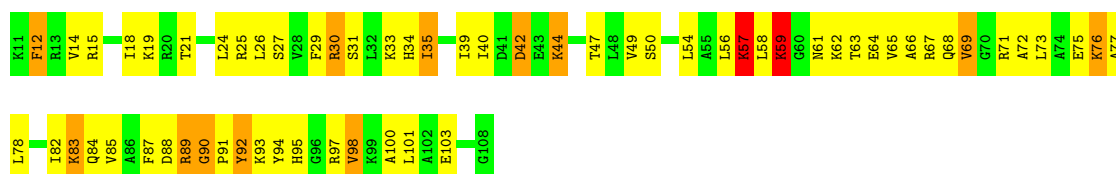


- Molecule 13: 50S ribosomal protein L17



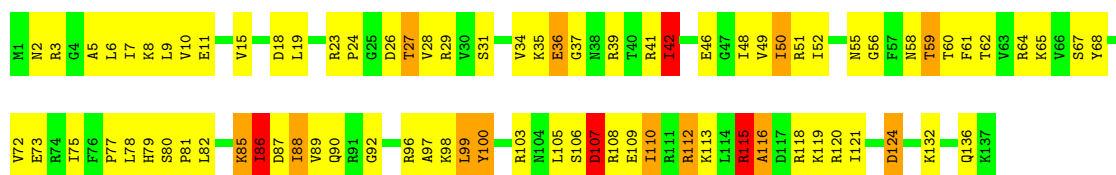
- Molecule 14: 50S ribosomal protein L18





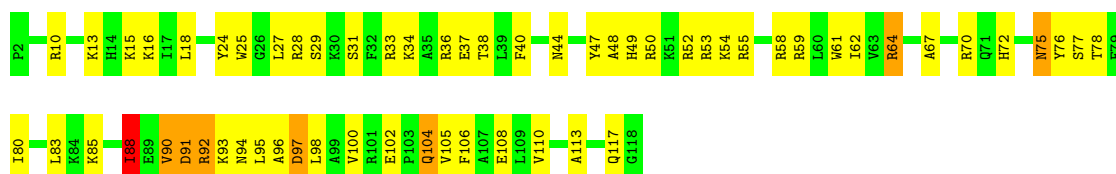
• Molecule 15: 50S ribosomal protein L19

Chain P:



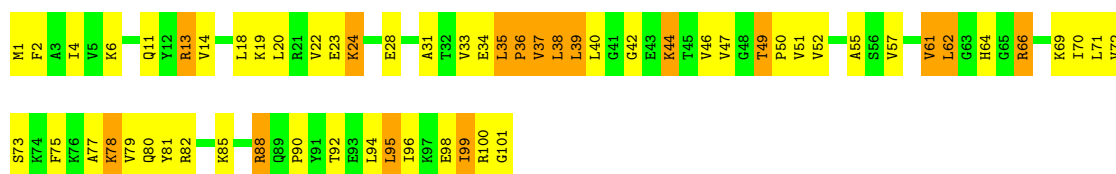
• Molecule 16: 50S ribosomal protein L20

Chain Q:



• Molecule 17: 50S ribosomal protein L21

Chain R:



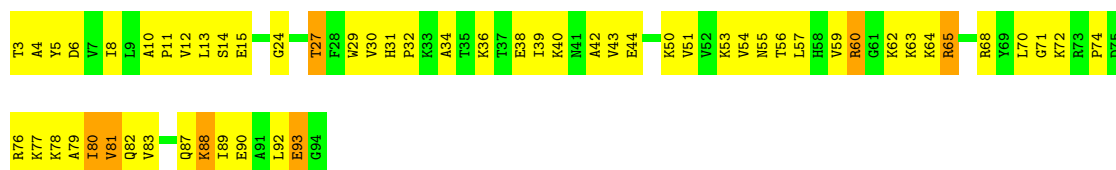
• Molecule 18: 50S ribosomal protein L22

Chain S:



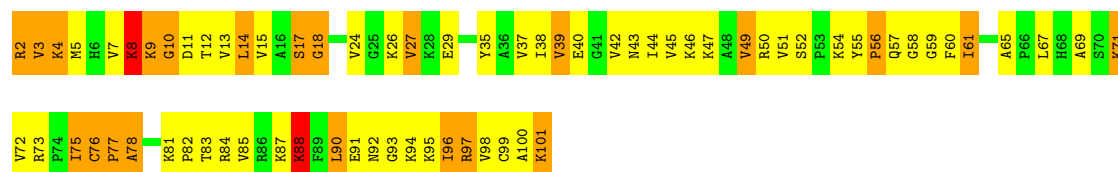
• Molecule 19: 50S ribosomal protein L23

Chain T:



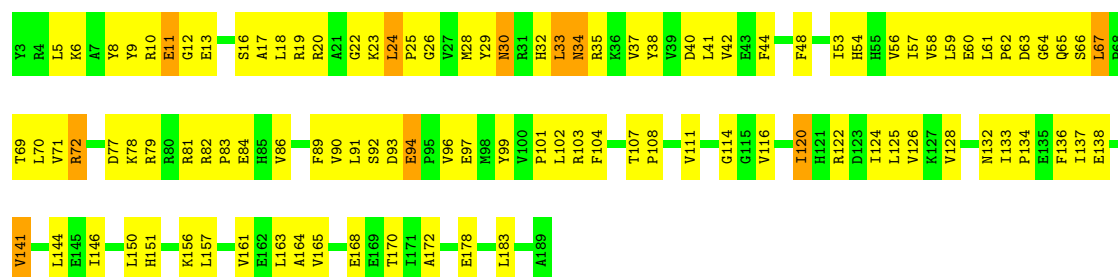
- Molecule 20: 50S ribosomal protein L24

Chain U: 



- Molecule 21: 50S ribosomal protein L25

Chain V: 



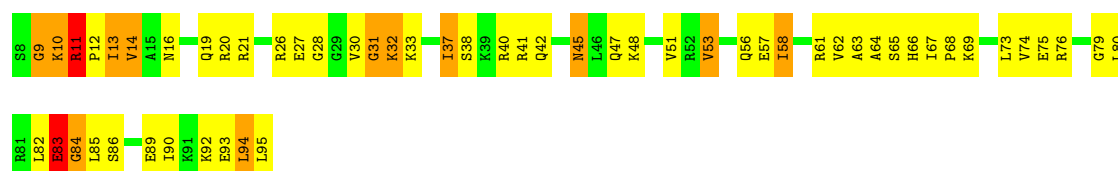
- Molecule 22: 50S ribosomal protein L27

Chain W: 



- Molecule 23: 50S ribosomal protein L28

Chain X: 



- Molecule 24: 50S ribosomal protein L29

Chain Y: 



- Molecule 25: 50S ribosomal protein L30

Chain Z: 



- Molecule 26: 50S ribosomal protein L31

Chain 1: 



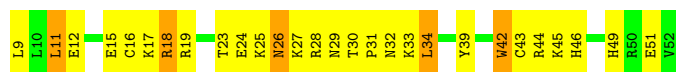
- Molecule 27: 50S ribosomal protein L32

Chain 2: 



- Molecule 28: 50S ribosomal protein L33

Chain 3: 



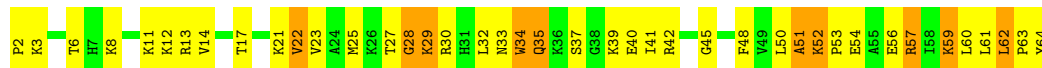
- Molecule 29: 50S ribosomal protein L34

Chain 4: 



- Molecule 30: 50S ribosomal protein L35

Chain 5: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.53Å 454.44Å 620.87Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.98 – 3.40 | Depositor |
| % Data completeness (in resolution range) | 99.8 (49.98-3.40) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | PHENIX (phenix.refine: 1.6.4_486) | Depositor |
| R, R_{free} | 0.231 , 0.268 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 93956 | wwPDB-VP |
| Average B, all atoms (Å ²) | 89.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.34 | 1/68308 (0.0%) | 0.64 | 11/106635 (0.0%) |
| 2 | B | 0.31 | 1/2857 (0.0%) | 0.52 | 0/4455 |
| 3 | D | 0.31 | 0/2155 | 0.52 | 0/2905 |
| 4 | E | 0.27 | 0/1597 | 0.49 | 0/2153 |
| 5 | F | 0.27 | 0/1622 | 0.47 | 0/2194 |
| 6 | G | 0.22 | 0/1500 | 0.41 | 0/2017 |
| 7 | H | 0.22 | 0/1246 | 0.43 | 0/1682 |
| 8 | I | 0.22 | 0/1148 | 0.42 | 0/1552 |
| 9 | J | 0.26 | 0/1124 | 0.49 | 0/1515 |
| 10 | K | 0.28 | 0/942 | 0.46 | 0/1268 |
| 11 | L | 0.31 | 0/1131 | 0.61 | 0/1504 |
| 12 | M | 0.28 | 0/1085 | 0.49 | 0/1449 |
| 13 | N | 0.28 | 0/974 | 0.47 | 0/1302 |
| 14 | O | 0.24 | 0/779 | 0.43 | 0/1036 |
| 15 | P | 0.27 | 0/1158 | 0.45 | 0/1544 |
| 16 | Q | 0.28 | 0/982 | 0.44 | 0/1306 |
| 17 | R | 0.29 | 0/790 | 0.51 | 0/1057 |
| 18 | S | 0.28 | 0/902 | 0.46 | 0/1209 |
| 19 | T | 0.29 | 0/740 | 0.46 | 0/993 |
| 20 | U | 0.30 | 0/789 | 0.46 | 0/1051 |
| 21 | V | 0.22 | 0/1515 | 0.42 | 0/2056 |
| 22 | W | 0.28 | 0/613 | 0.47 | 0/816 |
| 23 | X | 0.32 | 0/702 | 0.56 | 0/932 |
| 24 | Y | 0.27 | 0/523 | 0.49 | 0/690 |
| 25 | Z | 0.24 | 0/473 | 0.46 | 0/634 |
| 26 | 1 | 0.20 | 0/229 | 0.42 | 0/309 |
| 27 | 2 | 0.28 | 0/419 | 0.52 | 0/567 |
| 28 | 3 | 0.21 | 0/388 | 0.44 | 0/518 |
| 29 | 4 | 0.31 | 0/427 | 0.50 | 0/561 |
| 30 | 5 | 0.32 | 0/516 | 0.52 | 0/679 |
| All | All | 0.32 | 2/97634 (0.0%) | 0.60 | 11/146589 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 13 | N | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2 | B | 1 | U | OP3-P | -10.65 | 1.48 | 1.61 |
| 1 | A | 6 | A | OP3-P | -10.59 | 1.48 | 1.61 |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1420 | U | C2-N1-C1' | 6.88 | 125.96 | 117.70 |
| 1 | A | 1420 | U | C6-N1-C1' | -6.57 | 112.00 | 121.20 |
| 1 | A | 34 | C | C6-N1-C1' | -5.98 | 113.63 | 120.80 |
| 1 | A | 2593 | U | N3-C4-C5 | -5.67 | 111.20 | 114.60 |
| 1 | A | 34 | C | N3-C4-C5 | 5.57 | 124.13 | 121.90 |
| 1 | A | 676 | A | N7-C8-N9 | 5.43 | 116.51 | 113.80 |
| 1 | A | 944 | G | C4-N9-C1' | 5.42 | 133.55 | 126.50 |
| 1 | A | 2308 | G | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 1 | A | 676 | A | C5-N7-C8 | -5.15 | 101.32 | 103.90 |
| 1 | A | 676 | A | C2-N3-C4 | -5.13 | 108.03 | 110.60 |
| 1 | A | 783 | A | C5-N7-C8 | -5.13 | 101.33 | 103.90 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 13 | N | 10 | LEU | Peptide |

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 60991 | 0 | 30744 | 1326 | 0 |
| 2 | B | 2555 | 0 | 1294 | 52 | 0 |
| 3 | D | 2105 | 0 | 2182 | 184 | 0 |
| 4 | E | 1564 | 0 | 1629 | 103 | 0 |
| 5 | F | 1587 | 0 | 1632 | 102 | 0 |
| 6 | G | 1475 | 0 | 1537 | 124 | 0 |
| 7 | H | 1223 | 0 | 1282 | 65 | 0 |
| 8 | I | 1133 | 0 | 1220 | 75 | 0 |
| 9 | J | 1097 | 0 | 1168 | 80 | 0 |
| 10 | K | 932 | 0 | 994 | 50 | 0 |
| 11 | L | 1114 | 0 | 1187 | 196 | 0 |
| 12 | M | 1065 | 0 | 1114 | 93 | 0 |
| 13 | N | 960 | 0 | 1021 | 81 | 0 |
| 14 | O | 771 | 0 | 832 | 62 | 0 |
| 15 | P | 1144 | 0 | 1211 | 75 | 0 |
| 16 | Q | 964 | 0 | 1022 | 77 | 0 |
| 17 | R | 779 | 0 | 852 | 79 | 0 |
| 18 | S | 891 | 0 | 951 | 50 | 0 |
| 19 | T | 726 | 0 | 778 | 60 | 0 |
| 20 | U | 776 | 0 | 870 | 94 | 0 |
| 21 | V | 1483 | 0 | 1507 | 88 | 0 |
| 22 | W | 605 | 0 | 628 | 28 | 0 |
| 23 | X | 695 | 0 | 764 | 85 | 0 |
| 24 | Y | 521 | 0 | 575 | 62 | 0 |
| 25 | Z | 468 | 0 | 523 | 23 | 0 |
| 26 | 1 | 226 | 0 | 225 | 21 | 0 |
| 27 | 2 | 405 | 0 | 420 | 43 | 0 |
| 28 | 3 | 381 | 0 | 391 | 33 | 0 |
| 29 | 4 | 419 | 0 | 467 | 29 | 0 |
| 30 | 5 | 508 | 0 | 576 | 64 | 0 |
| 31 | A | 30 | 0 | 24 | 4 | 0 |
| 32 | 3 | 2 | 0 | 0 | 0 | 0 |
| 32 | 4 | 4 | 0 | 0 | 0 | 0 |
| 32 | A | 4209 | 0 | 0 | 0 | 0 |
| 32 | B | 50 | 0 | 0 | 0 | 0 |
| 32 | D | 20 | 0 | 0 | 0 | 0 |
| 32 | E | 4 | 0 | 0 | 0 | 0 |
| 32 | F | 6 | 0 | 0 | 0 | 0 |
| 32 | G | 7 | 0 | 0 | 0 | 0 |
| 32 | J | 1 | 0 | 0 | 0 | 0 |
| 32 | K | 15 | 0 | 0 | 0 | 0 |
| 32 | L | 2 | 0 | 0 | 0 | 0 |
| 32 | M | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | N | 4 | 0 | 0 | 0 | 0 |
| 32 | O | 1 | 0 | 0 | 0 | 0 |
| 32 | P | 13 | 0 | 0 | 0 | 0 |
| 32 | R | 5 | 0 | 0 | 0 | 0 |
| 32 | S | 6 | 0 | 0 | 0 | 0 |
| 32 | V | 2 | 0 | 0 | 0 | 0 |
| 32 | X | 7 | 0 | 0 | 0 | 0 |
| 32 | Y | 1 | 0 | 0 | 0 | 0 |
| All | All | 93956 | 0 | 59620 | 3121 | 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 20.

All (3121) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1541:U:H3' | 1:A:1542:G:H3' | 1.16 | 1.16 |
| 1:A:2502:G:H5' | 1:A:2503:A:H5'' | 1.28 | 1.14 |
| 1:A:2303:G:H2' | 1:A:2304:G:H5'' | 1.33 | 1.10 |
| 1:A:1899:G:N2 | 1:A:1902:C:H41 | 1.48 | 1.09 |
| 23:X:11:ARG:HB3 | 23:X:12:PRO:HD2 | 1.34 | 1.05 |
| 5:F:45:ARG:HH11 | 5:F:45:ARG:HG2 | 1.15 | 1.05 |
| 1:A:2393:A:H5' | 11:L:62:LEU:HD12 | 1.36 | 1.03 |
| 20:U:17:SER:HB2 | 20:U:71:LYS:HE2 | 1.38 | 1.03 |
| 1:A:274:G:H3' | 1:A:275:G:H4' | 1.41 | 1.02 |
| 1:A:34:C:O2' | 1:A:35:G:H5' | 1.60 | 1.00 |
| 11:L:23:PRO:HB2 | 11:L:33:ARG:HG3 | 1.37 | 1.00 |
| 11:L:49:ARG:HG3 | 11:L:49:ARG:HH11 | 1.25 | 1.00 |
| 23:X:19:GLN:HG2 | 23:X:41:ARG:HB3 | 1.44 | 1.00 |
| 20:U:76:CYS:SG | 20:U:77:PRO:HD2 | 2.02 | 1.00 |
| 1:A:2287:A:H62 | 1:A:2344:U:H3 | 1.06 | 1.00 |
| 7:H:42:ARG:HB2 | 7:H:53:GLU:HB2 | 1.44 | 0.99 |
| 11:L:41:ARG:HE | 11:L:41:ARG:HA | 1.23 | 0.99 |
| 27:2:4:HIS:HB3 | 27:2:5:PRO:HD3 | 1.44 | 0.98 |
| 8:I:93:THR:HG22 | 8:I:119:PRO:HB3 | 1.44 | 0.98 |
| 29:4:19:ARG:HH11 | 29:4:19:ARG:HG3 | 1.28 | 0.97 |
| 30:5:22:VAL:HB | 30:5:54:GLU:HG3 | 1.45 | 0.97 |
| 1:A:2579:C:O2' | 4:E:131:ALA:HB2 | 1.65 | 0.97 |
| 11:L:128:HIS:HA | 11:L:147:LEU:HB3 | 1.42 | 0.97 |
| 1:A:1190:G:H5'' | 11:L:35:HIS:HA | 1.47 | 0.96 |
| 3:D:103:ARG:HG2 | 3:D:103:ARG:HH11 | 1.27 | 0.96 |
| 1:A:960:A:H61 | 12:M:82:ARG:HH21 | 1.11 | 0.95 |
| 18:S:24:ILE:HG21 | 18:S:36:LEU:HD11 | 1.47 | 0.95 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1614:A:N1 | 18:S:93:ALA:HB2 | 1.82 | 0.95 |
| 1:A:676:A:H8 | 1:A:2069:G:H21 | 1.08 | 0.94 |
| 11:L:57:THR:HB | 11:L:59:LEU:H | 1.32 | 0.94 |
| 9:J:160:LYS:HZ2 | 9:J:161:LEU:H | 1.06 | 0.93 |
| 3:D:79:VAL:HG11 | 3:D:111:LEU:HD11 | 1.51 | 0.93 |
| 10:K:97:ARG:H | 10:K:117:LEU:HD23 | 1.34 | 0.93 |
| 1:A:1109:C:H5 | 1:A:1110:G:H1' | 1.32 | 0.92 |
| 17:R:49:THR:HG22 | 17:R:50:PRO:HD2 | 1.50 | 0.92 |
| 24:Y:50:ILE:HD12 | 24:Y:51:ARG:N | 1.84 | 0.92 |
| 9:J:132:LYS:H | 9:J:132:LYS:HD3 | 1.33 | 0.92 |
| 8:I:5:LEU:HD23 | 8:I:5:LEU:H | 1.35 | 0.92 |
| 1:A:1541:U:C3' | 1:A:1542:G:H3' | 2.00 | 0.91 |
| 1:A:846:C:H4' | 1:A:847:U:H5' | 1.53 | 0.91 |
| 1:A:1541:U:H3' | 1:A:1542:G:C3' | 2.00 | 0.91 |
| 1:A:774:A:H2 | 1:A:787:U:HO2' | 0.96 | 0.91 |
| 1:A:959:A:N6 | 12:M:82:ARG:HH22 | 1.68 | 0.91 |
| 3:D:106:ILE:H | 3:D:106:ILE:HD13 | 1.35 | 0.91 |
| 1:A:806:C:OP2 | 11:L:39:LYS:HG3 | 1.71 | 0.90 |
| 1:A:1899:G:H21 | 1:A:1902:C:H41 | 1.15 | 0.90 |
| 17:R:14:VAL:HG11 | 17:R:96:ILE:HG12 | 1.54 | 0.89 |
| 1:A:2473:U:O2' | 1:A:2474:C:H5' | 1.71 | 0.89 |
| 4:E:57:LYS:HG3 | 4:E:58:ARG:H | 1.37 | 0.88 |
| 1:A:1689:A:H62 | 1:A:1698:A:H2 | 1.19 | 0.88 |
| 11:L:91:PHE:HD1 | 11:L:91:PHE:H | 1.21 | 0.88 |
| 24:Y:14:ARG:HA | 24:Y:17:SER:HB2 | 1.57 | 0.87 |
| 3:D:108:PRO:HB3 | 3:D:143:HIS:CE1 | 2.09 | 0.87 |
| 1:A:2303:G:C2' | 1:A:2304:G:H5'' | 2.05 | 0.87 |
| 6:G:105:LYS:HD2 | 6:G:142:PRO:HG3 | 1.56 | 0.87 |
| 1:A:2090:G:H21 | 23:X:45:ASN:HD21 | 1.21 | 0.87 |
| 1:A:2729:G:H1' | 4:E:187:ALA:HB2 | 1.56 | 0.87 |
| 8:I:4:ILE:HG22 | 8:I:18:VAL:HG22 | 1.54 | 0.87 |
| 12:M:23:GLY:HA3 | 12:M:98:LYS:HB2 | 1.55 | 0.87 |
| 11:L:64:LYS:HB2 | 30:5:25:MET:HG3 | 1.55 | 0.87 |
| 20:U:81:LYS:HD3 | 20:U:97:ARG:HB3 | 1.56 | 0.87 |
| 1:A:1348:G:H2' | 1:A:1349:A:H5'' | 1.57 | 0.86 |
| 1:A:1678:G:H22 | 1:A:1989:G:H22 | 1.20 | 0.86 |
| 1:A:2681:C:H5 | 1:A:2725:A:H62 | 1.17 | 0.86 |
| 1:A:942:G:H5' | 11:L:35:HIS:HB2 | 1.56 | 0.86 |
| 1:A:273(G):C:H42 | 1:A:363(A):G:H1 | 1.24 | 0.86 |
| 20:U:50:ARG:HA | 20:U:58:GLY:HA3 | 1.57 | 0.86 |
| 6:G:88:ILE:HD13 | 6:G:89:GLY:H | 1.39 | 0.86 |
| 30:5:52:LYS:HA | 30:5:52:LYS:HE3 | 1.57 | 0.85 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:E:201:THR:HG22 | 4:E:202:LYS:N | 1.92 | 0.85 |
| 29:4:9:ARG:HE | 29:4:47:ARG:HB2 | 1.41 | 0.85 |
| 3:D:25:THR:CG2 | 3:D:82:ILE:H | 1.89 | 0.84 |
| 5:F:45:ARG:CG | 5:F:45:ARG:HH11 | 1.89 | 0.84 |
| 11:L:59:LEU:HA | 11:L:61:ARG:NE | 1.92 | 0.84 |
| 1:A:1174:A:H3' | 1:A:1175:U:H5'' | 1.60 | 0.84 |
| 1:A:140:A:H8 | 1:A:1408:C:O2' | 1.59 | 0.84 |
| 6:G:53:LEU:HD13 | 6:G:88:ILE:HG21 | 1.57 | 0.84 |
| 1:A:1210:A:H8 | 1:A:1210:A:H5' | 1.42 | 0.84 |
| 5:F:6:MET:HG2 | 5:F:7:TYR:HD1 | 1.40 | 0.84 |
| 3:D:108:PRO:HB3 | 3:D:143:HIS:HE1 | 1.40 | 0.84 |
| 4:E:201:THR:HG22 | 4:E:202:LYS:H | 1.43 | 0.84 |
| 1:A:1109:C:C5 | 1:A:1110:G:H1' | 2.12 | 0.83 |
| 12:M:10:ARG:CZ | 12:M:10:ARG:HA | 2.08 | 0.83 |
| 17:R:28:GLU:HB3 | 17:R:31:ALA:HB2 | 1.60 | 0.83 |
| 11:L:38:GLN:HG3 | 11:L:39:LYS:H | 1.41 | 0.83 |
| 1:A:908:C:OP1 | 12:M:22:LYS:HD2 | 1.78 | 0.83 |
| 16:Q:62:ILE:HD11 | 16:Q:93:LYS:HD3 | 1.61 | 0.83 |
| 12:M:43:THR:HA | 12:M:94:VAL:HG12 | 1.59 | 0.83 |
| 27:2:4:HIS:CB | 27:2:5:PRO:HD3 | 2.08 | 0.83 |
| 5:F:103:LYS:HA | 5:F:106:ARG:HG3 | 1.61 | 0.83 |
| 1:A:140:A:H8 | 1:A:1408:C:HO2' | 0.87 | 0.82 |
| 1:A:773:U:H4' | 3:D:47:GLY:HA3 | 1.61 | 0.82 |
| 1:A:780:G:H21 | 1:A:783:A:H62 | 1.24 | 0.82 |
| 1:A:1051:G:H1 | 1:A:1107:G:H22 | 1.27 | 0.82 |
| 11:L:45:LEU:HD23 | 11:L:46:LYS:H | 1.45 | 0.82 |
| 1:A:1420:U:O2' | 1:A:1421:G:H5' | 1.78 | 0.82 |
| 1:A:2790:A:H2' | 1:A:2791:C:H5'' | 1.62 | 0.82 |
| 11:L:125:VAL:HG11 | 11:L:138:LEU:HD21 | 1.59 | 0.82 |
| 1:A:1006:C:H1' | 9:J:129:MET:HG2 | 1.62 | 0.82 |
| 1:A:2447:G:H4' | 1:A:2448:A:O5' | 1.77 | 0.82 |
| 21:V:69:THR:HG22 | 21:V:90:VAL:HG22 | 1.60 | 0.81 |
| 9:J:156:GLN:C | 9:J:158:PRO:HD3 | 2.01 | 0.81 |
| 1:A:886:C:H2' | 1:A:887:A:O4' | 1.80 | 0.81 |
| 1:A:1537:C:H2' | 1:A:1538:G:O4' | 1.80 | 0.81 |
| 1:A:1902:C:H1' | 3:D:244:ARG:HD2 | 1.62 | 0.81 |
| 14:O:31:SER:HB3 | 14:O:34:HIS:HB2 | 1.61 | 0.81 |
| 1:A:1678:G:N2 | 1:A:1989:G:H22 | 1.78 | 0.81 |
| 1:A:661:C:O3' | 11:L:18:ARG:HG2 | 1.81 | 0.81 |
| 6:G:167:GLU:HA | 6:G:170:ARG:HB3 | 1.62 | 0.81 |
| 11:L:62:LEU:H | 11:L:62:LEU:HD22 | 1.44 | 0.81 |
| 2:B:89(A):G:H2' | 2:B:89(B):A:C8 | 2.16 | 0.81 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 23:X:13:ILE:HG21 | 23:X:63:ALA:H | 1.45 | 0.81 |
| 1:A:675:A:H4' | 5:F:67:GLN:NE2 | 1.95 | 0.80 |
| 7:H:169:VAL:C | 7:H:170:ARG:HE | 1.85 | 0.80 |
| 23:X:10:LYS:C | 23:X:13:ILE:HD11 | 2.01 | 0.80 |
| 23:X:13:ILE:HD12 | 23:X:14:VAL:H | 1.45 | 0.80 |
| 1:A:330:A:H2 | 1:A:1210:A:H2' | 1.47 | 0.80 |
| 1:A:602:G:H2' | 1:A:655:A:H61 | 1.45 | 0.80 |
| 6:G:43:LEU:H | 6:G:43:LEU:HD12 | 1.47 | 0.80 |
| 5:F:67:GLN:HG3 | 5:F:67:GLN:O | 1.81 | 0.80 |
| 15:P:24:PRO:HA | 15:P:49:VAL:HG13 | 1.62 | 0.80 |
| 1:A:1309:G:H4' | 29:4:7:PRO:HB2 | 1.61 | 0.80 |
| 1:A:2749:A:H4' | 7:H:62:LYS:HB3 | 1.64 | 0.79 |
| 15:P:50:ILE:HG12 | 15:P:99:LEU:HD12 | 1.64 | 0.79 |
| 1:A:274:G:H3' | 1:A:275:G:C4' | 2.12 | 0.79 |
| 11:L:16:ARG:NH2 | 11:L:18:ARG:H | 1.80 | 0.79 |
| 1:A:2502:G:H5' | 1:A:2503:A:C5' | 2.10 | 0.79 |
| 9:J:160:LYS:HZ3 | 9:J:160:LYS:HA | 1.48 | 0.79 |
| 1:A:2689:U:H4' | 1:A:2690:C:O5' | 1.81 | 0.79 |
| 5:F:107:LYS:HZ2 | 5:F:205:ARG:HG3 | 1.48 | 0.79 |
| 17:R:38:LEU:O | 17:R:39:LEU:HD13 | 1.83 | 0.79 |
| 23:X:11:ARG:HB3 | 23:X:12:PRO:CD | 2.13 | 0.79 |
| 1:A:302:C:H2' | 1:A:303:U:H6 | 1.45 | 0.78 |
| 3:D:255:LYS:HD2 | 3:D:255:LYS:H | 1.46 | 0.78 |
| 1:A:655:A:H2' | 1:A:656:G:O4' | 1.81 | 0.78 |
| 6:G:36:LYS:HB3 | 6:G:160:VAL:HB | 1.65 | 0.78 |
| 1:A:919:G:H5' | 2:B:81:G:H1' | 1.64 | 0.78 |
| 1:A:1287:A:N7 | 13:N:107:ASP:HB2 | 1.99 | 0.78 |
| 28:3:23:THR:HB | 30:5:35:GLN:HA | 1.65 | 0.78 |
| 1:A:2150:U:H2' | 1:A:2151:G:C8 | 2.18 | 0.78 |
| 1:A:959:A:H62 | 12:M:82:ARG:HH22 | 1.27 | 0.78 |
| 5:F:45:ARG:HG2 | 5:F:45:ARG:NH1 | 1.88 | 0.78 |
| 11:L:23:PRO:HB2 | 11:L:33:ARG:CG | 2.14 | 0.78 |
| 3:D:31:LYS:HG3 | 3:D:33:LEU:HG | 1.66 | 0.78 |
| 16:Q:90:VAL:HG13 | 16:Q:91:ASP:H | 1.49 | 0.78 |
| 19:T:60:ARG:HH21 | 29:4:47:ARG:CZ | 1.97 | 0.77 |
| 1:A:2807:G:H22 | 1:A:2893:G:H22 | 1.32 | 0.77 |
| 5:F:134:GLY:H | 5:F:162:LEU:HD22 | 1.48 | 0.77 |
| 29:4:9:ARG:HH21 | 29:4:47:ARG:HG3 | 1.48 | 0.77 |
| 16:Q:92:ARG:CD | 16:Q:94:ASN:HB3 | 2.14 | 0.77 |
| 1:A:141(A):A:H8 | 1:A:1595:G:H21 | 1.28 | 0.77 |
| 9:J:154:GLN:HE21 | 9:J:155:ALA:HB3 | 1.49 | 0.77 |
| 1:A:1019:U:H3 | 1:A:1142(B):A:H62 | 1.32 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 6:G:88:ILE:HD13 | 6:G:89:GLY:N | 2.00 | 0.77 |
| 29:4:19:ARG:CG | 29:4:19:ARG:HH11 | 1.96 | 0.77 |
| 30:5:50:LEU:HB2 | 30:5:54:GLU:HB2 | 1.66 | 0.77 |
| 13:N:57:ARG:HG2 | 13:N:58:GLY:H | 1.48 | 0.77 |
| 29:4:8:ASN:HD22 | 29:4:8:ASN:C | 1.88 | 0.77 |
| 1:A:910:A:C5 | 12:M:13:GLN:HG3 | 2.19 | 0.77 |
| 11:L:58:THR:O | 11:L:61:ARG:HG3 | 1.84 | 0.77 |
| 28:3:26:ASN:HD22 | 28:3:28:ARG:H | 1.30 | 0.77 |
| 4:E:47:VAL:HG21 | 4:E:86:PRO:HD3 | 1.67 | 0.77 |
| 11:L:148:LEU:HD13 | 11:L:148:LEU:H | 1.49 | 0.77 |
| 1:A:2015:A:H1' | 27:2:2:ALA:HA | 1.66 | 0.77 |
| 1:A:2287:A:N6 | 1:A:2344:U:H3 | 1.80 | 0.76 |
| 11:L:80:TYR:CD1 | 11:L:111:ARG:HB3 | 2.20 | 0.76 |
| 7:H:25:LYS:HD2 | 7:H:27:LYS:HE2 | 1.67 | 0.76 |
| 2:B:9:G:H5' | 14:O:25:ARG:HH22 | 1.51 | 0.76 |
| 1:A:1902:C:H4' | 3:D:244:ARG:HB2 | 1.67 | 0.76 |
| 9:J:160:LYS:HZ2 | 9:J:161:LEU:N | 1.84 | 0.76 |
| 3:D:25:THR:O | 3:D:27:THR:HG22 | 1.85 | 0.76 |
| 1:A:380:U:O2' | 23:X:20:ARG:HB3 | 1.85 | 0.76 |
| 3:D:227:ASN:HB3 | 3:D:228:PRO:HD2 | 1.68 | 0.76 |
| 18:S:1:MET:HG2 | 18:S:2:GLU:H | 1.51 | 0.76 |
| 1:A:1899:G:N2 | 1:A:1902:C:N4 | 2.32 | 0.75 |
| 4:E:91:VAL:HB | 4:E:95:ILE:HD11 | 1.67 | 0.75 |
| 14:O:61:ASN:HD22 | 14:O:64:GLU:H | 1.32 | 0.75 |
| 1:A:274:G:C3' | 1:A:275:G:H4' | 2.14 | 0.75 |
| 13:N:51:LEU:HD13 | 13:N:70:LEU:HD11 | 1.68 | 0.75 |
| 21:V:24:LEU:HD11 | 21:V:86:VAL:HG23 | 1.69 | 0.75 |
| 1:A:195:A:OP1 | 11:L:46:LYS:HE2 | 1.85 | 0.75 |
| 3:D:28:GLU:HB3 | 3:D:29:PRO:HD3 | 1.67 | 0.75 |
| 9:J:160:LYS:HA | 9:J:160:LYS:NZ | 2.00 | 0.75 |
| 4:E:57:LYS:HG3 | 4:E:58:ARG:N | 2.01 | 0.75 |
| 11:L:47:ASP:HB3 | 11:L:48:PRO:HA | 1.67 | 0.75 |
| 20:U:37:VAL:HG21 | 20:U:72:VAL:HG21 | 1.69 | 0.75 |
| 11:L:71:VAL:HB | 11:L:72:PRO:HD3 | 1.67 | 0.75 |
| 1:A:1379:A:H4' | 1:A:1380:G:OP2 | 1.86 | 0.74 |
| 5:F:63:LYS:HA | 5:F:76:GLY:O | 1.87 | 0.74 |
| 18:S:29:LEU:HD21 | 18:S:33:ARG:HH21 | 1.52 | 0.74 |
| 19:T:63:LYS:NZ | 19:T:72:LYS:HB3 | 2.02 | 0.74 |
| 1:A:773:U:C4' | 3:D:47:GLY:HA3 | 2.16 | 0.74 |
| 8:I:77:LEU:HD11 | 8:I:101:LEU:HB2 | 1.69 | 0.74 |
| 11:L:41:ARG:HE | 11:L:41:ARG:CA | 1.91 | 0.74 |
| 24:Y:46:GLN:HB2 | 24:Y:49:LYS:NZ | 2.02 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:273(F):U:H2' | 1:A:273(G):C:H5'' | 1.68 | 0.74 |
| 5:F:185:ASP:HA | 5:F:188:ARG:HD3 | 1.69 | 0.74 |
| 3:D:35:LYS:HG2 | 3:D:104:TYR:CE2 | 2.22 | 0.74 |
| 4:E:132:HIS:HA | 4:E:135:HIS:CE1 | 2.22 | 0.74 |
| 4:E:132:HIS:CD2 | 4:E:135:HIS:NE2 | 2.56 | 0.74 |
| 13:N:70:LEU:HD23 | 13:N:75:LEU:HD12 | 1.69 | 0.74 |
| 16:Q:92:ARG:HD3 | 16:Q:94:ASN:HB3 | 1.70 | 0.74 |
| 1:A:1024:G:H3' | 1:A:1025:G:H5'' | 1.70 | 0.73 |
| 1:A:2884:U:H5 | 1:A:2885:C:C2 | 2.06 | 0.73 |
| 12:M:74:TYR:HD2 | 12:M:91:GLU:HB2 | 1.53 | 0.73 |
| 15:P:26:ASP:O | 15:P:49:VAL:HG12 | 1.88 | 0.73 |
| 15:P:60:THR:HG22 | 15:P:77:PRO:HA | 1.70 | 0.73 |
| 23:X:51:VAL:HG21 | 23:X:74:VAL:HG21 | 1.70 | 0.73 |
| 23:X:86:SER:HB2 | 23:X:89:GLU:HB2 | 1.70 | 0.73 |
| 27:2:4:HIS:HB3 | 27:2:5:PRO:CD | 2.18 | 0.73 |
| 1:A:2119:A:N6 | 1:A:2170:A:N6 | 2.37 | 0.73 |
| 5:F:20:LEU:HD22 | 5:F:21:ALA:H | 1.54 | 0.73 |
| 3:D:7:LYS:HG2 | 3:D:8:PRO:HD2 | 1.69 | 0.72 |
| 4:E:24:THR:HB | 4:E:186:GLY:HA2 | 1.69 | 0.72 |
| 4:E:111:ARG:HB2 | 4:E:160:TYR:HB3 | 1.71 | 0.72 |
| 16:Q:58:ARG:O | 16:Q:62:ILE:HG12 | 1.89 | 0.72 |
| 1:A:322:A:OP2 | 5:F:169:ASN:HB2 | 1.89 | 0.72 |
| 1:A:2712:U:H1' | 1:A:712(B):A:C8 | 2.25 | 0.72 |
| 4:E:111:ARG:HG3 | 4:E:160:TYR:CD1 | 2.24 | 0.72 |
| 1:A:2680:C:H5' | 4:E:189:PRO:HA | 1.72 | 0.72 |
| 12:M:51:ARG:HH11 | 12:M:51:ARG:HB3 | 1.54 | 0.72 |
| 30:5:30:ARG:HA | 30:5:30:ARG:HE | 1.54 | 0.72 |
| 11:L:95:VAL:HA | 11:L:99:LEU:HD22 | 1.70 | 0.72 |
| 17:R:66:ARG:HD2 | 17:R:88:ARG:CZ | 2.19 | 0.72 |
| 1:A:83:G:N2 | 1:A:102:G:H2' | 2.05 | 0.72 |
| 20:U:17:SER:CB | 20:U:71:LYS:HE2 | 2.16 | 0.72 |
| 6:G:82:LEU:HA | 6:G:86:MET:HE1 | 1.72 | 0.72 |
| 1:A:388:G:OP1 | 23:X:33:LYS:HB3 | 1.90 | 0.71 |
| 11:L:50:ARG:HG2 | 11:L:51:PHE:N | 2.05 | 0.71 |
| 1:A:2001:A:H5'' | 1:A:2689:U:O2' | 1.89 | 0.71 |
| 1:A:276:C:H2' | 1:A:277:A:H8 | 1.54 | 0.71 |
| 8:I:72:LEU:HD11 | 8:I:101:LEU:HD11 | 1.71 | 0.71 |
| 1:A:887:A:H2' | 1:A:888:C:H5'' | 1.72 | 0.71 |
| 11:L:62:LEU:CD2 | 30:5:25:MET:HB2 | 2.20 | 0.71 |
| 17:R:35:LEU:C | 17:R:37:VAL:H | 1.93 | 0.71 |
| 9:J:80:ALA:O | 9:J:83:ILE:HG13 | 1.91 | 0.71 |
| 12:M:12:GLN:HB2 | 12:M:73:PRO:HD2 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 15:P:28:VAL:HG23 | 15:P:88:ILE:HA | 1.71 | 0.71 |
| 20:U:95:LYS:HG3 | 20:U:100:ALA:HA | 1.72 | 0.71 |
| 30:5:22:VAL:HB | 30:5:54:GLU:CG | 2.21 | 0.71 |
| 8:I:92:VAL:HG23 | 8:I:96:ASP:HB2 | 1.71 | 0.71 |
| 9:J:68:ASN:HD22 | 9:J:68:ASN:H | 1.37 | 0.71 |
| 16:Q:34:LYS:HA | 16:Q:34:LYS:HE2 | 1.73 | 0.71 |
| 1:A:2415:G:H4' | 11:L:67:MET:N | 2.05 | 0.71 |
| 13:N:57:ARG:HG2 | 13:N:58:GLY:N | 2.04 | 0.71 |
| 1:A:1386:C:H2' | 1:A:1387:C:H6 | 1.56 | 0.70 |
| 1:A:605:C:H1' | 1:A:657:U:O2' | 1.90 | 0.70 |
| 3:D:144:ALA:HB3 | 3:D:192:THR:HG23 | 1.73 | 0.70 |
| 1:A:2446:G:C2' | 1:A:2447:G:H5'' | 2.21 | 0.70 |
| 1:A:2807:G:H1 | 1:A:2893:G:H1 | 1.39 | 0.70 |
| 17:R:34:GLU:O | 17:R:36:PRO:HD3 | 1.91 | 0.70 |
| 23:X:80:LEU:HD22 | 23:X:82:LEU:HB3 | 1.72 | 0.70 |
| 5:F:157:VAL:HB | 5:F:194:MET:HB3 | 1.73 | 0.70 |
| 1:A:2094:G:H5' | 8:I:25:TYR:CD2 | 2.26 | 0.70 |
| 1:A:1359:A:H2' | 1:A:1360:A:H5' | 1.72 | 0.70 |
| 9:J:57:LEU:O | 9:J:72:GLY:HA3 | 1.91 | 0.70 |
| 1:A:2473:U:C2' | 1:A:2473:U:O2 | 2.40 | 0.70 |
| 5:F:113:ALA:HB1 | 5:F:186:ILE:HG21 | 1.74 | 0.70 |
| 7:H:123:PHE:HB3 | 7:H:133:VAL:HA | 1.73 | 0.70 |
| 7:H:168:PRO:HG2 | 7:H:170:ARG:HD3 | 1.71 | 0.70 |
| 8:I:88:ILE:O | 8:I:121:LYS:HE3 | 1.91 | 0.70 |
| 16:Q:108:GLU:HG3 | 17:R:44:LYS:HG2 | 1.74 | 0.70 |
| 16:Q:92:ARG:HH11 | 16:Q:92:ARG:CB | 2.05 | 0.70 |
| 1:A:1210:A:H8 | 1:A:1210:A:C5' | 2.05 | 0.70 |
| 1:A:2393:A:H5' | 11:L:62:LEU:CD1 | 2.20 | 0.70 |
| 20:U:81:LYS:CD | 20:U:97:ARG:HB3 | 2.22 | 0.70 |
| 21:V:126:VAL:HG12 | 21:V:163:LEU:HA | 1.72 | 0.70 |
| 21:V:30:ASN:HD22 | 21:V:32:HIS:H | 1.39 | 0.70 |
| 27:2:40:LYS:HD3 | 27:2:46:CYS:HB3 | 1.72 | 0.70 |
| 1:A:1405:U:H2' | 1:A:1406:U:C6 | 2.26 | 0.70 |
| 5:F:28:ILE:H | 5:F:28:ILE:HD13 | 1.57 | 0.70 |
| 11:L:64:LYS:O | 11:L:66:GLY:N | 2.20 | 0.70 |
| 4:E:10:GLY:HA3 | 15:P:8:LYS:HE3 | 1.73 | 0.70 |
| 22:W:23:VAL:HA | 22:W:38:VAL:HG22 | 1.74 | 0.70 |
| 1:A:1805:U:O2 | 3:D:50:THR:HB | 1.92 | 0.70 |
| 3:D:57:GLY:H | 3:D:216:GLY:HA2 | 1.55 | 0.70 |
| 8:I:92:VAL:HG13 | 8:I:120:ILE:HG13 | 1.73 | 0.70 |
| 11:L:62:LEU:HD22 | 11:L:62:LEU:N | 2.05 | 0.70 |
| 1:A:2446:G:H2' | 1:A:2447:G:H5'' | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 4:E:47:VAL:HG23 | 4:E:84:PHE:O | 1.92 | 0.69 |
| 10:K:71:ARG:HH21 | 10:K:77:ILE:HG21 | 1.56 | 0.69 |
| 12:M:10:ARG:NE | 12:M:10:ARG:HA | 2.06 | 0.69 |
| 15:P:56:GLY:O | 15:P:59:THR:HG22 | 1.92 | 0.69 |
| 25:Z:52:HIS:H | 25:Z:52:HIS:CD2 | 2.10 | 0.69 |
| 27:2:33:CYS:SG | 27:2:40:LYS:HE3 | 2.31 | 0.69 |
| 31:A:4001:BLS:H102 | 31:A:4001:BLS:H151 | 1.57 | 0.69 |
| 1:A:1858:G:H1' | 1:A:1884:A:N6 | 2.06 | 0.69 |
| 24:Y:14:ARG:HA | 24:Y:17:SER:CB | 2.23 | 0.69 |
| 1:A:2747:G:O6 | 1:A:2755:C:H5'' | 1.91 | 0.69 |
| 12:M:103:MET:HB2 | 12:M:104:PHE:HD1 | 1.57 | 0.69 |
| 1:A:960:A:N6 | 12:M:82:ARG:HH21 | 1.89 | 0.69 |
| 23:X:53:VAL:HG22 | 23:X:74:VAL:HG13 | 1.74 | 0.69 |
| 25:Z:8:LEU:HB2 | 25:Z:28:LEU:HD23 | 1.74 | 0.69 |
| 4:E:9:VAL:HG13 | 4:E:25:VAL:O | 1.92 | 0.69 |
| 11:L:29:LYS:N | 11:L:29:LYS:HD2 | 2.06 | 0.69 |
| 15:P:27:THR:HG23 | 15:P:90:GLN:HB3 | 1.74 | 0.69 |
| 20:U:90:LEU:HD23 | 20:U:90:LEU:H | 1.56 | 0.69 |
| 10:K:4:PRO:O | 10:K:5:GLN:HB2 | 1.92 | 0.69 |
| 20:U:7:VAL:C | 20:U:8:LYS:HG3 | 2.11 | 0.69 |
| 23:X:51:VAL:HG13 | 23:X:58:ILE:HG23 | 1.75 | 0.69 |
| 3:D:21:PHE:HB3 | 3:D:24:ILE:HD12 | 1.72 | 0.69 |
| 5:F:6:MET:HG2 | 5:F:7:TYR:CD1 | 2.27 | 0.69 |
| 23:X:10:LYS:O | 23:X:13:ILE:HD11 | 1.92 | 0.69 |
| 24:Y:13:ALA:O | 24:Y:17:SER:HA | 1.92 | 0.69 |
| 1:A:118:A:H5' | 1:A:119:A:H8 | 1.58 | 0.69 |
| 9:J:79:ASN:H | 9:J:148:GLY:HA3 | 1.58 | 0.69 |
| 24:Y:14:ARG:HG2 | 24:Y:17:SER:OG | 1.92 | 0.69 |
| 11:L:29:LYS:H | 11:L:29:LYS:HD2 | 1.58 | 0.69 |
| 1:A:494:G:H21 | 18:S:57:ASN:HD21 | 1.41 | 0.69 |
| 3:D:255:LYS:O | 3:D:255:LYS:HD3 | 1.93 | 0.68 |
| 1:A:860:U:H5 | 1:A:917:A:N7 | 1.91 | 0.68 |
| 30:5:51:ALA:O | 30:5:54:GLU:HB3 | 1.93 | 0.68 |
| 1:A:1854:A:H62 | 1:A:1888:G:H8 | 1.40 | 0.68 |
| 1:A:2210:G:H3' | 1:A:2210:G:N3 | 2.08 | 0.68 |
| 4:E:103:ASP:OD1 | 4:E:201:THR:HG23 | 1.93 | 0.68 |
| 1:A:1529:A:H62 | 1:A:1542:G:N2 | 1.91 | 0.68 |
| 23:X:40:ARG:NH1 | 23:X:42:GLN:HG2 | 2.09 | 0.68 |
| 15:P:115:ARG:HD3 | 15:P:115:ARG:H | 1.59 | 0.68 |
| 1:A:602:G:H2' | 1:A:655:A:N6 | 2.07 | 0.68 |
| 5:F:133:ASN:HA | 5:F:162:LEU:HD13 | 1.76 | 0.68 |
| 12:M:58:PHE:HD1 | 12:M:58:PHE:O | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 20:U:42:VAL:HG12 | 20:U:65:ALA:HB3 | 1.75 | 0.68 |
| 11:L:62:LEU:HD23 | 30:5:25:MET:HB2 | 1.75 | 0.68 |
| 1:A:1045:A:H5' | 1:A:1047:G:H5' | 1.74 | 0.68 |
| 1:A:1659:U:OP2 | 4:E:132:HIS:HE1 | 1.76 | 0.68 |
| 1:A:1386:C:H2' | 1:A:1387:C:C6 | 2.29 | 0.68 |
| 1:A:1709:U:H2' | 1:A:1710:C:C6 | 2.28 | 0.68 |
| 1:A:2394:C:OP1 | 11:L:63:PRO:HD2 | 1.94 | 0.68 |
| 1:A:744:G:OP1 | 4:E:132:HIS:HB3 | 1.93 | 0.68 |
| 11:L:23:PRO:HD2 | 11:L:33:ARG:NH2 | 2.09 | 0.68 |
| 1:A:270(T):G:H2' | 1:A:270(U):G:H8 | 1.58 | 0.68 |
| 17:R:14:VAL:CG1 | 17:R:96:ILE:HG12 | 2.24 | 0.68 |
| 11:L:77:ARG:HB2 | 11:L:78:PRO:HD2 | 1.75 | 0.68 |
| 4:E:2:LYS:HD3 | 4:E:95:ILE:HG22 | 1.76 | 0.67 |
| 7:H:118:PRO:HG2 | 7:H:121:ILE:HD13 | 1.76 | 0.67 |
| 23:X:27:GLU:HB2 | 23:X:33:LYS:HA | 1.76 | 0.67 |
| 1:A:1416:G:H2' | 1:A:1417:C:C6 | 2.29 | 0.67 |
| 8:I:63:ALA:O | 8:I:66:GLU:HB3 | 1.94 | 0.67 |
| 23:X:40:ARG:HD2 | 23:X:41:ARG:N | 2.09 | 0.67 |
| 24:Y:14:ARG:HG2 | 24:Y:17:SER:CB | 2.24 | 0.67 |
| 4:E:49:LEU:HD23 | 4:E:81:ILE:HG12 | 1.75 | 0.67 |
| 6:G:71:THR:HG22 | 6:G:89:GLY:N | 2.08 | 0.67 |
| 11:L:23:PRO:HB3 | 11:L:29:LYS:HB3 | 1.77 | 0.67 |
| 12:M:10:ARG:HD3 | 12:M:11:LYS:H | 1.57 | 0.67 |
| 6:G:41:GLN:HB2 | 6:G:43:LEU:HD11 | 1.76 | 0.67 |
| 1:A:2840:C:H4' | 13:N:53:HIS:CD2 | 2.30 | 0.67 |
| 1:A:1045:A:H5'' | 1:A:1046:A:H3' | 1.76 | 0.67 |
| 1:A:2756:U:H4' | 1:A:2757:A:OP1 | 1.93 | 0.67 |
| 1:A:480:A:OP2 | 20:U:46:LYS:HE2 | 1.93 | 0.67 |
| 1:A:1332:G:H21 | 1:A:1610:A:H8 | 1.43 | 0.67 |
| 1:A:1981:A:H5'' | 1:A:1982:C:OP2 | 1.94 | 0.67 |
| 19:T:55:ASN:HB2 | 19:T:80:ILE:HG13 | 1.76 | 0.67 |
| 1:A:1005:C:O2' | 9:J:51:THR:HG21 | 1.95 | 0.67 |
| 5:F:12:LEU:HD13 | 5:F:124:LEU:HD11 | 1.77 | 0.67 |
| 9:J:157:ARG:N | 9:J:158:PRO:HD3 | 2.09 | 0.67 |
| 11:L:41:ARG:NE | 11:L:41:ARG:HA | 2.06 | 0.67 |
| 1:A:943:U:OP1 | 11:L:38:GLN:HB3 | 1.95 | 0.66 |
| 3:D:238:GLY:O | 3:D:239:ARG:C | 2.33 | 0.66 |
| 1:A:127:A:H5'' | 1:A:128:C:C6 | 2.30 | 0.66 |
| 1:A:1902:C:C4' | 3:D:244:ARG:HB2 | 2.25 | 0.66 |
| 7:H:33:LEU:HD11 | 7:H:136:ILE:HG22 | 1.76 | 0.66 |
| 18:S:73:ALA:HB3 | 18:S:106:ILE:HD11 | 1.76 | 0.66 |
| 13:N:29:LEU:HD12 | 13:N:70:LEU:HD21 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 21:V:9:TYR:OH | 21:V:61:LEU:HD13 | 1.95 | 0.66 |
| 1:A:1270:C:H5'' | 1:A:1271:G:O5' | 1.95 | 0.66 |
| 1:A:2116:G:N2 | 1:A:2163:C:H41 | 1.92 | 0.66 |
| 3:D:103:ARG:HG2 | 3:D:103:ARG:NH1 | 2.06 | 0.66 |
| 1:A:2562:U:H1' | 10:K:23:ARG:NH1 | 2.10 | 0.66 |
| 11:L:6:LEU:HD23 | 11:L:6:LEU:H | 1.60 | 0.66 |
| 19:T:50:LYS:N | 19:T:87:GLN:HE22 | 1.93 | 0.66 |
| 1:A:2039:C:H2' | 1:A:2040:C:H6 | 1.60 | 0.66 |
| 1:A:784:A:C5 | 3:D:229:VAL:HG21 | 2.31 | 0.66 |
| 27:2:40:LYS:CD | 27:2:46:CYS:HB3 | 2.24 | 0.66 |
| 1:A:996:A:H4' | 16:Q:92:ARG:NH1 | 2.10 | 0.66 |
| 8:I:56:LYS:HZ2 | 8:I:56:LYS:HB3 | 1.61 | 0.66 |
| 11:L:46:LYS:HB3 | 11:L:52:GLU:HG3 | 1.78 | 0.66 |
| 15:P:98:LYS:HB3 | 15:P:100:TYR:CE1 | 2.30 | 0.66 |
| 21:V:125:LEU:HD13 | 21:V:164:ALA:HB3 | 1.77 | 0.66 |
| 21:V:72:ARG:HG2 | 21:V:89:PHE:HB2 | 1.78 | 0.66 |
| 22:W:53:MET:HB3 | 22:W:59:LEU:HD23 | 1.77 | 0.66 |
| 22:W:56:ASP:O | 22:W:57:PHE:HB2 | 1.96 | 0.66 |
| 1:A:2688:U:H5 | 1:A:2720:U:OP2 | 1.79 | 0.66 |
| 1:A:547:A:H2' | 1:A:548:A:C2 | 2.31 | 0.66 |
| 4:E:7:VAL:HG22 | 4:E:27:LEU:HB3 | 1.76 | 0.66 |
| 1:A:528:A:H2 | 1:A:2043:C:H5' | 1.61 | 0.66 |
| 1:A:2147:G:H2' | 1:A:2148:G:O4' | 1.96 | 0.66 |
| 1:A:2601:C:H3' | 1:A:2602:A:H5'' | 1.77 | 0.66 |
| 6:G:90:LEU:HD22 | 6:G:90:LEU:H | 1.61 | 0.66 |
| 19:T:5:TYR:CE2 | 24:Y:30:ARG:HG3 | 2.31 | 0.66 |
| 27:2:29:ILE:O | 27:2:29:ILE:HD12 | 1.95 | 0.66 |
| 1:A:1270:C:H5'' | 1:A:1271:G:C5' | 2.26 | 0.66 |
| 1:A:2267:A:H5'' | 1:A:2268:A:H5' | 1.78 | 0.66 |
| 15:P:107:ASP:H | 15:P:110:ILE:HB | 1.60 | 0.66 |
| 16:Q:92:ARG:NH2 | 17:R:11:GLN:H | 1.93 | 0.66 |
| 12:M:62:GLY:HA2 | 21:V:116:VAL:HG21 | 1.76 | 0.66 |
| 1:A:2115:G:H2' | 1:A:2116:G:C8 | 2.32 | 0.65 |
| 1:A:2225:A:H4' | 1:A:2226:C:O5' | 1.94 | 0.65 |
| 6:G:137:GLU:HG2 | 6:G:152:LEU:HD22 | 1.78 | 0.65 |
| 15:P:8:LYS:O | 15:P:11:GLU:HB3 | 1.96 | 0.65 |
| 23:X:27:GLU:HG3 | 23:X:33:LYS:CE | 2.26 | 0.65 |
| 1:A:273(G):C:N4 | 1:A:363(A):G:H1 | 1.92 | 0.65 |
| 13:N:2:ARG:O | 13:N:2:ARG:HD2 | 1.96 | 0.65 |
| 1:A:518:G:H4' | 18:S:18:ARG:NH1 | 2.11 | 0.65 |
| 20:U:54:LYS:HG2 | 20:U:55:TYR:H | 1.60 | 0.65 |
| 1:A:1647:G:H3' | 1:A:1647:G:OP2 | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 4:E:172:VAL:HG13 | 4:E:182:LEU:HD11 | 1.77 | 0.65 |
| 5:F:34:TRP:CZ2 | 11:L:12:ALA:HB2 | 2.31 | 0.65 |
| 11:L:51:PHE:H | 11:L:57:THR:HG23 | 1.61 | 0.65 |
| 20:U:81:LYS:HG3 | 20:U:82:PRO:HD2 | 1.79 | 0.65 |
| 28:3:42:TRP:HA | 28:3:42:TRP:CE3 | 2.30 | 0.65 |
| 1:A:1478:G:HO2' | 1:A:1558:A:H2 | 1.45 | 0.65 |
| 2:B:115:G:H5' | 14:O:50:SER:OG | 1.97 | 0.65 |
| 1:A:2320:A:N3 | 1:A:2320:A:H2' | 2.12 | 0.65 |
| 1:A:814:C:H41 | 11:L:27:HIS:CD2 | 2.14 | 0.65 |
| 16:Q:24:TYR:HB2 | 16:Q:29:SER:HB3 | 1.79 | 0.65 |
| 1:A:1175:U:H5 | 1:A:1177:A:N6 | 1.95 | 0.65 |
| 1:A:34:C:O2' | 1:A:35:G:C5' | 2.41 | 0.65 |
| 16:Q:92:ARG:HD2 | 16:Q:95:LEU:HG | 1.78 | 0.65 |
| 1:A:302:C:H2' | 1:A:303:U:C6 | 2.30 | 0.65 |
| 1:A:534:U:O2' | 16:Q:49:HIS:CD2 | 2.50 | 0.65 |
| 11:L:89:ALA:HB1 | 11:L:121:LYS:HD3 | 1.78 | 0.65 |
| 5:F:11:VAL:HG22 | 5:F:125:LEU:HB2 | 1.79 | 0.65 |
| 11:L:16:ARG:NH1 | 11:L:18:ARG:HB2 | 2.12 | 0.65 |
| 30:5:52:LYS:HD2 | 30:5:52:LYS:N | 2.12 | 0.65 |
| 1:A:270(R):C:H2' | 1:A:270(S):G:H8 | 1.61 | 0.65 |
| 11:L:49:ARG:CG | 11:L:49:ARG:HH11 | 2.05 | 0.65 |
| 25:Z:40:THR:HG23 | 25:Z:43:ILE:HG12 | 1.77 | 0.65 |
| 5:F:20:LEU:CD2 | 5:F:21:ALA:H | 2.09 | 0.64 |
| 1:A:1490:A:H5' | 1:A:1494:A:N1 | 2.13 | 0.64 |
| 1:A:2090:G:H21 | 23:X:45:ASN:ND2 | 1.94 | 0.64 |
| 3:D:238:GLY:O | 3:D:240:ALA:N | 2.30 | 0.64 |
| 19:T:24:GLY:O | 19:T:83:VAL:HG22 | 1.97 | 0.64 |
| 1:A:1899:G:O2' | 1:A:1900:A:H5'' | 1.98 | 0.64 |
| 20:U:98:VAL:HG13 | 20:U:99:CYS:H | 1.63 | 0.64 |
| 28:3:25:LYS:HD3 | 30:5:34:TRP:CZ3 | 2.32 | 0.64 |
| 1:A:1113:U:H2' | 1:A:1114:G:C8 | 2.32 | 0.64 |
| 5:F:8:GLN:HA | 5:F:20:LEU:O | 1.97 | 0.64 |
| 27:2:4:HIS:CB | 27:2:5:PRO:CD | 2.76 | 0.64 |
| 28:3:39:TYR:HB3 | 28:3:49:HIS:CE1 | 2.31 | 0.64 |
| 4:E:77:ILE:HD13 | 4:E:195:LEU:HD13 | 1.79 | 0.64 |
| 11:L:18:ARG:O | 11:L:18:ARG:HD2 | 1.97 | 0.64 |
| 23:X:13:ILE:HG21 | 23:X:63:ALA:HB3 | 1.79 | 0.64 |
| 23:X:13:ILE:HG23 | 23:X:62:VAL:HG22 | 1.80 | 0.64 |
| 1:A:1348:G:C2' | 1:A:1349:A:H5'' | 2.26 | 0.64 |
| 1:A:2630:G:O4' | 1:A:2894:G:H1' | 1.98 | 0.64 |
| 10:K:107:ARG:HH22 | 15:P:36:GLU:HG3 | 1.63 | 0.64 |
| 3:D:25:THR:HG23 | 3:D:82:ILE:H | 1.61 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 6:G:114:ILE:HD13 | 6:G:140:ILE:HG21 | 1.80 | 0.64 |
| 12:M:22:LYS:HD3 | 12:M:22:LYS:C | 2.18 | 0.64 |
| 1:A:1416:G:H2' | 1:A:1417:C:H6 | 1.62 | 0.64 |
| 5:F:123:LEU:HD12 | 5:F:124:LEU:H | 1.61 | 0.64 |
| 8:I:133:HIS:HE1 | 8:I:135:GLU:HB3 | 1.63 | 0.64 |
| 11:L:126:VAL:HG22 | 11:L:145:PRO:HG2 | 1.78 | 0.64 |
| 1:A:271(C):G:H4' | 1:A:271(D):U:H5' | 1.80 | 0.64 |
| 1:A:276:C:H2' | 1:A:277:A:C8 | 2.31 | 0.64 |
| 1:A:892:G:H2' | 1:A:893:C:C6 | 2.33 | 0.64 |
| 16:Q:90:VAL:HG22 | 16:Q:91:ASP:N | 2.13 | 0.64 |
| 26:1:46:ASN:HD22 | 26:1:47:VAL:H | 1.44 | 0.64 |
| 1:A:1567:A:H5' | 3:D:58:HIS:ND1 | 2.12 | 0.64 |
| 1:A:2473:U:H2' | 1:A:2473:U:O2 | 1.98 | 0.63 |
| 1:A:655:A:O2' | 1:A:656:G:H5' | 1.98 | 0.63 |
| 5:F:14:PRO:HD3 | 5:F:128:ALA:HB2 | 1.79 | 0.63 |
| 1:A:7:G:H4' | 9:J:152:PRO:HB3 | 1.79 | 0.63 |
| 10:K:119:PRO:HB2 | 15:P:68:TYR:CE2 | 2.33 | 0.63 |
| 1:A:1796:U:H2' | 1:A:1797:C:C6 | 2.33 | 0.63 |
| 13:N:2:ARG:HD2 | 13:N:2:ARG:C | 2.18 | 0.63 |
| 21:V:5:LEU:HD23 | 21:V:6:LYS:N | 2.13 | 0.63 |
| 6:G:115:ARG:HH22 | 6:G:136:ARG:H | 1.45 | 0.63 |
| 1:A:2469:A:H2 | 1:A:2481:G:H21 | 1.46 | 0.63 |
| 9:J:154:GLN:NE2 | 9:J:155:ALA:HB3 | 2.13 | 0.63 |
| 1:A:270(L):C:H2' | 1:A:270(M):U:H2' | 1.79 | 0.63 |
| 1:A:2787:C:O4' | 4:E:62:PRO:HB3 | 1.99 | 0.63 |
| 4:E:92:THR:O | 4:E:95:ILE:HG13 | 1.98 | 0.63 |
| 1:A:1011:G:H5'' | 16:Q:77:SER:OG | 1.99 | 0.63 |
| 1:A:1514:U:H2' | 1:A:1515:C:H6 | 1.62 | 0.63 |
| 1:A:185:U:H4' | 1:A:218:A:H4' | 1.79 | 0.63 |
| 3:D:125:ILE:HG12 | 3:D:137:PRO:CD | 2.28 | 0.63 |
| 3:D:8:PRO:HB3 | 3:D:14:ARG:HB2 | 1.79 | 0.63 |
| 14:O:26:LEU:HG | 14:O:39:ILE:HD11 | 1.79 | 0.63 |
| 1:A:1658:C:OP1 | 4:E:132:HIS:ND1 | 2.32 | 0.63 |
| 10:K:76:ALA:HB3 | 15:P:75:ILE:HD13 | 1.81 | 0.63 |
| 1:A:534:U:O2' | 16:Q:49:HIS:HD2 | 1.80 | 0.63 |
| 1:A:1639:U:H2' | 1:A:1640:C:H5'' | 1.79 | 0.63 |
| 1:A:2115:G:H4' | 1:A:2166:G:H2' | 1.79 | 0.63 |
| 5:F:155:LEU:HA | 5:F:174:VAL:HG23 | 1.80 | 0.63 |
| 8:I:25:TYR:CE1 | 8:I:30:LEU:HD11 | 2.33 | 0.63 |
| 17:R:39:LEU:HA | 17:R:47:VAL:CG1 | 2.28 | 0.63 |
| 24:Y:17:SER:HB3 | 24:Y:18:PRO:HD3 | 1.79 | 0.63 |
| 27:2:33:CYS:HB3 | 27:2:40:LYS:HD2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1493:C:O2 | 1:A:1493:C:H2' | 1.99 | 0.63 |
| 1:A:1678:G:N2 | 1:A:1989:G:N2 | 2.47 | 0.63 |
| 8:I:3:VAL:HG23 | 8:I:37:VAL:O | 1.98 | 0.63 |
| 11:L:41:ARG:NE | 11:L:41:ARG:CA | 2.62 | 0.63 |
| 15:P:107:ASP:O | 15:P:110:ILE:HG22 | 1.99 | 0.63 |
| 15:P:86:ILE:O | 15:P:86:ILE:HG12 | 1.97 | 0.63 |
| 17:R:13:ARG:HD3 | 17:R:13:ARG:O | 1.99 | 0.63 |
| 1:A:1155:A:OP2 | 16:Q:55:ARG:HD3 | 1.99 | 0.62 |
| 1:A:2131:G:H5' | 1:A:2132:U:H3' | 1.81 | 0.62 |
| 1:A:2572:A:OP1 | 1:A:2574:G:H4' | 1.99 | 0.62 |
| 15:P:55:ASN:H | 15:P:59:THR:HB | 1.63 | 0.62 |
| 1:A:1187:G:H5'' | 17:R:81:TYR:CE2 | 2.34 | 0.62 |
| 1:A:1899:G:H22 | 1:A:1902:C:H41 | 1.43 | 0.62 |
| 3:D:139:GLY:H | 3:D:165:ILE:HB | 1.64 | 0.62 |
| 1:A:2113:U:H2' | 1:A:2114:A:C8 | 2.35 | 0.62 |
| 5:F:143:ALA:HB1 | 5:F:148:LEU:HB2 | 1.81 | 0.62 |
| 8:I:91:SER:OG | 8:I:119:PRO:HB2 | 1.97 | 0.62 |
| 1:A:2308:G:O2' | 1:A:2309:A:OP2 | 2.15 | 0.62 |
| 6:G:117:PHE:HD1 | 6:G:118:ARG:N | 1.96 | 0.62 |
| 11:L:94:GLU:HG3 | 11:L:124:LYS:HB3 | 1.81 | 0.62 |
| 11:L:64:LYS:HB2 | 30:5:25:MET:CG | 2.26 | 0.62 |
| 1:A:2287:A:N1 | 1:A:2346:A:H2 | 1.97 | 0.62 |
| 3:D:186:HIS:CD2 | 3:D:188:GLU:H | 2.18 | 0.62 |
| 16:Q:85:LYS:HD3 | 16:Q:85:LYS:O | 1.98 | 0.62 |
| 1:A:1174:A:H3' | 1:A:1175:U:C5' | 2.27 | 0.62 |
| 1:A:1871:A:H2' | 1:A:1872:A:C8 | 2.34 | 0.62 |
| 6:G:106:LEU:HA | 6:G:110:ALA:HB3 | 1.80 | 0.62 |
| 8:I:133:HIS:CE1 | 8:I:135:GLU:HB3 | 2.33 | 0.62 |
| 1:A:2814:C:O2' | 27:2:29:ILE:HG21 | 1.99 | 0.62 |
| 13:N:104:ARG:NH1 | 13:N:109:ALA:HB3 | 2.14 | 0.62 |
| 30:5:61:LEU:HB3 | 30:5:64:TYR:HB2 | 1.80 | 0.62 |
| 1:A:404:C:H4' | 1:A:405:U:H5' | 1.80 | 0.62 |
| 2:B:40:U:H3' | 2:B:41:U:C5' | 2.30 | 0.62 |
| 12:M:54:MET:HE3 | 12:M:64:ILE:HD12 | 1.82 | 0.62 |
| 20:U:14:LEU:HB2 | 20:U:24:VAL:HG22 | 1.82 | 0.62 |
| 20:U:13:VAL:CG1 | 20:U:27:VAL:HG12 | 2.30 | 0.62 |
| 24:Y:2:LYS:HA | 24:Y:5:GLU:CD | 2.20 | 0.62 |
| 1:A:1009:A:H5'' | 16:Q:59:ARG:HD3 | 1.82 | 0.62 |
| 2:B:66:A:H61 | 2:B:107:U:H2' | 1.65 | 0.62 |
| 23:X:11:ARG:HG2 | 23:X:61:ARG:O | 2.00 | 0.62 |
| 24:Y:11:GLU:O | 24:Y:14:ARG:HG3 | 1.99 | 0.62 |
| 24:Y:24:LEU:HD22 | 24:Y:60:LEU:HD11 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 26:1:39:ARG:HE | 26:1:39:ARG:HA | 1.65 | 0.61 |
| 1:A:1466:G:H2' | 1:A:1547:C:H41 | 1.65 | 0.61 |
| 1:A:2473:U:O2' | 1:A:2474:C:C5' | 2.46 | 0.61 |
| 5:F:131:GLY:HA2 | 5:F:138:GLU:OE1 | 1.99 | 0.61 |
| 17:R:47:VAL:HG12 | 17:R:52:VAL:HB | 1.82 | 0.61 |
| 15:P:132:LYS:O | 15:P:136:GLN:HG3 | 2.00 | 0.61 |
| 23:X:13:ILE:O | 23:X:14:VAL:HB | 2.01 | 0.61 |
| 1:A:1420:U:O2' | 1:A:1421:G:C5' | 2.48 | 0.61 |
| 1:A:2096:U:H2' | 1:A:2097:C:C6 | 2.35 | 0.61 |
| 1:A:2134:A:H8 | 1:A:2157:G:H21 | 1.49 | 0.61 |
| 1:A:2792:G:H1' | 1:A:2805:G:H22 | 1.63 | 0.61 |
| 3:D:154:LYS:HA | 3:D:157:ARG:HD3 | 1.81 | 0.61 |
| 16:Q:83:LEU:HD12 | 16:Q:113:ALA:HB2 | 1.82 | 0.61 |
| 12:M:64:ILE:HG12 | 21:V:178:GLU:HG3 | 1.81 | 0.61 |
| 1:A:1731:G:HO2' | 1:A:1732:A:H8 | 1.48 | 0.61 |
| 1:A:207:A:H2' | 1:A:208:C:O4' | 2.00 | 0.61 |
| 1:A:2364:C:H4' | 22:W:56:ASP:OD1 | 2.01 | 0.61 |
| 1:A:2577:A:H5'' | 1:A:2578:G:H5' | 1.82 | 0.61 |
| 1:A:270(O):G:O2' | 1:A:270(Q):C:H5' | 2.00 | 0.61 |
| 11:L:47:ASP:HB3 | 11:L:48:PRO:CA | 2.30 | 0.61 |
| 17:R:18:LEU:HD22 | 17:R:19:LYS:N | 2.15 | 0.61 |
| 27:2:25:LEU:HD12 | 27:2:25:LEU:H | 1.64 | 0.61 |
| 1:A:1019:U:H2' | 1:A:1021:A:H2 | 1.66 | 0.61 |
| 1:A:1022:G:O2' | 1:A:1023:U:OP2 | 2.15 | 0.61 |
| 3:D:38:LYS:N | 3:D:38:LYS:HD2 | 2.15 | 0.61 |
| 5:F:78:ILE:H | 5:F:78:ILE:HD12 | 1.65 | 0.61 |
| 16:Q:75:ASN:ND2 | 16:Q:78:THR:H | 1.97 | 0.61 |
| 18:S:70:TYR:H | 18:S:70:TYR:HD2 | 1.47 | 0.61 |
| 18:S:73:ALA:O | 18:S:106:ILE:HG13 | 2.00 | 0.61 |
| 23:X:13:ILE:CG2 | 23:X:63:ALA:HB3 | 2.30 | 0.61 |
| 1:A:528:A:C2 | 1:A:2043:C:H5' | 2.35 | 0.61 |
| 1:A:2119:A:N6 | 1:A:2170:A:H61 | 1.98 | 0.61 |
| 1:A:273(F):U:C2' | 1:A:273(G):C:H5'' | 2.30 | 0.61 |
| 3:D:43:ARG:HB2 | 3:D:48:ARG:O | 2.01 | 0.61 |
| 4:E:201:THR:CG2 | 4:E:202:LYS:N | 2.62 | 0.61 |
| 13:N:13:HIS:HE1 | 13:N:15:SER:HB2 | 1.64 | 0.61 |
| 21:V:28:MET:HE1 | 21:V:67:LEU:HD13 | 1.82 | 0.61 |
| 1:A:394:A:O2' | 1:A:395:U:H5' | 2.01 | 0.61 |
| 1:A:2729:G:H1' | 4:E:187:ALA:CB | 2.28 | 0.61 |
| 6:G:77:ILE:HB | 6:G:82:LEU:HD12 | 1.82 | 0.61 |
| 8:I:8:PRO:HD3 | 8:I:15:VAL:HG22 | 1.82 | 0.61 |
| 12:M:24:GLY:HA2 | 12:M:101:ARG:HA | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 23:X:10:LYS:O | 23:X:11:ARG:HB2 | 2.01 | 0.61 |
| 1:A:1858:G:H1' | 1:A:1884:A:H62 | 1.66 | 0.61 |
| 1:A:2392:A:H2 | 1:A:2424:C:H42 | 1.49 | 0.61 |
| 11:L:125:VAL:HG13 | 11:L:144:GLU:HB3 | 1.82 | 0.61 |
| 16:Q:95:LEU:HD13 | 17:R:4:ILE:HD12 | 1.82 | 0.61 |
| 3:D:27:THR:O | 3:D:27:THR:HG23 | 2.00 | 0.61 |
| 11:L:7:ARG:O | 11:L:10:PRO:HD2 | 2.01 | 0.61 |
| 14:O:56:LEU:HD23 | 14:O:57:LYS:NZ | 2.15 | 0.61 |
| 20:U:76:CYS:HB3 | 20:U:96:ILE:HD13 | 1.83 | 0.61 |
| 28:3:42:TRP:HA | 28:3:42:TRP:HE3 | 1.66 | 0.60 |
| 29:4:8:ASN:ND2 | 29:4:11:LYS:H | 1.99 | 0.60 |
| 4:E:28:ALA:HB3 | 4:E:93:VAL:HG22 | 1.82 | 0.60 |
| 21:V:10:ARG:HG2 | 21:V:11:GLU:H | 1.66 | 0.60 |
| 30:5:61:LEU:O | 30:5:63:PRO:HD2 | 1.99 | 0.60 |
| 1:A:2309:A:O5' | 1:A:2309:A:H8 | 1.84 | 0.60 |
| 7:H:94:TYR:H | 7:H:94:TYR:HD1 | 1.47 | 0.60 |
| 9:J:59:GLY:O | 9:J:61:HIS:N | 2.33 | 0.60 |
| 17:R:35:LEU:HB2 | 17:R:57:VAL:HG13 | 1.83 | 0.60 |
| 21:V:78:LYS:O | 21:V:79:ARG:HB3 | 2.01 | 0.60 |
| 23:X:13:ILE:HG21 | 23:X:63:ALA:CB | 2.31 | 0.60 |
| 25:Z:54:VAL:O | 25:Z:55:ARG:HD3 | 2.00 | 0.60 |
| 28:3:26:ASN:ND2 | 28:3:28:ARG:H | 1.99 | 0.60 |
| 3:D:30:GLU:HG3 | 3:D:63:ARG:CZ | 2.30 | 0.60 |
| 24:Y:57:ILE:HG22 | 24:Y:61:LEU:HD23 | 1.82 | 0.60 |
| 1:A:2023:G:H5' | 1:A:2617:C:H4' | 1.83 | 0.60 |
| 2:B:81:G:H5' | 2:B:82:G:OP2 | 2.02 | 0.60 |
| 3:D:133:LEU:HB3 | 3:D:173:VAL:HG11 | 1.84 | 0.60 |
| 17:R:52:VAL:HG13 | 17:R:55:ALA:HB3 | 1.83 | 0.60 |
| 1:A:1614:A:H61 | 18:S:88:ARG:H | 1.47 | 0.60 |
| 1:A:784:A:H5' | 1:A:785:G:OP1 | 2.01 | 0.60 |
| 6:G:19:LEU:HD11 | 6:G:172:LEU:HD13 | 1.84 | 0.60 |
| 11:L:17:LYS:HB3 | 11:L:19:VAL:HG22 | 1.82 | 0.60 |
| 14:O:26:LEU:HD13 | 14:O:87:PHE:HD1 | 1.67 | 0.60 |
| 1:A:1840:G:H1 | 1:A:1902:C:H42 | 1.50 | 0.60 |
| 1:A:2698:U:H2' | 1:A:2699:C:C6 | 2.37 | 0.60 |
| 1:A:2306:C:H4' | 6:G:136:ARG:NH1 | 2.16 | 0.60 |
| 1:A:1022:G:H22 | 1:A:1142(B):A:H2 | 1.47 | 0.60 |
| 3:D:131:LEU:HA | 3:D:190:TYR:CE2 | 2.37 | 0.60 |
| 6:G:60:LEU:O | 6:G:64:THR:HG22 | 2.01 | 0.60 |
| 20:U:13:VAL:HG12 | 20:U:27:VAL:HG12 | 1.81 | 0.60 |
| 25:Z:6:VAL:HG22 | 25:Z:56:VAL:HG12 | 1.84 | 0.60 |
| 1:A:1270:C:H5'' | 1:A:1271:G:H5' | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1510:A:H2' | 1:A:1511:A:C8 | 2.37 | 0.60 |
| 1:A:277:A:C5 | 1:A:278:A:H1' | 2.36 | 0.60 |
| 6:G:141:PHE:HB3 | 6:G:142:PRO:HD2 | 1.84 | 0.60 |
| 1:A:494:G:N2 | 18:S:57:ASN:HD21 | 1.98 | 0.60 |
| 21:V:94:GLU:CD | 21:V:94:GLU:H | 2.04 | 0.60 |
| 23:X:13:ILE:HD12 | 23:X:14:VAL:N | 2.15 | 0.60 |
| 1:A:2306:C:H4' | 6:G:136:ARG:HH12 | 1.67 | 0.60 |
| 1:A:86:C:H4' | 1:A:104:U:H1' | 1.83 | 0.60 |
| 3:D:106:ILE:O | 3:D:108:PRO:HD3 | 2.02 | 0.60 |
| 3:D:31:LYS:HE3 | 3:D:33:LEU:HD11 | 1.84 | 0.60 |
| 8:I:71:ILE:HG13 | 8:I:72:LEU:HD22 | 1.84 | 0.60 |
| 19:T:57:LEU:HD11 | 19:T:78:LYS:HD2 | 1.84 | 0.60 |
| 20:U:2:ARG:N | 20:U:4:LYS:HZ2 | 2.00 | 0.60 |
| 21:V:120:ILE:HG12 | 21:V:172:ALA:HA | 1.82 | 0.60 |
| 1:A:1019:U:C2' | 1:A:1021:A:H2 | 2.15 | 0.60 |
| 2:B:86:G:H2' | 2:B:87:G:C8 | 2.36 | 0.60 |
| 4:E:201:THR:CG2 | 4:E:202:LYS:H | 2.13 | 0.60 |
| 5:F:181:LEU:HD21 | 5:F:186:ILE:HD11 | 1.84 | 0.60 |
| 5:F:52:LYS:HB3 | 5:F:56:GLU:HB2 | 1.84 | 0.60 |
| 10:K:63:VAL:HB | 10:K:102:VAL:HG12 | 1.83 | 0.60 |
| 13:N:33:ARG:NE | 13:N:115:GLU:HG3 | 2.16 | 0.60 |
| 13:N:4:LEU:O | 13:N:4:LEU:HD13 | 2.01 | 0.60 |
| 18:S:9:TYR:H | 18:S:102:HIS:HD2 | 1.50 | 0.60 |
| 23:X:57:GLU:HG2 | 23:X:58:ILE:H | 1.67 | 0.60 |
| 1:A:32:C:O2' | 1:A:33:U:H5' | 2.01 | 0.59 |
| 15:P:23:ARG:HE | 15:P:120:ARG:HD3 | 1.67 | 0.59 |
| 1:A:2236:C:H2' | 1:A:2237:G:O4' | 2.02 | 0.59 |
| 1:A:2529:G:H5'' | 1:A:2530:A:H5'' | 1.84 | 0.59 |
| 1:A:2531:A:H5'' | 7:H:157:TYR:CE2 | 2.37 | 0.59 |
| 1:A:2688:U:C5 | 1:A:2720:U:OP2 | 2.56 | 0.59 |
| 3:D:172:TYR:CD1 | 3:D:186:HIS:HA | 2.37 | 0.59 |
| 3:D:186:HIS:HD2 | 3:D:188:GLU:H | 1.50 | 0.59 |
| 1:A:2598:A:OP1 | 3:D:235:GLY:HA3 | 2.01 | 0.59 |
| 12:M:52:VAL:HA | 12:M:55:VAL:HG13 | 1.84 | 0.59 |
| 1:A:2867:G:C5 | 15:P:23:ARG:NH1 | 2.70 | 0.59 |
| 1:A:847:U:H5 | 1:A:933:A:H62 | 1.50 | 0.59 |
| 13:N:56:LYS:HE3 | 13:N:87:TYR:O | 2.02 | 0.59 |
| 15:P:35:LYS:O | 15:P:35:LYS:HG3 | 2.02 | 0.59 |
| 1:A:1227:G:OP1 | 16:Q:13:LYS:HG2 | 2.01 | 0.59 |
| 1:A:2615:U:C2 | 27:2:7:PRO:HA | 2.36 | 0.59 |
| 1:A:154:G:H2' | 1:A:155:C:O4' | 2.02 | 0.59 |
| 1:A:2645:G:H3' | 1:A:2646:C:H5' | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:E:192:ASN:HD22 | 4:E:192:ASN:N | 1.99 | 0.59 |
| 5:F:202:PHE:CE1 | 5:F:206:ILE:HD11 | 2.36 | 0.59 |
| 11:L:125:VAL:CG1 | 11:L:138:LEU:HD21 | 2.30 | 0.59 |
| 1:A:245:G:H5' | 11:L:73:GLY:HA3 | 1.83 | 0.59 |
| 16:Q:83:LEU:HG | 16:Q:88:ILE:HD12 | 1.84 | 0.59 |
| 19:T:12:VAL:HG12 | 19:T:29:TRP:CE2 | 2.37 | 0.59 |
| 20:U:47:LYS:HA | 20:U:60:PHE:CD2 | 2.36 | 0.59 |
| 1:A:1025:G:OP1 | 1:A:1025:G:H8 | 1.85 | 0.59 |
| 3:D:57:GLY:N | 3:D:216:GLY:HA2 | 2.16 | 0.59 |
| 17:R:72:VAL:HG23 | 17:R:85:LYS:HB2 | 1.85 | 0.59 |
| 1:A:2567:G:H2' | 1:A:2568:C:C6 | 2.37 | 0.59 |
| 6:G:107:LEU:HD21 | 6:G:178:PHE:CD1 | 2.37 | 0.59 |
| 13:N:70:LEU:HD12 | 13:N:70:LEU:H | 1.67 | 0.59 |
| 19:T:3:THR:HA | 19:T:6:ASP:OD2 | 2.02 | 0.59 |
| 1:A:2564:A:C2 | 1:A:2647:U:H4' | 2.38 | 0.59 |
| 5:F:117:ARG:HD2 | 5:F:190:GLU:O | 2.02 | 0.59 |
| 11:L:23:PRO:CB | 11:L:33:ARG:HG3 | 2.25 | 0.59 |
| 17:R:77:ALA:O | 17:R:79:VAL:HG22 | 2.01 | 0.59 |
| 1:A:2090:G:N2 | 23:X:45:ASN:HD21 | 1.97 | 0.59 |
| 28:3:26:ASN:ND2 | 28:3:27:LYS:H | 2.00 | 0.59 |
| 6:G:7:LEU:HD11 | 6:G:107:LEU:HD12 | 1.83 | 0.59 |
| 7:H:137:ASP:HB3 | 7:H:140:LYS:HG3 | 1.84 | 0.59 |
| 19:T:50:LYS:H | 19:T:87:GLN:HE22 | 1.51 | 0.59 |
| 1:A:1544:C:OP1 | 1:A:1544:C:H6 | 1.86 | 0.59 |
| 1:A:674:G:H1' | 5:F:74:ARG:HD3 | 1.85 | 0.59 |
| 3:D:206:LEU:HD22 | 3:D:211:ARG:HG2 | 1.83 | 0.59 |
| 3:D:62:TYR:HA | 3:D:87:ASN:HD21 | 1.67 | 0.59 |
| 17:R:38:LEU:HD23 | 17:R:39:LEU:H | 1.67 | 0.59 |
| 1:A:495:G:H1' | 18:S:57:ASN:ND2 | 2.17 | 0.59 |
| 25:Z:7:LYS:HE2 | 25:Z:32:GLN:NE2 | 2.17 | 0.59 |
| 1:A:1598:C:H5' | 19:T:36:LYS:HB2 | 1.84 | 0.59 |
| 3:D:79:VAL:HG23 | 3:D:113:VAL:HA | 1.85 | 0.59 |
| 6:G:130:ASN:OD1 | 6:G:160:VAL:HA | 2.02 | 0.59 |
| 7:H:13:LYS:HD3 | 7:H:14:GLY:N | 2.18 | 0.59 |
| 11:L:61:ARG:C | 11:L:62:LEU:HD13 | 2.23 | 0.59 |
| 21:V:92:SER:HB2 | 21:V:94:GLU:OE1 | 2.03 | 0.59 |
| 1:A:203:C:H3' | 1:A:204:A:H5'' | 1.85 | 0.58 |
| 1:A:2543:G:H2' | 1:A:2544:G:C8 | 2.38 | 0.58 |
| 1:A:34:C:H41 | 1:A:447:A:H61 | 1.51 | 0.58 |
| 4:E:69:LYS:HD3 | 4:E:69:LYS:O | 2.02 | 0.58 |
| 9:J:132:LYS:HD3 | 9:J:132:LYS:N | 2.12 | 0.58 |
| 10:K:3:GLN:HB2 | 10:K:4:PRO:HD2 | 1.83 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 15:P:118:ARG:HA | 15:P:121:ILE:HB | 1.84 | 0.58 |
| 15:P:36:GLU:HB2 | 15:P:41:ARG:HD3 | 1.84 | 0.58 |
| 16:Q:44:ASN:HD21 | 17:R:75:PHE:HB3 | 1.67 | 0.58 |
| 24:Y:9:GLN:O | 24:Y:12:GLU:HB3 | 2.03 | 0.58 |
| 1:A:1546:A:H2' | 1:A:1546(B):C:H5' | 1.84 | 0.58 |
| 1:A:2356:C:O3' | 22:W:20:ARG:HD3 | 2.02 | 0.58 |
| 3:D:264:LYS:HD3 | 3:D:266:SER:HB3 | 1.85 | 0.58 |
| 3:D:58:HIS:O | 3:D:58:HIS:CG | 2.57 | 0.58 |
| 16:Q:47:TYR:HA | 16:Q:50:ARG:NH2 | 2.19 | 0.58 |
| 23:X:56:GLN:HE21 | 23:X:85:LEU:HD23 | 1.68 | 0.58 |
| 23:X:64:ALA:HA | 23:X:67:ILE:HG13 | 1.83 | 0.58 |
| 23:X:67:ILE:N | 23:X:68:PRO:HD2 | 2.18 | 0.58 |
| 29:4:8:ASN:ND2 | 29:4:8:ASN:C | 2.57 | 0.58 |
| 23:X:9:GLY:O | 23:X:13:ILE:CD1 | 2.51 | 0.58 |
| 1:A:1021:A:N6 | 1:A:1141:U:H3 | 2.02 | 0.58 |
| 1:A:1578:U:H2' | 1:A:1579:A:H5' | 1.84 | 0.58 |
| 1:A:2150:U:H2' | 1:A:2151:G:H8 | 1.68 | 0.58 |
| 7:H:65:HIS:CE1 | 7:H:69:ARG:HD3 | 2.39 | 0.58 |
| 20:U:13:VAL:HG23 | 20:U:73:ARG:O | 2.02 | 0.58 |
| 20:U:51:VAL:HG13 | 20:U:52:SER:H | 1.69 | 0.58 |
| 21:V:30:ASN:OD1 | 21:V:90:VAL:HB | 2.02 | 0.58 |
| 1:A:860:U:C5 | 1:A:917:A:N7 | 2.71 | 0.58 |
| 1:A:95:G:H4' | 24:Y:46:GLN:HB3 | 1.85 | 0.58 |
| 7:H:168:PRO:HG2 | 7:H:170:ARG:NH1 | 2.18 | 0.58 |
| 21:V:10:ARG:HH21 | 21:V:26:GLY:H | 1.49 | 0.58 |
| 23:X:31:GLY:O | 23:X:32:LYS:HB2 | 2.02 | 0.58 |
| 1:A:270(R):C:H2' | 1:A:270(S):G:C8 | 2.38 | 0.58 |
| 10:K:68:GLU:HA | 10:K:78:ARG:HB3 | 1.85 | 0.58 |
| 11:L:16:ARG:CZ | 11:L:18:ARG:HB2 | 2.34 | 0.58 |
| 13:N:33:ARG:HA | 13:N:115:GLU:HB2 | 1.85 | 0.58 |
| 3:D:75:ILE:HG21 | 3:D:99:ASP:HB2 | 1.85 | 0.58 |
| 12:M:45:GLN:CD | 12:M:45:GLN:H | 2.07 | 0.58 |
| 15:P:24:PRO:HD3 | 15:P:52:ILE:HD12 | 1.85 | 0.58 |
| 21:V:136:PHE:C | 21:V:137:ILE:HD12 | 2.24 | 0.58 |
| 1:A:2355:C:H1' | 22:W:39:ARG:HE | 1.68 | 0.58 |
| 3:D:132:PRO:HD3 | 3:D:190:TYR:CZ | 2.38 | 0.58 |
| 4:E:24:THR:HG22 | 4:E:184:VAL:HG23 | 1.86 | 0.58 |
| 9:J:90:LEU:H | 9:J:90:LEU:HD12 | 1.67 | 0.58 |
| 10:K:7:TYR:CE1 | 10:K:20:MET:HB2 | 2.39 | 0.58 |
| 1:A:941:A:H4' | 11:L:35:HIS:CD2 | 2.38 | 0.58 |
| 1:A:2196:C:O2' | 1:A:2197:U:H5' | 2.03 | 0.58 |
| 1:A:2447:G:H4' | 1:A:2448:A:C5' | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:323:G:H2' | 5:F:169:ASN:OD1 | 2.03 | 0.58 |
| 6:G:73:ALA:HB3 | 6:G:85:GLY:HA2 | 1.86 | 0.58 |
| 9:J:127:LYS:HB2 | 9:J:140:PHE:CE1 | 2.38 | 0.58 |
| 1:A:1266:G:C8 | 18:S:15:ARG:NH2 | 2.72 | 0.58 |
| 24:Y:49:LYS:O | 24:Y:53:LEU:HB2 | 2.04 | 0.58 |
| 1:A:1389:G:C2 | 1:A:1399:C:O2 | 2.56 | 0.58 |
| 1:A:1408:C:H2' | 1:A:1409:C:C6 | 2.39 | 0.58 |
| 1:A:1494:A:O2' | 1:A:1495:A:H5'' | 2.04 | 0.58 |
| 1:A:2809:A:N1 | 1:A:2892:A:H1' | 2.19 | 0.58 |
| 11:L:92:GLU:HG3 | 11:L:123:LEU:HD13 | 1.86 | 0.58 |
| 15:P:100:TYR:HD2 | 15:P:103:ARG:HH22 | 1.51 | 0.58 |
| 26:I:53:THR:O | 26:I:54:LYS:HG2 | 2.04 | 0.57 |
| 1:A:1794:U:H1' | 1:A:1900:A:C2 | 2.39 | 0.57 |
| 1:A:2233:U:H2' | 1:A:2234:G:C8 | 2.39 | 0.57 |
| 3:D:131:LEU:HG | 3:D:136:ILE:HD11 | 1.87 | 0.57 |
| 1:A:1796:U:H4' | 3:D:256:GLY:H | 1.69 | 0.57 |
| 11:L:23:PRO:HD2 | 11:L:33:ARG:HH21 | 1.67 | 0.57 |
| 11:L:59:LEU:HA | 11:L:61:ARG:CZ | 2.34 | 0.57 |
| 1:A:244:A:H4' | 11:L:74:GLU:HB2 | 1.86 | 0.57 |
| 18:S:15:ARG:NE | 27:2:20:ARG:HH12 | 2.02 | 0.57 |
| 1:A:1921:G:H2' | 1:A:1922:G:H8 | 1.69 | 0.57 |
| 1:A:2146:C:H4' | 1:A:2147:G:C8 | 2.39 | 0.57 |
| 1:A:49:A:H5'' | 1:A:51:G:O4' | 2.04 | 0.57 |
| 3:D:255:LYS:CD | 3:D:255:LYS:H | 2.15 | 0.57 |
| 6:G:107:LEU:HD23 | 6:G:111:LEU:HD12 | 1.85 | 0.57 |
| 1:A:2414:G:H21 | 11:L:67:MET:CE | 2.17 | 0.57 |
| 14:O:14:VAL:O | 14:O:18:ILE:HG12 | 2.04 | 0.57 |
| 17:R:38:LEU:O | 17:R:52:VAL:HG12 | 2.04 | 0.57 |
| 18:S:83:LYS:C | 18:S:84:ARG:HD2 | 2.24 | 0.57 |
| 1:A:245:G:O6 | 30:5:8:LYS:HE3 | 2.04 | 0.57 |
| 1:A:1048:A:H2' | 1:A:1048:A:N3 | 2.18 | 0.57 |
| 1:A:265:A:H1' | 1:A:266:G:O4' | 2.04 | 0.57 |
| 6:G:77:ILE:N | 6:G:82:LEU:HB2 | 2.19 | 0.57 |
| 7:H:20:ALA:HB1 | 7:H:21:PRO:HD2 | 1.86 | 0.57 |
| 7:H:92:ILE:HD12 | 7:H:92:ILE:H | 1.68 | 0.57 |
| 11:L:49:ARG:NH1 | 11:L:49:ARG:HG3 | 2.05 | 0.57 |
| 17:R:39:LEU:HA | 17:R:47:VAL:HG13 | 1.85 | 0.57 |
| 20:U:14:LEU:HD12 | 20:U:15:VAL:N | 2.20 | 0.57 |
| 24:Y:9:GLN:HA | 24:Y:12:GLU:HB3 | 1.86 | 0.57 |
| 24:Y:46:GLN:H | 24:Y:49:LYS:HE2 | 1.67 | 0.57 |
| 1:A:1493:C:H4' | 1:A:1494:A:OP1 | 2.04 | 0.57 |
| 1:A:1824:G:OP1 | 3:D:52:ARG:HD3 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2210:G:N2 | 1:A:2211:G:H5' | 2.19 | 0.57 |
| 4:E:47:VAL:HG12 | 4:E:49:LEU:HD22 | 1.86 | 0.57 |
| 6:G:117:PHE:HD1 | 6:G:118:ARG:H | 1.51 | 0.57 |
| 8:I:109:ILE:HB | 8:I:130:TYR:CE1 | 2.39 | 0.57 |
| 13:N:49:ASP:OD2 | 13:N:95:THR:HB | 2.04 | 0.57 |
| 14:O:61:ASN:ND2 | 14:O:64:GLU:H | 2.01 | 0.57 |
| 21:V:24:LEU:HD12 | 21:V:25:PRO:O | 2.04 | 0.57 |
| 1:A:1406:U:H2' | 1:A:1407:C:C6 | 2.39 | 0.57 |
| 1:A:2294:C:H2' | 1:A:2295:C:H6 | 1.70 | 0.57 |
| 1:A:2593:U:H2' | 1:A:2594:C:C6 | 2.39 | 0.57 |
| 6:G:83:ARG:HB2 | 6:G:86:MET:SD | 2.44 | 0.57 |
| 8:I:23:PRO:O | 8:I:27:ARG:HB2 | 2.05 | 0.57 |
| 8:I:6:LEU:O | 8:I:15:VAL:HG13 | 2.03 | 0.57 |
| 9:J:85:VAL:HG22 | 9:J:89:LYS:HG3 | 1.85 | 0.57 |
| 1:A:1495:A:N3 | 1:A:1495:A:H2' | 2.17 | 0.57 |
| 1:A:1794:U:H1' | 1:A:1900:A:N3 | 2.20 | 0.57 |
| 6:G:139:LEU:HD23 | 6:G:139:LEU:H | 1.69 | 0.57 |
| 11:L:91:PHE:N | 11:L:91:PHE:CD1 | 2.70 | 0.57 |
| 10:K:73:ASP:HB2 | 15:P:82:LEU:CD1 | 2.34 | 0.57 |
| 17:R:39:LEU:HD12 | 17:R:47:VAL:HG21 | 1.86 | 0.57 |
| 17:R:39:LEU:HD12 | 17:R:50:PRO:O | 2.05 | 0.57 |
| 21:V:157:LEU:HD11 | 21:V:163:LEU:HD22 | 1.87 | 0.57 |
| 24:Y:35:LEU:HD12 | 24:Y:53:LEU:HD12 | 1.87 | 0.57 |
| 30:5:50:LEU:O | 30:5:51:ALA:CB | 2.51 | 0.57 |
| 1:A:1221(A):C:H2' | 1:A:1222:C:H6 | 1.69 | 0.57 |
| 1:A:2712:U:O2' | 1:A:712(B):A:P | 2.62 | 0.57 |
| 10:K:2:ILE:HD11 | 10:K:82:ASN:HB3 | 1.86 | 0.57 |
| 11:L:112:LEU:HD23 | 11:L:113:LYS:N | 2.18 | 0.57 |
| 15:P:120:ARG:O | 15:P:124:ASP:HB2 | 2.05 | 0.57 |
| 27:2:36:CYS:SG | 27:2:37:LYS:N | 2.78 | 0.57 |
| 1:A:2285:C:OP2 | 28:3:27:LYS:HD2 | 2.05 | 0.57 |
| 20:U:81:LYS:HD2 | 20:U:98:VAL:HG12 | 1.87 | 0.57 |
| 1:A:1292:U:H2' | 1:A:1293:C:C6 | 2.39 | 0.57 |
| 1:A:2398:U:H2' | 1:A:2399:G:C8 | 2.40 | 0.57 |
| 1:A:2645:G:OP2 | 1:A:2645:G:H8 | 1.88 | 0.57 |
| 1:A:999:U:O2' | 1:A:1000:A:H5' | 2.04 | 0.57 |
| 10:K:101:PRO:O | 10:K:102:VAL:HG13 | 2.05 | 0.57 |
| 17:R:69:LYS:O | 17:R:70:ILE:HD12 | 2.05 | 0.57 |
| 29:4:36:GLN:HG2 | 29:4:36:GLN:O | 2.05 | 0.57 |
| 1:A:330:A:C2 | 1:A:1210:A:H2' | 2.36 | 0.57 |
| 1:A:1328:G:H2' | 1:A:1330:C:C5 | 2.40 | 0.57 |
| 1:A:2262:U:H4' | 1:A:2328:A:C2 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:2889:C:H2' | 1:A:2891:G:O4' | 2.04 | 0.57 |
| 3:D:70:TRP:CH2 | 3:D:150:LYS:HA | 2.40 | 0.57 |
| 6:G:105:LYS:CD | 6:G:142:PRO:HG3 | 2.33 | 0.57 |
| 6:G:77:ILE:H | 6:G:82:LEU:HB2 | 1.70 | 0.57 |
| 1:A:832:G:H21 | 11:L:53:GLY:HA3 | 1.70 | 0.57 |
| 11:L:59:LEU:HA | 11:L:61:ARG:CD | 2.35 | 0.57 |
| 18:S:6:ILE:HG12 | 18:S:104:THR:HG23 | 1.87 | 0.57 |
| 25:Z:31:LEU:HD23 | 25:Z:32:GLN:HG2 | 1.86 | 0.57 |
| 1:A:2291:U:H2' | 1:A:2292:C:C6 | 2.40 | 0.56 |
| 1:A:2446:G:C3' | 1:A:2447:G:H5'' | 2.34 | 0.56 |
| 12:M:27:VAL:HB | 12:M:134:ARG:HD2 | 1.86 | 0.56 |
| 17:R:39:LEU:HB3 | 17:R:47:VAL:CG2 | 2.35 | 0.56 |
| 18:S:24:ILE:HG21 | 18:S:36:LEU:CD1 | 2.29 | 0.56 |
| 20:U:81:LYS:HZ3 | 20:U:98:VAL:HB | 1.70 | 0.56 |
| 30:5:52:LYS:HA | 30:5:52:LYS:CE | 2.29 | 0.56 |
| 1:A:2307:G:C5 | 1:A:2308:G:C5 | 2.93 | 0.56 |
| 1:A:278:A:H61 | 1:A:362:U:H3 | 1.52 | 0.56 |
| 3:D:161:THR:O | 3:D:196:VAL:HG23 | 2.04 | 0.56 |
| 13:N:78:LYS:O | 13:N:83:ILE:HG12 | 2.05 | 0.56 |
| 1:A:1607:C:H5'' | 1:A:1608:A:H5' | 1.86 | 0.56 |
| 1:A:2738:A:C2 | 1:A:2739:U:H1' | 2.40 | 0.56 |
| 1:A:2808:U:C2' | 1:A:2809:A:H5' | 2.35 | 0.56 |
| 5:F:34:TRP:HB2 | 11:L:10:PRO:O | 2.05 | 0.56 |
| 11:L:40:SER:O | 11:L:41:ARG:NE | 2.39 | 0.56 |
| 16:Q:91:ASP:OD1 | 16:Q:96:ALA:HB2 | 2.05 | 0.56 |
| 20:U:2:ARG:N | 20:U:4:LYS:HD2 | 2.19 | 0.56 |
| 25:Z:2:PRO:O | 25:Z:3:ARG:HG3 | 2.05 | 0.56 |
| 1:A:1766:U:H2' | 1:A:1767:C:H6 | 1.70 | 0.56 |
| 1:A:247:G:H4' | 1:A:386:G:C5 | 2.40 | 0.56 |
| 1:A:654:U:H5' | 1:A:655:A:OP2 | 2.05 | 0.56 |
| 13:N:78:LYS:HE2 | 13:N:83:ILE:HD11 | 1.87 | 0.56 |
| 14:O:49:VAL:HG13 | 14:O:76:LYS:HZ2 | 1.70 | 0.56 |
| 24:Y:47:ASN:O | 24:Y:50:ILE:HG13 | 2.06 | 0.56 |
| 1:A:61:G:H5' | 24:Y:50:ILE:CD1 | 2.36 | 0.56 |
| 1:A:2272:U:H5'' | 1:A:2273:A:OP1 | 2.05 | 0.56 |
| 1:A:2645:G:H3' | 1:A:2646:C:C5' | 2.35 | 0.56 |
| 1:A:780:G:N2 | 1:A:783:A:H62 | 2.00 | 0.56 |
| 10:K:88:ASN:HD21 | 10:K:92:GLU:HB2 | 1.70 | 0.56 |
| 13:N:87:TYR:HD1 | 13:N:90:ARG:HD3 | 1.70 | 0.56 |
| 24:Y:6:VAL:O | 24:Y:10:LEU:HG | 2.06 | 0.56 |
| 1:A:2130:U:H3' | 1:A:2130:U:OP2 | 2.06 | 0.56 |
| 1:A:545:G:H21 | 1:A:548:A:H62 | 1.53 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:58:G:N2 | 1:A:70:G:C4 | 2.74 | 0.56 |
| 2:B:43:C:H2' | 2:B:44:G:H5'' | 1.86 | 0.56 |
| 14:O:26:LEU:HD13 | 14:O:87:PHE:CD1 | 2.40 | 0.56 |
| 20:U:73:ARG:NH2 | 20:U:82:PRO:HD3 | 2.20 | 0.56 |
| 1:A:1021:A:H3' | 1:A:1021:A:C8 | 2.40 | 0.56 |
| 1:A:2282:G:H4' | 1:A:2389:G:O2' | 2.05 | 0.56 |
| 1:A:2709:G:O2' | 1:A:2710:C:H5' | 2.06 | 0.56 |
| 1:A:2808:U:H2' | 1:A:2809:A:H5' | 1.86 | 0.56 |
| 1:A:2879:C:H4' | 1:A:2880:C:OP1 | 2.04 | 0.56 |
| 6:G:107:LEU:HD21 | 6:G:178:PHE:CE1 | 2.40 | 0.56 |
| 16:Q:75:ASN:HD21 | 16:Q:78:THR:H | 1.51 | 0.56 |
| 16:Q:92:ARG:CG | 16:Q:92:ARG:HH11 | 2.19 | 0.56 |
| 17:R:39:LEU:HB3 | 17:R:47:VAL:HG21 | 1.88 | 0.56 |
| 18:S:15:ARG:CZ | 27:2:20:ARG:HH12 | 2.18 | 0.56 |
| 25:Z:17:LYS:HD3 | 25:Z:18:ASP:N | 2.20 | 0.56 |
| 1:A:108:U:H2' | 1:A:109:G:C8 | 2.41 | 0.56 |
| 1:A:2320:A:C8 | 1:A:2333:A:N6 | 2.73 | 0.56 |
| 1:A:2821:A:OP2 | 1:A:2822:G:OP2 | 2.23 | 0.56 |
| 1:A:528:A:C2 | 1:A:2043:C:H4' | 2.41 | 0.56 |
| 1:A:616:A:C4' | 1:A:617:G:OP1 | 2.54 | 0.56 |
| 7:H:121:ILE:HD11 | 7:H:140:LYS:HB3 | 1.87 | 0.56 |
| 8:I:4:ILE:HD13 | 8:I:4:ILE:H | 1.71 | 0.56 |
| 9:J:160:LYS:NZ | 9:J:161:LEU:H | 1.91 | 0.56 |
| 10:K:1:MET:HE3 | 10:K:67:LYS:HG2 | 1.86 | 0.56 |
| 1:A:2690:C:H5'' | 13:N:8:ARG:HH12 | 1.71 | 0.56 |
| 14:O:64:GLU:HG2 | 14:O:67:ARG:HH21 | 1.70 | 0.56 |
| 1:A:2355:C:O2' | 22:W:39:ARG:HD2 | 2.06 | 0.56 |
| 24:Y:18:PRO:O | 24:Y:22:GLU:HG3 | 2.05 | 0.56 |
| 1:A:1217:C:P | 16:Q:15:LYS:HZ1 | 2.29 | 0.56 |
| 15:P:51:ARG:HG3 | 15:P:98:LYS:HG3 | 1.87 | 0.56 |
| 22:W:51:VAL:HG22 | 22:W:81:VAL:HG23 | 1.86 | 0.56 |
| 1:A:1500:G:H21 | 3:D:100:GLY:HA3 | 1.70 | 0.56 |
| 1:A:2029:G:H2' | 1:A:2031:A:OP1 | 2.05 | 0.56 |
| 1:A:2777:G:C5' | 1:A:2778:A:H5' | 2.36 | 0.56 |
| 1:A:796:C:H2' | 1:A:797:C:C6 | 2.41 | 0.56 |
| 2:B:40:U:H3' | 2:B:41:U:H5'' | 1.87 | 0.56 |
| 19:T:89:ILE:HG22 | 19:T:92:LEU:H | 1.71 | 0.56 |
| 21:V:82:ARG:HG3 | 21:V:83:PRO:HD2 | 1.88 | 0.56 |
| 2:B:83:G:H5'' | 25:Z:52:HIS:CE1 | 2.41 | 0.56 |
| 1:A:1052:C:C5 | 1:A:1101:U:H5' | 2.41 | 0.56 |
| 1:A:1731:G:O2' | 1:A:1732:A:H8 | 1.89 | 0.56 |
| 1:A:1980:G:O2' | 1:A:1982:C:OP2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:2584:U:H2' | 1:A:2585:U:H2' | 1.88 | 0.56 |
| 1:A:330:A:H2 | 1:A:1210:A:C2' | 2.19 | 0.56 |
| 2:B:51:G:N2 | 2:B:52:A:H62 | 2.04 | 0.56 |
| 6:G:41:GLN:HG2 | 6:G:155:MET:HB3 | 1.88 | 0.56 |
| 9:J:68:ASN:HD22 | 9:J:68:ASN:N | 2.04 | 0.56 |
| 11:L:57:THR:HB | 11:L:59:LEU:N | 2.14 | 0.56 |
| 11:L:93:GLY:H | 11:L:123:LEU:HD12 | 1.71 | 0.56 |
| 1:A:1732:A:H2' | 1:A:1733:G:O4' | 2.06 | 0.55 |
| 1:A:830:G:H4' | 1:A:831:G:OP2 | 2.05 | 0.55 |
| 3:D:36:PRO:HA | 3:D:62:TYR:O | 2.06 | 0.55 |
| 6:G:124:SER:HB2 | 6:G:131:TYR:CE1 | 2.41 | 0.55 |
| 7:H:25:LYS:HG3 | 7:H:34:GLU:HG2 | 1.87 | 0.55 |
| 9:J:93:LYS:HE2 | 9:J:95:TYR:CZ | 2.41 | 0.55 |
| 19:T:10:ALA:HB1 | 19:T:11:PRO:HD2 | 1.88 | 0.55 |
| 1:A:1153:C:C2' | 1:A:1154:G:H5' | 2.36 | 0.55 |
| 1:A:163:U:H2' | 1:A:164:U:O4' | 2.06 | 0.55 |
| 1:A:2115:G:C6 | 1:A:2117:A:H5'' | 2.42 | 0.55 |
| 1:A:2212:A:H1' | 1:A:2215:G:C4 | 2.42 | 0.55 |
| 7:H:87:LEU:HB2 | 7:H:131:VAL:HB | 1.88 | 0.55 |
| 1:A:631:A:OP1 | 11:L:64:LYS:HE3 | 2.06 | 0.55 |
| 12:M:83:MET:SD | 12:M:83:MET:C | 2.84 | 0.55 |
| 13:N:9:LYS:O | 13:N:10:LEU:HB3 | 2.06 | 0.55 |
| 17:R:2:PHE:CZ | 17:R:13:ARG:NH2 | 2.74 | 0.55 |
| 21:V:54:HIS:CG | 21:V:101:PRO:HG3 | 2.41 | 0.55 |
| 21:V:59:LEU:HD12 | 21:V:69:THR:HG21 | 1.87 | 0.55 |
| 24:Y:53:LEU:O | 24:Y:57:ILE:HG13 | 2.04 | 0.55 |
| 26:1:40:ILE:HD12 | 26:1:40:ILE:H | 1.70 | 0.55 |
| 1:A:2123:G:H2' | 1:A:2124:G:C8 | 2.42 | 0.55 |
| 6:G:59:GLU:O | 6:G:63:ILE:HG23 | 2.06 | 0.55 |
| 11:L:116:GLY:N | 11:L:134:ALA:HB2 | 2.21 | 0.55 |
| 12:M:116:GLU:O | 12:M:120:ILE:HG12 | 2.05 | 0.55 |
| 16:Q:61:TRP:CH2 | 16:Q:94:ASN:HB2 | 2.41 | 0.55 |
| 19:T:44:GLU:HG3 | 19:T:51:VAL:HG22 | 1.88 | 0.55 |
| 23:X:27:GLU:HB3 | 23:X:33:LYS:HG3 | 1.88 | 0.55 |
| 23:X:27:GLU:HG3 | 23:X:33:LYS:CD | 2.36 | 0.55 |
| 23:X:51:VAL:O | 23:X:58:ILE:HG22 | 2.06 | 0.55 |
| 1:A:1210:A:C8 | 1:A:1210:A:C5' | 2.88 | 0.55 |
| 1:A:2262:U:H4' | 1:A:2328:A:H2 | 1.71 | 0.55 |
| 1:A:2579:C:O2' | 4:E:131:ALA:CB | 2.49 | 0.55 |
| 1:A:448:U:O4 | 1:A:583:G:H1' | 2.07 | 0.55 |
| 3:D:103:ARG:CG | 3:D:103:ARG:HH11 | 2.07 | 0.55 |
| 6:G:16:ARG:O | 6:G:20:ILE:HG13 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 7:H:88:LEU:HD12 | 7:H:129:THR:O | 2.06 | 0.55 |
| 8:I:72:LEU:HD12 | 8:I:140:LEU:HD13 | 1.86 | 0.55 |
| 8:I:72:LEU:HD21 | 8:I:107:ILE:HG12 | 1.89 | 0.55 |
| 9:J:33:GLU:CD | 9:J:34:PRO:HD2 | 2.27 | 0.55 |
| 14:O:30:ARG:HA | 14:O:35:ILE:HA | 1.88 | 0.55 |
| 17:R:6:LYS:O | 17:R:37:VAL:HG21 | 2.05 | 0.55 |
| 20:U:4:LYS:N | 20:U:4:LYS:HD3 | 2.21 | 0.55 |
| 1:A:2287:A:N1 | 1:A:2346:A:C2 | 2.74 | 0.55 |
| 1:A:270(Z):G:C2 | 1:A:271(A):U:O4 | 2.59 | 0.55 |
| 6:G:63:ILE:HG22 | 6:G:144:ILE:HD11 | 1.89 | 0.55 |
| 7:H:86:GLU:CD | 7:H:86:GLU:H | 2.10 | 0.55 |
| 9:J:79:ASN:HD21 | 9:J:149:PRO:HD3 | 1.70 | 0.55 |
| 17:R:39:LEU:O | 17:R:40:LEU:HB2 | 2.06 | 0.55 |
| 21:V:104:PHE:HB3 | 21:V:141:VAL:HG11 | 1.87 | 0.55 |
| 26:1:61:VAL:HG13 | 26:1:65:CYS:HB2 | 1.87 | 0.55 |
| 1:A:1006:C:H1' | 9:J:129:MET:CG | 2.35 | 0.55 |
| 1:A:310:A:OP1 | 20:U:18:GLY:HA2 | 2.06 | 0.55 |
| 3:D:130:ALA:HA | 3:D:192:THR:HA | 1.89 | 0.55 |
| 6:G:11:TYR:HA | 6:G:15:VAL:HB | 1.89 | 0.55 |
| 6:G:39:ILE:HD12 | 6:G:39:ILE:H | 1.71 | 0.55 |
| 13:N:98:LEU:HB2 | 13:N:113:LEU:CD2 | 2.37 | 0.55 |
| 19:T:53:LYS:HB3 | 19:T:82:GLN:HB3 | 1.88 | 0.55 |
| 20:U:50:ARG:NH2 | 20:U:55:TYR:HB3 | 2.21 | 0.55 |
| 1:A:1021:A:H62 | 1:A:1141:U:H3 | 1.53 | 0.55 |
| 1:A:1036:G:OP1 | 7:H:59:ARG:HB2 | 2.06 | 0.55 |
| 1:A:1126:A:H4' | 1:A:1127:A:O5' | 2.07 | 0.55 |
| 1:A:26:G:C6 | 1:A:27:G:N1 | 2.74 | 0.55 |
| 3:D:148:GLU:HB2 | 3:D:151:LYS:HD2 | 1.89 | 0.55 |
| 3:D:17:THR:O | 3:D:204:ILE:HG22 | 2.06 | 0.55 |
| 9:J:69:VAL:O | 9:J:70:ALA:HB3 | 2.07 | 0.55 |
| 11:L:116:GLY:H | 11:L:134:ALA:HB2 | 1.72 | 0.55 |
| 1:A:2278:A:OP1 | 12:M:10:ARG:HD2 | 2.06 | 0.55 |
| 12:M:38:GLU:HB2 | 12:M:127:ILE:HD12 | 1.89 | 0.55 |
| 1:A:2126:A:H1' | 1:A:2127:G:H1' | 1.88 | 0.55 |
| 1:A:832:G:H21 | 11:L:53:GLY:CA | 2.19 | 0.55 |
| 1:A:881:G:H1 | 1:A:895:U:H3 | 1.54 | 0.55 |
| 3:D:177:LEU:HD11 | 3:D:183:ARG:HD2 | 1.87 | 0.55 |
| 3:D:37:LEU:C | 3:D:38:LYS:HD2 | 2.27 | 0.55 |
| 9:J:154:GLN:HG2 | 9:J:155:ALA:N | 2.21 | 0.55 |
| 17:R:62:LEU:HD22 | 17:R:95:LEU:HB2 | 1.88 | 0.55 |
| 19:T:12:VAL:HG22 | 19:T:27:THR:O | 2.06 | 0.55 |
| 1:A:2086:U:H2' | 1:A:2087:G:C8 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:296:C:H2' | 1:A:297:C:H6 | 1.72 | 0.55 |
| 20:U:54:LYS:HG2 | 20:U:55:TYR:N | 2.22 | 0.55 |
| 1:A:1657:C:H2' | 1:A:1658:C:H6 | 1.72 | 0.55 |
| 1:A:286:C:H2' | 1:A:287:C:H6 | 1.70 | 0.55 |
| 3:D:231:HIS:CG | 3:D:232:PRO:HD2 | 2.41 | 0.55 |
| 3:D:95:LEU:HD12 | 3:D:95:LEU:O | 2.07 | 0.55 |
| 5:F:110:LEU:HD11 | 5:F:181:LEU:HD22 | 1.89 | 0.55 |
| 1:A:451:C:H4' | 5:F:52:LYS:NZ | 2.21 | 0.55 |
| 16:Q:62:ILE:HD12 | 16:Q:76:TYR:CZ | 2.42 | 0.55 |
| 1:A:947:G:H2' | 1:A:948:G:H8 | 1.72 | 0.54 |
| 3:D:235:GLY:O | 3:D:237:GLU:N | 2.40 | 0.54 |
| 3:D:57:GLY:H | 3:D:216:GLY:CA | 2.19 | 0.54 |
| 7:H:17:VAL:HG12 | 7:H:26:VAL:HG22 | 1.89 | 0.54 |
| 8:I:101:LEU:HD22 | 8:I:109:ILE:HD12 | 1.88 | 0.54 |
| 8:I:75:LEU:HD12 | 8:I:76:THR:H | 1.72 | 0.54 |
| 15:P:105:LEU:HD21 | 15:P:109:GLU:HG3 | 1.89 | 0.54 |
| 1:A:1587:A:H2' | 1:A:1588:C:C6 | 2.41 | 0.54 |
| 1:A:188:G:H2' | 1:A:189:G:H5' | 1.89 | 0.54 |
| 1:A:2563:U:H2' | 1:A:2565:A:OP2 | 2.07 | 0.54 |
| 3:D:131:LEU:HG | 3:D:136:ILE:CD1 | 2.37 | 0.54 |
| 4:E:101:ARG:HD3 | 4:E:169:ASN:ND2 | 2.21 | 0.54 |
| 7:H:123:PHE:HA | 7:H:132:ARG:O | 2.07 | 0.54 |
| 14:O:27:SER:HA | 14:O:88:ASP:HB3 | 1.88 | 0.54 |
| 15:P:115:ARG:H | 15:P:115:ARG:CD | 2.17 | 0.54 |
| 18:S:31:GLU:O | 18:S:35:ILE:HG13 | 2.06 | 0.54 |
| 21:V:34:ASN:O | 21:V:35:ARG:HG2 | 2.07 | 0.54 |
| 1:A:108:U:H2' | 1:A:109:G:H8 | 1.73 | 0.54 |
| 1:A:1668:A:H4' | 1:A:1669:A:O5' | 2.07 | 0.54 |
| 1:A:1889:A:H2' | 1:A:1890:A:C8 | 2.43 | 0.54 |
| 1:A:252:G:OP2 | 11:L:50:ARG:NH1 | 2.40 | 0.54 |
| 1:A:2789:C:H5'' | 1:A:2790:A:OP1 | 2.07 | 0.54 |
| 3:D:155:LEU:HD23 | 3:D:177:LEU:HD22 | 1.89 | 0.54 |
| 4:E:24:THR:CB | 4:E:186:GLY:HA2 | 2.36 | 0.54 |
| 15:P:31:SER:OG | 15:P:85:LYS:HE2 | 2.06 | 0.54 |
| 23:X:13:ILE:HG21 | 23:X:63:ALA:N | 2.21 | 0.54 |
| 29:4:9:ARG:HE | 29:4:47:ARG:CB | 2.14 | 0.54 |
| 1:A:1514:U:H2' | 1:A:1515:C:C6 | 2.41 | 0.54 |
| 1:A:1656:C:H2' | 1:A:1657:C:C6 | 2.43 | 0.54 |
| 1:A:2630:G:C8 | 1:A:2894:G:C2 | 2.96 | 0.54 |
| 9:J:154:GLN:HE21 | 9:J:155:ALA:CB | 2.18 | 0.54 |
| 13:N:96:ARG:NH2 | 13:N:117:VAL:HG23 | 2.22 | 0.54 |
| 15:P:23:ARG:HH21 | 15:P:120:ARG:HD3 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 20:U:11:ASP:O | 20:U:27:VAL:HG13 | 2.08 | 0.54 |
| 1:A:85:G:OP1 | 20:U:9:LYS:HB2 | 2.07 | 0.54 |
| 1:A:2420:C:OP1 | 30:5:34:TRP:HA | 2.08 | 0.54 |
| 1:A:1656:C:H2' | 1:A:1657:C:H6 | 1.73 | 0.54 |
| 1:A:1854:A:N6 | 1:A:1888:G:H8 | 2.06 | 0.54 |
| 1:A:2562:U:H1' | 10:K:23:ARG:HH11 | 1.73 | 0.54 |
| 1:A:655:A:C2' | 1:A:656:G:H5' | 2.37 | 0.54 |
| 7:H:105:LEU:HD12 | 7:H:105:LEU:O | 2.08 | 0.54 |
| 7:H:168:PRO:HG2 | 7:H:170:ARG:HH11 | 1.72 | 0.54 |
| 1:A:2758:A:C4 | 7:H:67:LEU:HD21 | 2.42 | 0.54 |
| 9:J:96:THR:HB | 9:J:105:LEU:HD11 | 1.88 | 0.54 |
| 19:T:29:TRP:CZ3 | 19:T:78:LYS:HB2 | 2.43 | 0.54 |
| 30:5:8:LYS:O | 30:5:12:LYS:HG3 | 2.07 | 0.54 |
| 1:A:2271:G:H2' | 1:A:2272:U:C6 | 2.42 | 0.54 |
| 1:A:2698:U:H2' | 1:A:2699:C:H6 | 1.73 | 0.54 |
| 2:B:95:U:H2' | 2:B:96:G:C8 | 2.43 | 0.54 |
| 12:M:10:ARG:HD3 | 12:M:11:LYS:N | 2.23 | 0.54 |
| 17:R:49:THR:HG22 | 17:R:50:PRO:CD | 2.33 | 0.54 |
| 21:V:60:GLU:OE1 | 21:V:66:SER:HB3 | 2.08 | 0.54 |
| 1:A:2880:C:H1' | 13:N:92:GLY:O | 2.07 | 0.54 |
| 1:A:479:A:H4' | 1:A:480:A:O5' | 2.08 | 0.54 |
| 3:D:132:PRO:HD3 | 3:D:190:TYR:CE2 | 2.42 | 0.54 |
| 5:F:101:LEU:HD12 | 5:F:102:PRO:HD2 | 1.89 | 0.54 |
| 19:T:31:HIS:ND1 | 19:T:32:PRO:HD2 | 2.23 | 0.54 |
| 21:V:58:VAL:HA | 21:V:67:LEU:O | 2.07 | 0.54 |
| 24:Y:42:GLY:O | 24:Y:44:LEU:N | 2.40 | 0.54 |
| 1:A:1344:G:H4' | 1:A:1384:A:C5 | 2.43 | 0.54 |
| 1:A:1730:U:H2' | 1:A:1730:U:O2 | 2.07 | 0.54 |
| 1:A:2125:G:H2' | 1:A:2126:A:C8 | 2.42 | 0.54 |
| 1:A:389:G:C6 | 11:L:71:VAL:HG23 | 2.43 | 0.54 |
| 3:D:10:THR:OG1 | 3:D:13:ARG:HB2 | 2.07 | 0.54 |
| 3:D:27:THR:CG2 | 3:D:83:GLU:HG2 | 2.38 | 0.54 |
| 8:I:25:TYR:O | 8:I:29:TYR:HB3 | 2.07 | 0.54 |
| 27:2:42:PRO:O | 27:2:44:THR:HG23 | 2.08 | 0.54 |
| 1:A:1005:C:H2' | 1:A:1006:C:C6 | 2.43 | 0.54 |
| 1:A:996:A:H4' | 16:Q:92:ARG:CZ | 2.38 | 0.54 |
| 4:E:203:LYS:O | 4:E:203:LYS:HD2 | 2.08 | 0.54 |
| 6:G:173:LEU:HD13 | 6:G:178:PHE:CE2 | 2.43 | 0.54 |
| 7:H:16:SER:HB2 | 7:H:27:LYS:HB2 | 1.90 | 0.54 |
| 9:J:59:GLY:H | 9:J:65:TRP:HZ3 | 1.55 | 0.54 |
| 13:N:63:ARG:HA | 13:N:80:PHE:CZ | 2.43 | 0.54 |
| 13:N:90:ARG:HG3 | 13:N:90:ARG:O | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 23:X:13:ILE:HG13 | 23:X:62:VAL:HG23 | 1.90 | 0.54 |
| 23:X:27:GLU:CB | 23:X:33:LYS:HG3 | 2.38 | 0.54 |
| 1:A:1529:A:N6 | 1:A:1542:G:N2 | 2.56 | 0.54 |
| 1:A:1299:G:H22 | 1:A:1640:C:H5' | 1.73 | 0.54 |
| 1:A:508:G:O2' | 1:A:509:C:H5'' | 2.08 | 0.54 |
| 1:A:2275:C:O2 | 12:M:83:MET:HG3 | 2.08 | 0.54 |
| 13:N:70:LEU:HD12 | 13:N:70:LEU:N | 2.22 | 0.54 |
| 15:P:27:THR:HA | 15:P:48:ILE:HA | 1.89 | 0.54 |
| 15:P:48:ILE:H | 15:P:48:ILE:HD12 | 1.72 | 0.54 |
| 1:A:1558:A:H1' | 1:A:1559:G:OP2 | 2.08 | 0.53 |
| 1:A:2822:G:H2' | 1:A:2823:A:H5'' | 1.90 | 0.53 |
| 1:A:860:U:O2 | 1:A:860:U:O4' | 2.24 | 0.53 |
| 1:A:881:G:C2 | 1:A:882:G:H1' | 2.43 | 0.53 |
| 1:A:2311:A:H5' | 6:G:77:ILE:HD11 | 1.91 | 0.53 |
| 19:T:59:VAL:HG23 | 19:T:59:VAL:O | 2.09 | 0.53 |
| 1:A:2764:A:N6 | 1:A:2766:G:C2 | 2.76 | 0.53 |
| 1:A:586:A:N1 | 1:A:809:G:O2' | 2.35 | 0.53 |
| 10:K:17:ARG:HE | 10:K:47:ILE:HD12 | 1.72 | 0.53 |
| 13:N:22:ARG:O | 13:N:26:LYS:HG3 | 2.08 | 0.53 |
| 14:O:71:ARG:O | 14:O:75:GLU:HG2 | 2.08 | 0.53 |
| 15:P:35:LYS:HE2 | 15:P:37:GLY:O | 2.08 | 0.53 |
| 16:Q:76:TYR:CZ | 16:Q:80:ILE:HG13 | 2.43 | 0.53 |
| 21:V:48:PHE:HE2 | 21:V:71:VAL:HG11 | 1.72 | 0.53 |
| 1:A:593:G:O3' | 30:5:62:LEU:HD22 | 2.08 | 0.53 |
| 1:A:1396:U:H2' | 1:A:1396:U:O2 | 2.07 | 0.53 |
| 1:A:2307:G:C8 | 1:A:2308:G:N7 | 2.76 | 0.53 |
| 1:A:2341:G:H2' | 1:A:2342:C:O4' | 2.07 | 0.53 |
| 1:A:405:U:H3' | 1:A:406:G:C5' | 2.37 | 0.53 |
| 6:G:72:ARG:HD2 | 6:G:85:GLY:O | 2.09 | 0.53 |
| 7:H:131:VAL:HG12 | 7:H:133:VAL:HG23 | 1.91 | 0.53 |
| 9:J:66:THR:O | 9:J:69:VAL:HG12 | 2.08 | 0.53 |
| 10:K:79:PHE:HD2 | 15:P:72:VAL:HG22 | 1.72 | 0.53 |
| 20:U:2:ARG:HD2 | 20:U:3:VAL:HG23 | 1.89 | 0.53 |
| 20:U:77:PRO:O | 20:U:78:ALA:HB2 | 2.08 | 0.53 |
| 1:A:1543:A:H5' | 1:A:1544:C:OP2 | 2.08 | 0.53 |
| 1:A:2114:A:N6 | 1:A:2115:G:C2 | 2.77 | 0.53 |
| 1:A:2850:A:OP2 | 1:A:2866:U:H5 | 1.91 | 0.53 |
| 1:A:2853:C:H2' | 1:A:2854:G:C8 | 2.43 | 0.53 |
| 5:F:45:ARG:CG | 5:F:45:ARG:NH1 | 2.59 | 0.53 |
| 6:G:16:ARG:NH1 | 6:G:31:VAL:HG11 | 2.24 | 0.53 |
| 7:H:103:LEU:HD23 | 7:H:104:GLU:N | 2.23 | 0.53 |
| 1:A:806:C:P | 11:L:39:LYS:HG3 | 2.49 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:411:G:N2 | 11:L:71:VAL:HG11 | 2.23 | 0.53 |
| 12:M:9:TYR:O | 12:M:9:TYR:CD2 | 2.61 | 0.53 |
| 17:R:35:LEU:HB3 | 17:R:37:VAL:HG23 | 1.91 | 0.53 |
| 19:T:71:GLY:C | 19:T:72:LYS:HG3 | 2.27 | 0.53 |
| 21:V:53:ILE:HD11 | 21:V:99:TYR:HB2 | 1.89 | 0.53 |
| 1:A:2795:G:H3' | 1:A:2797:U:C5' | 2.38 | 0.53 |
| 1:A:886:C:N3 | 1:A:890:A:N6 | 2.57 | 0.53 |
| 1:A:960:A:H61 | 12:M:82:ARG:NH2 | 1.94 | 0.53 |
| 2:B:103:U:O2' | 2:B:104:A:H5' | 2.08 | 0.53 |
| 4:E:104:VAL:HG12 | 4:E:196:VAL:CG2 | 2.39 | 0.53 |
| 1:A:1142(B):A:H4' | 9:J:48:ARG:HH22 | 1.73 | 0.53 |
| 19:T:53:LYS:NZ | 19:T:55:ASN:HD21 | 2.06 | 0.53 |
| 28:3:18:ARG:HH21 | 28:3:44:ARG:HH11 | 1.57 | 0.53 |
| 1:A:212:G:O2' | 1:A:213:A:H5' | 2.08 | 0.53 |
| 1:A:38:A:H2' | 1:A:39:C:C6 | 2.43 | 0.53 |
| 1:A:443:A:H1' | 1:A:1201:C:O4' | 2.08 | 0.53 |
| 3:D:147:LEU:HD13 | 3:D:155:LEU:HD11 | 1.91 | 0.53 |
| 8:I:5:LEU:CD2 | 8:I:5:LEU:H | 2.14 | 0.53 |
| 24:Y:16:LEU:HB2 | 24:Y:20:GLU:HG2 | 1.90 | 0.53 |
| 30:5:14:VAL:CG1 | 30:5:22:VAL:HG13 | 2.39 | 0.53 |
| 1:A:2349:G:OP2 | 30:5:42:ARG:HD3 | 2.09 | 0.53 |
| 1:A:1437:C:H2' | 1:A:1438:U:C6 | 2.44 | 0.53 |
| 1:A:286:C:H2' | 1:A:287:C:C6 | 2.43 | 0.53 |
| 1:A:352:G:O2' | 1:A:353:G:C8 | 2.62 | 0.53 |
| 1:A:363(F):U:O2' | 1:A:363(G):A:O5' | 2.27 | 0.53 |
| 1:A:1659:U:OP2 | 4:E:132:HIS:CE1 | 2.60 | 0.53 |
| 11:L:51:PHE:CE1 | 11:L:59:LEU:HD13 | 2.44 | 0.53 |
| 17:R:96:ILE:N | 17:R:96:ILE:HD12 | 2.24 | 0.53 |
| 1:A:1323:U:H5' | 18:S:84:ARG:HH21 | 1.74 | 0.53 |
| 1:A:153:C:OP1 | 23:X:92:LYS:HD2 | 2.09 | 0.53 |
| 18:S:15:ARG:NE | 27:2:20:ARG:NH1 | 2.57 | 0.53 |
| 28:3:15:GLU:HG2 | 28:3:16:CYS:N | 2.23 | 0.53 |
| 1:A:1358:G:O2' | 1:A:1359:A:H5'' | 2.08 | 0.53 |
| 4:E:101:ARG:HD3 | 4:E:169:ASN:HD21 | 1.74 | 0.53 |
| 7:H:168:PRO:CG | 7:H:170:ARG:HD3 | 2.37 | 0.53 |
| 9:J:53:ILE:O | 9:J:57:LEU:HD22 | 2.09 | 0.53 |
| 1:A:390:A:C5 | 11:L:71:VAL:HG21 | 2.44 | 0.53 |
| 14:O:61:ASN:HB3 | 14:O:64:GLU:HB2 | 1.91 | 0.53 |
| 16:Q:102:GLU:HG3 | 17:R:2:PHE:CE1 | 2.44 | 0.53 |
| 17:R:99:ILE:HD13 | 17:R:99:ILE:N | 2.24 | 0.53 |
| 30:5:59:LYS:HB3 | 30:5:59:LYS:HZ2 | 1.74 | 0.53 |
| 1:A:1288:U:C2 | 1:A:1327:C:O2 | 2.61 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 1:A:2681:C:H5 | 1:A:2725:A:N6 | 1.96 | 0.53 |
| 9:J:66:THR:HG22 | 9:J:68:ASN:ND2 | 2.23 | 0.53 |
| 11:L:16:ARG:C | 11:L:16:ARG:HE | 2.12 | 0.53 |
| 12:M:9:TYR:C | 12:M:9:TYR:CD2 | 2.82 | 0.53 |
| 18:S:68:ARG:O | 18:S:110:LYS:HB2 | 2.09 | 0.53 |
| 23:X:10:LYS:O | 23:X:11:ARG:CB | 2.56 | 0.53 |
| 23:X:13:ILE:HG23 | 23:X:62:VAL:CG2 | 2.38 | 0.53 |
| 1:A:1278:A:H2' | 1:A:1279:G:C8 | 2.44 | 0.53 |
| 1:A:2068:U:H3 | 1:A:2430:A:H2 | 1.56 | 0.53 |
| 1:A:214:G:H1' | 1:A:216:A:O2' | 2.08 | 0.53 |
| 1:A:2211:G:H3' | 1:A:2211:G:N3 | 2.24 | 0.53 |
| 1:A:2506:U:H3' | 1:A:2506:U:H6 | 1.74 | 0.53 |
| 1:A:2730:C:O2' | 1:A:2731:G:H5' | 2.09 | 0.53 |
| 1:A:2439:A:OP1 | 31:A:4001:BLS:H102 | 2.09 | 0.53 |
| 1:A:611:C:O2' | 1:A:612:G:H5' | 2.09 | 0.53 |
| 4:E:24:THR:CG2 | 4:E:184:VAL:HG23 | 2.39 | 0.53 |
| 11:L:45:LEU:HD23 | 11:L:46:LYS:N | 2.18 | 0.53 |
| 12:M:54:MET:CE | 12:M:64:ILE:HD12 | 2.38 | 0.53 |
| 14:O:40:ILE:HG22 | 14:O:47:THR:HA | 1.91 | 0.53 |
| 23:X:51:VAL:HG13 | 23:X:58:ILE:CG2 | 2.39 | 0.53 |
| 1:A:1022:G:C6 | 1:A:1140:C:C4 | 2.97 | 0.52 |
| 1:A:195:A:N7 | 1:A:197:A:OP1 | 2.42 | 0.52 |
| 1:A:2130:U:H3' | 1:A:2130:U:P | 2.49 | 0.52 |
| 1:A:1824:G:O3' | 3:D:249:PRO:HD3 | 2.09 | 0.52 |
| 6:G:86:MET:SD | 6:G:87:PRO:HD3 | 2.49 | 0.52 |
| 12:M:10:ARG:HH11 | 12:M:11:LYS:N | 2.07 | 0.52 |
| 12:M:58:PHE:CD1 | 12:M:58:PHE:O | 2.58 | 0.52 |
| 16:Q:92:ARG:HD2 | 16:Q:95:LEU:H | 1.75 | 0.52 |
| 17:R:24:LYS:HA | 17:R:92:THR:HG23 | 1.91 | 0.52 |
| 21:V:10:ARG:HG2 | 21:V:11:GLU:N | 2.24 | 0.52 |
| 21:V:40:ASP:OD1 | 21:V:42:VAL:HG12 | 2.10 | 0.52 |
| 6:G:109:VAL:HG22 | 26:1:59:VAL:HG21 | 1.91 | 0.52 |
| 1:A:1916:A:H2' | 1:A:1917:U:O4' | 2.09 | 0.52 |
| 1:A:322:A:C5 | 1:A:340:A:C2 | 2.96 | 0.52 |
| 2:B:28:C:H2' | 2:B:29:A:C8 | 2.45 | 0.52 |
| 1:A:1843:C:H5' | 3:D:253:GLN:OE1 | 2.09 | 0.52 |
| 5:F:148:LEU:HD11 | 5:F:193:VAL:HG21 | 1.91 | 0.52 |
| 11:L:122:PRO:O | 11:L:123:LEU:HB3 | 2.08 | 0.52 |
| 15:P:106:SER:HA | 15:P:110:ILE:HB | 1.90 | 0.52 |
| 16:Q:25:TRP:C | 16:Q:25:TRP:CD1 | 2.82 | 0.52 |
| 21:V:8:TYR:HB2 | 21:V:38:TYR:CE2 | 2.44 | 0.52 |
| 1:A:850:C:O2' | 25:Z:46:ASN:ND2 | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 26:1:38:ALA:HA | 26:1:55:PRO:HA | 1.92 | 0.52 |
| 1:A:57:C:H2' | 1:A:58:G:O4' | 2.09 | 0.52 |
| 1:A:1971:A:C2 | 3:D:241:PRO:HD3 | 2.44 | 0.52 |
| 16:Q:62:ILE:HD12 | 16:Q:76:TYR:CE1 | 2.44 | 0.52 |
| 1:A:498:G:H1' | 20:U:47:LYS:NZ | 2.24 | 0.52 |
| 21:V:70:LEU:HD12 | 21:V:91:LEU:HD21 | 1.92 | 0.52 |
| 21:V:53:ILE:CD1 | 21:V:99:TYR:HB2 | 2.39 | 0.52 |
| 1:A:572:A:H5'' | 1:A:573:G:OP2 | 2.09 | 0.52 |
| 1:A:973:A:H5' | 1:A:1188:U:H1' | 1.90 | 0.52 |
| 4:E:11:MET:HB2 | 4:E:23:VAL:O | 2.10 | 0.52 |
| 5:F:107:LYS:NZ | 5:F:205:ARG:HG3 | 2.23 | 0.52 |
| 2:B:78:A:O3' | 12:M:21:THR:HG22 | 2.10 | 0.52 |
| 12:M:68:ILE:HD13 | 12:M:68:ILE:H | 1.73 | 0.52 |
| 16:Q:61:TRP:CZ3 | 16:Q:94:ASN:HB2 | 2.44 | 0.52 |
| 1:A:1210:A:C8 | 1:A:1210:A:H5' | 2.33 | 0.52 |
| 1:A:162:U:H2' | 1:A:163:U:C6 | 2.43 | 0.52 |
| 1:A:363(F):U:O2' | 1:A:363(G):A:O4' | 2.27 | 0.52 |
| 31:A:4001:BLS:H102 | 31:A:4001:BLS:N15 | 2.25 | 0.52 |
| 1:A:466:A:N3 | 1:A:683:C:H1' | 2.24 | 0.52 |
| 3:D:58:HIS:O | 3:D:59:LYS:O | 2.28 | 0.52 |
| 4:E:117:MET:HE1 | 4:E:124:GLY:HA3 | 1.91 | 0.52 |
| 5:F:150:GLY:HA2 | 5:F:172:TRP:CD2 | 2.44 | 0.52 |
| 12:M:70:PRO:HA | 12:M:95:ALA:HB2 | 1.90 | 0.52 |
| 20:U:81:LYS:NZ | 20:U:98:VAL:HB | 2.24 | 0.52 |
| 1:A:1544:C:C6 | 1:A:1544:C:OP1 | 2.62 | 0.52 |
| 1:A:2307:G:N7 | 1:A:2308:G:C5 | 2.78 | 0.52 |
| 1:A:273(B):G:C2 | 1:A:364:C:N3 | 2.77 | 0.52 |
| 1:A:2784:C:H1' | 4:E:37:ARG:HH12 | 1.75 | 0.52 |
| 1:A:773:U:C5' | 3:D:47:GLY:HA3 | 2.38 | 0.52 |
| 7:H:13:LYS:HD3 | 7:H:13:LYS:C | 2.30 | 0.52 |
| 8:I:50:ARG:O | 8:I:54:GLN:HB2 | 2.10 | 0.52 |
| 10:K:102:VAL:HB | 10:K:106:LEU:HD12 | 1.92 | 0.52 |
| 11:L:124:LYS:HA | 11:L:143:GLY:O | 2.10 | 0.52 |
| 11:L:23:PRO:O | 11:L:33:ARG:HD2 | 2.10 | 0.52 |
| 13:N:53:HIS:HD2 | 13:N:94:TYR:OH | 1.92 | 0.52 |
| 1:A:498:G:O2' | 20:U:47:LYS:HD3 | 2.09 | 0.52 |
| 21:V:6:LYS:HD2 | 21:V:60:GLU:O | 2.08 | 0.52 |
| 23:X:57:GLU:O | 23:X:58:ILE:HB | 2.09 | 0.52 |
| 26:1:48:ILE:HG22 | 26:1:49:GLU:N | 2.25 | 0.52 |
| 1:A:1024:G:OP2 | 1:A:1025:G:H3' | 2.10 | 0.52 |
| 1:A:2068:U:N3 | 1:A:2430:A:H2 | 2.07 | 0.52 |
| 1:A:2128:C:H2' | 1:A:2129:C:N1 | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:784:A:N7 | 3:D:229:VAL:HG21 | 2.24 | 0.52 |
| 1:A:826:U:H2' | 1:A:828:U:O4' | 2.10 | 0.52 |
| 9:J:66:THR:HG22 | 9:J:68:ASN:HD22 | 1.74 | 0.52 |
| 15:P:92:GLY:HA2 | 15:P:116:ALA:HA | 1.91 | 0.52 |
| 19:T:63:LYS:HD2 | 19:T:72:LYS:HG2 | 1.91 | 0.52 |
| 1:A:1529:A:H62 | 1:A:1542:G:H22 | 1.55 | 0.52 |
| 1:A:747:U:O2 | 1:A:2014:A:H1' | 2.10 | 0.52 |
| 1:A:2134:A:O2' | 1:A:2159:G:H1' | 2.10 | 0.52 |
| 1:A:2392:A:H2 | 1:A:2424:C:N4 | 2.07 | 0.52 |
| 8:I:31:LEU:HB2 | 8:I:32:PRO:HD3 | 1.92 | 0.52 |
| 12:M:80:GLU:OE2 | 12:M:80:GLU:HA | 2.09 | 0.52 |
| 13:N:79:LEU:HD22 | 13:N:83:ILE:HB | 1.92 | 0.52 |
| 26:1:60:GLU:CD | 26:1:60:GLU:H | 2.14 | 0.52 |
| 28:3:18:ARG:HG2 | 28:3:19:ARG:H | 1.74 | 0.52 |
| 1:A:1434:A:H61 | 1:A:1558:A:H62 | 1.57 | 0.52 |
| 1:A:926:A:H2' | 1:A:928:G:H8 | 1.75 | 0.52 |
| 5:F:65:TRP:CZ2 | 5:F:75:HIS:HD2 | 2.27 | 0.52 |
| 9:J:149:PRO:O | 9:J:150:ASP:HB2 | 2.10 | 0.52 |
| 15:P:88:ILE:O | 15:P:88:ILE:HG13 | 2.10 | 0.52 |
| 18:S:72:LYS:HB3 | 18:S:106:ILE:HD12 | 1.92 | 0.52 |
| 21:V:63:ASP:HB3 | 21:V:65:GLN:HG3 | 1.92 | 0.52 |
| 28:3:33:LYS:HB2 | 28:3:34:LEU:HD13 | 1.91 | 0.52 |
| 29:4:19:ARG:NH1 | 29:4:19:ARG:HG3 | 2.08 | 0.52 |
| 30:5:21:LYS:HA | 30:5:54:GLU:OE2 | 2.10 | 0.52 |
| 3:D:70:TRP:CZ2 | 3:D:150:LYS:HA | 2.44 | 0.52 |
| 4:E:10:GLY:O | 4:E:25:VAL:HG23 | 2.09 | 0.52 |
| 1:A:2882:A:H5' | 13:N:96:ARG:HG3 | 1.90 | 0.52 |
| 21:V:29:TYR:HB3 | 21:V:34:ASN:HB2 | 1.91 | 0.52 |
| 24:Y:43:GLN:O | 24:Y:44:LEU:HG | 2.10 | 0.52 |
| 27:2:16:ARG:CG | 27:2:20:ARG:HE | 2.23 | 0.51 |
| 29:4:5:TRP:NE1 | 29:4:7:PRO:HG3 | 2.26 | 0.51 |
| 1:A:405:U:H3' | 1:A:406:G:H5' | 1.92 | 0.51 |
| 1:A:747:U:C4 | 27:2:2:ALA:N | 2.78 | 0.51 |
| 11:L:49:ARG:O | 11:L:50:ARG:HB3 | 2.09 | 0.51 |
| 1:A:2415:G:O3' | 11:L:66:GLY:HA3 | 2.10 | 0.51 |
| 15:P:65:LYS:HE3 | 15:P:67:SER:HB2 | 1.91 | 0.51 |
| 11:L:61:ARG:HD2 | 30:5:13:ARG:HD2 | 1.92 | 0.51 |
| 1:A:1005:C:H2' | 1:A:1006:C:H6 | 1.75 | 0.51 |
| 1:A:2321:G:H5'' | 1:A:2322:A:OP2 | 2.11 | 0.51 |
| 1:A:2330:G:H2' | 1:A:2331:G:O4' | 2.10 | 0.51 |
| 1:A:2427:C:H5'' | 1:A:2428:G:OP1 | 2.10 | 0.51 |
| 1:A:2787:C:H1' | 4:E:62:PRO:HG3 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:426:C:H2' | 1:A:427:U:H6 | 1.75 | 0.51 |
| 1:A:1903:G:OP2 | 3:D:241:PRO:HB2 | 2.10 | 0.51 |
| 8:I:129:THR:HA | 8:I:138:ILE:O | 2.10 | 0.51 |
| 13:N:88:ARG:HH21 | 13:N:88:ARG:HA | 1.75 | 0.51 |
| 16:Q:95:LEU:O | 16:Q:98:LEU:HG | 2.11 | 0.51 |
| 21:V:163:LEU:HD23 | 21:V:163:LEU:H | 1.75 | 0.51 |
| 1:A:1278:A:H2' | 1:A:1279:G:H8 | 1.75 | 0.51 |
| 1:A:2015:A:N3 | 27:2:2:ALA:N | 2.57 | 0.51 |
| 1:A:2163:C:H2' | 1:A:2163:C:O2 | 2.09 | 0.51 |
| 1:A:2311:A:N3 | 6:G:82:LEU:HD11 | 2.25 | 0.51 |
| 1:A:2476:A:H2' | 1:A:2477:C:H5'' | 1.92 | 0.51 |
| 4:E:117:MET:O | 4:E:121:ASN:HA | 2.09 | 0.51 |
| 7:H:40:GLU:C | 7:H:41:MET:HG2 | 2.30 | 0.51 |
| 8:I:31:LEU:HD11 | 8:I:38:LEU:HD22 | 1.92 | 0.51 |
| 10:K:112:MET:O | 10:K:115:VAL:HG22 | 2.10 | 0.51 |
| 11:L:59:LEU:CA | 11:L:61:ARG:NE | 2.69 | 0.51 |
| 21:V:17:ALA:HA | 21:V:20:ARG:HD3 | 1.92 | 0.51 |
| 21:V:19:ARG:HH12 | 21:V:84:GLU:CA | 2.23 | 0.51 |
| 1:A:2285:C:C5 | 28:3:27:LYS:HE3 | 2.46 | 0.51 |
| 1:A:1019:U:O2' | 1:A:1021:A:H2 | 1.92 | 0.51 |
| 1:A:1190:G:H5'' | 11:L:35:HIS:CA | 2.31 | 0.51 |
| 1:A:733:G:C8 | 1:A:761:A:N6 | 2.79 | 0.51 |
| 2:B:66:A:N6 | 2:B:107:U:H2' | 2.26 | 0.51 |
| 4:E:4:ILE:HD13 | 4:E:28:ALA:HB1 | 1.91 | 0.51 |
| 4:E:38:THR:H | 4:E:42:ASP:HB2 | 1.75 | 0.51 |
| 5:F:140:LEU:HD21 | 5:F:170:LEU:HD21 | 1.92 | 0.51 |
| 7:H:136:ILE:HD12 | 7:H:136:ILE:N | 2.25 | 0.51 |
| 8:I:56:LYS:NZ | 8:I:56:LYS:HB3 | 2.24 | 0.51 |
| 8:I:67:ARG:HE | 8:I:67:ARG:HA | 1.75 | 0.51 |
| 18:S:12:ILE:HD13 | 18:S:17:VAL:HG12 | 1.93 | 0.51 |
| 1:A:498:G:H1' | 20:U:47:LYS:HZ2 | 1.74 | 0.51 |
| 23:X:69:LYS:O | 23:X:73:LEU:HB2 | 2.09 | 0.51 |
| 1:A:1858:G:O2' | 1:A:1859:A:H8 | 1.93 | 0.51 |
| 1:A:2892:A:N7 | 1:A:2893:G:C4 | 2.79 | 0.51 |
| 5:F:129:PHE:O | 5:F:132:VAL:HG13 | 2.11 | 0.51 |
| 13:N:115:GLU:HG2 | 13:N:116:LEU:N | 2.24 | 0.51 |
| 14:O:33:LYS:O | 14:O:54:LEU:HG | 2.10 | 0.51 |
| 18:S:29:LEU:HD22 | 18:S:69:LEU:HD11 | 1.91 | 0.51 |
| 23:X:73:LEU:HD21 | 23:X:94:LEU:O | 2.11 | 0.51 |
| 24:Y:24:LEU:HD13 | 24:Y:60:LEU:HD21 | 1.92 | 0.51 |
| 29:4:8:ASN:HD21 | 29:4:10:ARG:HB3 | 1.74 | 0.51 |
| 1:A:1153:C:O2' | 1:A:1154:G:H5' | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:274:G:H4' | 1:A:275:G:OP2 | 2.10 | 0.51 |
| 1:A:807:U:OP2 | 11:L:39:LYS:HG2 | 2.11 | 0.51 |
| 3:D:145:VAL:HB | 3:D:155:LEU:HB2 | 1.92 | 0.51 |
| 6:G:163:ALA:HB3 | 6:G:169:ALA:HB2 | 1.92 | 0.51 |
| 11:L:61:ARG:HA | 11:L:62:LEU:HD13 | 1.92 | 0.51 |
| 12:M:109:VAL:HB | 12:M:113:GLN:HB2 | 1.93 | 0.51 |
| 12:M:78:PRO:O | 12:M:79:LEU:HB2 | 2.11 | 0.51 |
| 14:O:57:LYS:HD2 | 14:O:58:LEU:N | 2.24 | 0.51 |
| 25:Z:26:LEU:HB2 | 25:Z:28:LEU:HD13 | 1.92 | 0.51 |
| 1:A:1174:A:C3' | 1:A:1175:U:H5'' | 2.34 | 0.51 |
| 1:A:1578:U:C2' | 1:A:1579:A:H5' | 2.41 | 0.51 |
| 1:A:2472:G:H3' | 1:A:2473:U:H5'' | 1.92 | 0.51 |
| 1:A:947:G:H2' | 1:A:948:G:C8 | 2.46 | 0.51 |
| 3:D:174:ILE:N | 3:D:174:ILE:HD12 | 2.26 | 0.51 |
| 1:A:1844:C:O3' | 3:D:258:LYS:HE2 | 2.11 | 0.51 |
| 4:E:57:LYS:CG | 4:E:58:ARG:H | 2.18 | 0.51 |
| 8:I:4:ILE:HG12 | 8:I:4:ILE:O | 2.10 | 0.51 |
| 20:U:17:SER:OG | 20:U:18:GLY:N | 2.43 | 0.51 |
| 30:5:51:ALA:H | 30:5:54:GLU:HB2 | 1.75 | 0.51 |
| 1:A:118:A:H1' | 1:A:178:G:O4' | 2.11 | 0.51 |
| 1:A:1336:A:H2' | 1:A:1337:G:H8 | 1.75 | 0.51 |
| 1:A:1996:C:H4' | 1:A:1997:G:OP1 | 2.10 | 0.51 |
| 1:A:1998:G:H2' | 1:A:1999:C:H6 | 1.76 | 0.51 |
| 1:A:277:A:C6 | 1:A:278:A:H1' | 2.46 | 0.51 |
| 1:A:580:C:H2' | 1:A:581:C:C6 | 2.46 | 0.51 |
| 2:B:11:C:OP2 | 2:B:12:C:H5 | 1.94 | 0.51 |
| 5:F:205:ARG:HG2 | 5:F:206:ILE:HG23 | 1.93 | 0.51 |
| 14:O:25:ARG:HG2 | 14:O:88:ASP:HB2 | 1.92 | 0.51 |
| 23:X:30:VAL:HG12 | 23:X:30:VAL:O | 2.11 | 0.51 |
| 11:L:62:LEU:HD11 | 30:5:27:THR:HA | 1.92 | 0.51 |
| 1:A:1766:U:H2' | 1:A:1767:C:C6 | 2.46 | 0.51 |
| 1:A:676:A:H2 | 1:A:802:A:H61 | 1.55 | 0.51 |
| 3:D:125:ILE:O | 3:D:125:ILE:HG22 | 2.10 | 0.51 |
| 4:E:33:VAL:HG23 | 4:E:47:VAL:HG13 | 1.93 | 0.51 |
| 4:E:6:GLY:HA2 | 4:E:51:PHE:CZ | 2.46 | 0.51 |
| 13:N:10:LEU:HD22 | 13:N:17:ARG:CZ | 2.41 | 0.51 |
| 13:N:12:ARG:HH11 | 13:N:12:ARG:HG3 | 1.75 | 0.51 |
| 17:R:4:ILE:HB | 17:R:39:LEU:O | 2.10 | 0.51 |
| 1:A:1665:A:H1' | 10:K:1:MET:HG2 | 1.92 | 0.51 |
| 1:A:2712:U:H1' | 1:A:712(B):A:H8 | 1.74 | 0.51 |
| 1:A:483:A:H4' | 20:U:49:VAL:HG22 | 1.93 | 0.51 |
| 1:A:616:A:H4' | 1:A:617:G:OP1 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:D:159:ALA:HB1 | 3:D:198:ASN:O | 2.11 | 0.51 |
| 8:I:75:LEU:HD11 | 8:I:105:HIS:NE2 | 2.26 | 0.51 |
| 11:L:128:HIS:HA | 11:L:147:LEU:CB | 2.30 | 0.51 |
| 19:T:11:PRO:HB3 | 19:T:92:LEU:HD21 | 1.91 | 0.51 |
| 30:5:61:LEU:O | 30:5:62:LEU:HB2 | 2.10 | 0.50 |
| 1:A:1590:U:H2' | 1:A:1591:G:C8 | 2.46 | 0.50 |
| 1:A:2074:U:H2' | 1:A:2075:U:C6 | 2.46 | 0.50 |
| 1:A:2307:G:N7 | 1:A:2308:G:C6 | 2.79 | 0.50 |
| 1:A:273(B):G:C2 | 1:A:364:C:C2 | 2.99 | 0.50 |
| 1:A:588:U:H2' | 1:A:589:C:C6 | 2.45 | 0.50 |
| 6:G:111:LEU:HB3 | 6:G:117:PHE:HE2 | 1.75 | 0.50 |
| 11:L:30:THR:O | 11:L:32:THR:N | 2.44 | 0.50 |
| 20:U:83:THR:HG22 | 20:U:84:ARG:N | 2.27 | 0.50 |
| 1:A:1019:U:HO2' | 1:A:1021:A:H2 | 1.57 | 0.50 |
| 1:A:1139:G:O2' | 1:A:1143:A:N1 | 2.41 | 0.50 |
| 1:A:2542:A:N3 | 1:A:2542:A:H5'' | 2.25 | 0.50 |
| 1:A:270(T):G:H2' | 1:A:270(U):G:C8 | 2.43 | 0.50 |
| 1:A:322:A:H3' | 5:F:169:ASN:HD21 | 1.76 | 0.50 |
| 4:E:192:ASN:HD22 | 4:E:192:ASN:H | 1.59 | 0.50 |
| 7:H:169:VAL:HG13 | 7:H:170:ARG:H | 1.76 | 0.50 |
| 8:I:61:ARG:HH12 | 8:I:133:HIS:HB2 | 1.75 | 0.50 |
| 9:J:37:VAL:HG12 | 9:J:38:LEU:N | 2.27 | 0.50 |
| 11:L:6:LEU:HG | 11:L:8:PRO:HD2 | 1.91 | 0.50 |
| 14:O:93:LYS:HD3 | 14:O:95:HIS:HB2 | 1.93 | 0.50 |
| 17:R:66:ARG:HD2 | 17:R:88:ARG:NH1 | 2.27 | 0.50 |
| 20:U:29:GLU:HB3 | 20:U:38:ILE:HB | 1.92 | 0.50 |
| 26:1:40:ILE:HD12 | 26:1:40:ILE:N | 2.26 | 0.50 |
| 1:A:2017:U:O2 | 27:2:10:LYS:HB2 | 2.11 | 0.50 |
| 1:A:1427:A:H4' | 1:A:1428:C:O5' | 2.12 | 0.50 |
| 1:A:1509:A:O3' | 1:A:1510:A:O4' | 2.29 | 0.50 |
| 1:A:1658:C:OP1 | 4:E:132:HIS:O | 2.28 | 0.50 |
| 1:A:994:C:OP1 | 16:Q:53:ARG:NH2 | 2.43 | 0.50 |
| 9:J:35:ARG:O | 9:J:73:ASP:HB3 | 2.12 | 0.50 |
| 11:L:50:ARG:HG2 | 11:L:51:PHE:HB2 | 1.93 | 0.50 |
| 11:L:58:THR:C | 11:L:61:ARG:HE | 2.13 | 0.50 |
| 9:J:63:PRO:O | 16:Q:64:ARG:HD2 | 2.11 | 0.50 |
| 17:R:35:LEU:C | 17:R:37:VAL:N | 2.63 | 0.50 |
| 1:A:1615:C:O2' | 1:A:1616:A:H5' | 2.11 | 0.50 |
| 1:A:559:G:H22 | 16:Q:49:HIS:CD2 | 2.29 | 0.50 |
| 1:A:611:C:C2' | 1:A:612:G:H5' | 2.41 | 0.50 |
| 1:A:778:G:C6 | 1:A:779:U:N3 | 2.80 | 0.50 |
| 10:K:71:ARG:NH2 | 10:K:77:ILE:HG21 | 2.23 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 11:L:85:LEU:HD23 | 11:L:88:LEU:HD23 | 1.93 | 0.50 |
| 18:S:36:LEU:HD12 | 18:S:36:LEU:N | 2.25 | 0.50 |
| 23:X:27:GLU:HG2 | 23:X:28:GLY:N | 2.26 | 0.50 |
| 1:A:195:A:H5'' | 1:A:196:A:OP2 | 2.11 | 0.50 |
| 1:A:2056:G:H22 | 27:2:4:HIS:C | 2.15 | 0.50 |
| 3:D:264:LYS:HG2 | 3:D:266:SER:HB3 | 1.94 | 0.50 |
| 3:D:63:ARG:HD3 | 3:D:63:ARG:N | 2.27 | 0.50 |
| 11:L:62:LEU:HD13 | 11:L:62:LEU:N | 2.27 | 0.50 |
| 15:P:28:VAL:HA | 15:P:89:VAL:HG12 | 1.94 | 0.50 |
| 16:Q:85:LYS:HD3 | 16:Q:85:LYS:C | 2.31 | 0.50 |
| 17:R:71:LEU:HD12 | 17:R:71:LEU:N | 2.26 | 0.50 |
| 21:V:125:LEU:HD22 | 21:V:126:VAL:N | 2.27 | 0.50 |
| 22:W:56:ASP:O | 22:W:57:PHE:CB | 2.60 | 0.50 |
| 1:A:270(S):G:H1' | 23:X:79:GLY:HA3 | 1.94 | 0.50 |
| 24:Y:14:ARG:HG2 | 24:Y:17:SER:HB2 | 1.91 | 0.50 |
| 1:A:1184:G:OP1 | 25:Z:29:ARG:HD3 | 2.11 | 0.50 |
| 1:A:1252:G:C2 | 1:A:1253:A:C2 | 3.00 | 0.50 |
| 1:A:1373:A:H2' | 1:A:1374:G:O4' | 2.10 | 0.50 |
| 1:A:1587:A:H2' | 1:A:1588:C:H6 | 1.75 | 0.50 |
| 1:A:1641:A:H2' | 1:A:1642:G:O4' | 2.11 | 0.50 |
| 1:A:1657:C:H2' | 1:A:1658:C:C6 | 2.47 | 0.50 |
| 1:A:2428:G:H5'' | 1:A:2429:G:O5' | 2.11 | 0.50 |
| 1:A:2695:C:H2' | 1:A:2696:U:C6 | 2.46 | 0.50 |
| 1:A:2712:U:O2' | 1:A:712(B):A:OP2 | 2.28 | 0.50 |
| 5:F:183:VAL:O | 5:F:187:VAL:HG23 | 2.12 | 0.50 |
| 11:L:23:PRO:HA | 11:L:29:LYS:HB2 | 1.93 | 0.50 |
| 13:N:55:ALA:HA | 13:N:80:PHE:CE1 | 2.47 | 0.50 |
| 16:Q:33:ARG:O | 16:Q:37:GLU:HG3 | 2.12 | 0.50 |
| 16:Q:95:LEU:HD12 | 17:R:11:GLN:HE21 | 1.75 | 0.50 |
| 17:R:39:LEU:HA | 17:R:47:VAL:HG11 | 1.94 | 0.50 |
| 18:S:29:LEU:HG | 18:S:33:ARG:HE | 1.76 | 0.50 |
| 24:Y:34:GLU:O | 24:Y:38:GLN:HG2 | 2.11 | 0.50 |
| 24:Y:51:ARG:O | 24:Y:55:ARG:HG2 | 2.12 | 0.50 |
| 26:1:46:ASN:HD22 | 26:1:47:VAL:N | 2.09 | 0.50 |
| 1:A:1108:U:H2' | 1:A:1109:C:C5 | 2.47 | 0.50 |
| 1:A:1496:A:C8 | 1:A:1577:C:O2' | 2.65 | 0.50 |
| 1:A:528:A:C2 | 1:A:2043:C:C5' | 2.94 | 0.50 |
| 1:A:280:C:C2 | 1:A:361:G:N2 | 2.80 | 0.50 |
| 1:A:631:A:H2' | 1:A:632:A:O4' | 2.11 | 0.50 |
| 2:B:28:C:H2' | 2:B:29:A:O4' | 2.11 | 0.50 |
| 2:B:51:G:H21 | 2:B:52:A:H62 | 1.58 | 0.50 |
| 3:D:145:VAL:HG12 | 3:D:146:GLU:O | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 5:F:47:GLY:HA3 | 5:F:95:ARG:H | 1.76 | 0.50 |
| 7:H:67:LEU:HG | 7:H:71:LEU:CD2 | 2.42 | 0.50 |
| 9:J:114:LEU:HA | 9:J:118:PRO:HB3 | 1.94 | 0.50 |
| 11:L:114:ILE:HD13 | 11:L:130:PHE:CE1 | 2.47 | 0.50 |
| 1:A:1049:C:C5 | 1:A:1050:A:N7 | 2.79 | 0.50 |
| 1:A:1496:A:O2' | 1:A:1497:U:H5'' | 2.12 | 0.50 |
| 1:A:1952:A:C6 | 1:A:1953:A:N1 | 2.79 | 0.50 |
| 1:A:2773:C:H2' | 1:A:2774:C:H6 | 1.77 | 0.50 |
| 1:A:943:U:OP2 | 11:L:38:GLN:CD | 2.51 | 0.50 |
| 2:B:38:C:O2 | 2:B:48:A:H1' | 2.12 | 0.50 |
| 3:D:154:LYS:C | 3:D:155:LEU:HD12 | 2.33 | 0.50 |
| 3:D:172:TYR:HB3 | 3:D:184:LYS:HB3 | 1.92 | 0.50 |
| 13:N:98:LEU:HB2 | 13:N:113:LEU:HD21 | 1.94 | 0.50 |
| 1:A:106:C:H2' | 1:A:107:C:H6 | 1.77 | 0.50 |
| 1:A:1388:G:H4' | 1:A:1525:G:O2' | 2.11 | 0.50 |
| 1:A:2823:A:OP1 | 4:E:113:PHE:HB2 | 2.11 | 0.50 |
| 5:F:107:LYS:HZ2 | 5:F:205:ARG:CG | 2.20 | 0.50 |
| 5:F:184:TYR:O | 5:F:188:ARG:HG3 | 2.12 | 0.50 |
| 5:F:206:ILE:HG12 | 5:F:206:ILE:O | 2.10 | 0.50 |
| 1:A:2312:U:H4' | 6:G:71:THR:HG21 | 1.93 | 0.50 |
| 9:J:161:LEU:N | 9:J:161:LEU:HD23 | 2.26 | 0.50 |
| 11:L:38:GLN:O | 11:L:39:LYS:HB2 | 2.12 | 0.50 |
| 13:N:38:VAL:HB | 13:N:39:PRO:HD3 | 1.94 | 0.50 |
| 19:T:89:ILE:O | 19:T:93:GLU:HG2 | 2.12 | 0.50 |
| 21:V:22:GLY:O | 21:V:41:LEU:HB2 | 2.12 | 0.50 |
| 1:A:1019:U:H2' | 1:A:1021:A:C2 | 2.45 | 0.49 |
| 1:A:1023:U:H2' | 1:A:1024:G:H5' | 1.93 | 0.49 |
| 1:A:1050:A:C2 | 1:A:2751:G:C4 | 3.00 | 0.49 |
| 1:A:1568:G:H5' | 3:D:60:ARG:HA | 1.94 | 0.49 |
| 1:A:2557:G:H2' | 1:A:2558:C:C6 | 2.47 | 0.49 |
| 1:A:244:A:C2 | 1:A:255:A:C4 | 3.00 | 0.49 |
| 1:A:2853:C:H2' | 1:A:2854:G:H8 | 1.77 | 0.49 |
| 1:A:30:G:H2' | 1:A:31:C:O4' | 2.12 | 0.49 |
| 1:A:713:G:H2' | 1:A:714:U:C6 | 2.47 | 0.49 |
| 6:G:131:TYR:HB3 | 6:G:159:VAL:HG13 | 1.94 | 0.49 |
| 7:H:94:TYR:CD1 | 7:H:94:TYR:N | 2.80 | 0.49 |
| 11:L:14:LYS:O | 11:L:15:ARG:HB2 | 2.11 | 0.49 |
| 12:M:81:VAL:O | 12:M:82:ARG:HG2 | 2.12 | 0.49 |
| 18:S:4:LYS:HG2 | 18:S:5:ALA:N | 2.27 | 0.49 |
| 27:2:47:PRO:O | 27:2:48:GLU:HB3 | 2.12 | 0.49 |
| 1:A:1045:A:O2' | 1:A:1047:G:C6 | 2.65 | 0.49 |
| 1:A:1495:A:N3 | 1:A:1496:A:C2 | 2.81 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:307:G:H21 | 1:A:330:A:H62 | 1.60 | 0.49 |
| 1:A:813:U:H2' | 1:A:814:C:C6 | 2.47 | 0.49 |
| 7:H:98:LEU:HD12 | 7:H:99:VAL:H | 1.77 | 0.49 |
| 12:M:87:LYS:O | 12:M:89:ASN:OD1 | 2.30 | 0.49 |
| 13:N:13:HIS:CE1 | 13:N:15:SER:HB2 | 2.47 | 0.49 |
| 1:A:17:G:H4' | 16:Q:25:TRP:CZ3 | 2.47 | 0.49 |
| 19:T:70:LEU:HD13 | 19:T:71:GLY:N | 2.28 | 0.49 |
| 20:U:13:VAL:HG23 | 20:U:73:ARG:C | 2.32 | 0.49 |
| 23:X:21:ARG:HB2 | 23:X:38:SER:O | 2.12 | 0.49 |
| 1:A:1512:G:H2' | 1:A:1513:C:O4' | 2.11 | 0.49 |
| 1:A:1559:G:N3 | 1:A:1559:G:H5' | 2.28 | 0.49 |
| 1:A:2115:G:H2' | 1:A:2116:G:N7 | 2.28 | 0.49 |
| 1:A:2562:U:H2' | 1:A:2563:U:H5' | 1.95 | 0.49 |
| 1:A:2630:G:H2' | 1:A:2631:G:H8 | 1.76 | 0.49 |
| 3:D:134:ARG:HG3 | 3:D:135:PHE:CD1 | 2.47 | 0.49 |
| 3:D:269:PHE:CD1 | 3:D:269:PHE:N | 2.81 | 0.49 |
| 1:A:1570:A:H4' | 3:D:38:LYS:NZ | 2.27 | 0.49 |
| 4:E:137:HIS:HB3 | 4:E:138:PRO:HD2 | 1.94 | 0.49 |
| 5:F:34:TRP:CE2 | 11:L:12:ALA:HB2 | 2.48 | 0.49 |
| 10:K:97:ARG:N | 10:K:117:LEU:HD23 | 2.15 | 0.49 |
| 10:K:8:LEU:N | 10:K:8:LEU:HD23 | 2.27 | 0.49 |
| 11:L:41:ARG:HH22 | 11:L:45:LEU:HD12 | 1.76 | 0.49 |
| 14:O:56:LEU:HD23 | 14:O:57:LYS:HZ1 | 1.77 | 0.49 |
| 18:S:9:TYR:H | 18:S:102:HIS:CD2 | 2.27 | 0.49 |
| 19:T:63:LYS:HZ2 | 19:T:72:LYS:HB3 | 1.75 | 0.49 |
| 22:W:27:GLU:HG3 | 22:W:68:GLU:HA | 1.94 | 0.49 |
| 1:A:593:G:O2' | 30:5:62:LEU:HD13 | 2.12 | 0.49 |
| 1:A:2211:G:C2' | 1:A:2212:A:H5'' | 2.42 | 0.49 |
| 1:A:885:C:H2' | 1:A:886:C:H5'' | 1.94 | 0.49 |
| 1:A:894:C:O2' | 1:A:895:U:H5' | 2.12 | 0.49 |
| 2:B:78:A:C2 | 2:B:99:A:C4 | 3.00 | 0.49 |
| 4:E:132:HIS:O | 4:E:135:HIS:CD2 | 2.65 | 0.49 |
| 6:G:2:PRO:C | 6:G:3:LEU:HD12 | 2.33 | 0.49 |
| 13:N:94:TYR:C | 13:N:117:VAL:HG12 | 2.33 | 0.49 |
| 21:V:48:PHE:CE2 | 21:V:71:VAL:HG11 | 2.47 | 0.49 |
| 1:A:1349:A:N6 | 1:A:1598:C:N4 | 2.61 | 0.49 |
| 1:A:1899:G:H21 | 1:A:1902:C:N4 | 1.96 | 0.49 |
| 1:A:193:U:H2' | 1:A:194:G:H8 | 1.78 | 0.49 |
| 1:A:2393:A:C5' | 11:L:62:LEU:HB3 | 2.43 | 0.49 |
| 1:A:443:A:N7 | 5:F:45:ARG:HD2 | 2.27 | 0.49 |
| 1:A:892:G:H2' | 1:A:893:C:C5 | 2.47 | 0.49 |
| 4:E:23:VAL:HA | 4:E:184:VAL:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1438:U:O2' | 1:A:1439:A:H5' | 2.13 | 0.49 |
| 1:A:1459:G:H5'' | 1:A:1460:A:P | 2.52 | 0.49 |
| 1:A:192:C:H2' | 1:A:193:U:H5' | 1.95 | 0.49 |
| 1:A:2119:A:H61 | 1:A:2170:A:N6 | 2.07 | 0.49 |
| 1:A:1790:C:O2' | 3:D:209:ALA:HB2 | 2.12 | 0.49 |
| 4:E:132:HIS:CD2 | 4:E:135:HIS:CE1 | 3.00 | 0.49 |
| 12:M:20:ALA:HA | 12:M:98:LYS:HB3 | 1.94 | 0.49 |
| 13:N:57:ARG:HD3 | 13:N:59:ASP:CG | 2.33 | 0.49 |
| 25:Z:40:THR:HG23 | 25:Z:43:ILE:CG1 | 2.42 | 0.49 |
| 1:A:1485:G:H2' | 1:A:1486:A:H8 | 1.76 | 0.49 |
| 1:A:1932:A:H2' | 1:A:1933:G:O4' | 2.13 | 0.49 |
| 1:A:2117:A:N6 | 1:A:2172:U:C2 | 2.81 | 0.49 |
| 1:A:2605:U:H2' | 1:A:2606:C:C6 | 2.47 | 0.49 |
| 1:A:49:A:H4' | 1:A:50:U:H5'' | 1.93 | 0.49 |
| 1:A:844:C:C2' | 1:A:845:G:H5' | 2.43 | 0.49 |
| 4:E:31:CYS:HB3 | 4:E:49:LEU:HD12 | 1.93 | 0.49 |
| 4:E:93:VAL:HG11 | 4:E:181:LEU:O | 2.13 | 0.49 |
| 5:F:167:ALA:HB1 | 5:F:173:VAL:HG11 | 1.94 | 0.49 |
| 1:A:451:C:H4' | 5:F:52:LYS:HZ2 | 1.77 | 0.49 |
| 1:A:1009:A:H4' | 16:Q:59:ARG:HG3 | 1.95 | 0.49 |
| 18:S:28:SER:OG | 18:S:31:GLU:HG2 | 2.13 | 0.49 |
| 20:U:81:LYS:HD3 | 20:U:97:ARG:CB | 2.34 | 0.49 |
| 23:X:12:PRO:O | 23:X:14:VAL:HG23 | 2.13 | 0.49 |
| 1:A:1488:G:C5 | 1:A:1489:U:C5 | 3.00 | 0.49 |
| 1:A:1963:U:O2 | 1:A:1963:U:H2' | 2.12 | 0.49 |
| 1:A:580:C:H2' | 1:A:581:C:H6 | 1.77 | 0.49 |
| 2:B:29:A:C2 | 2:B:56:G:C2 | 3.01 | 0.49 |
| 2:B:81:G:O6 | 2:B:95:U:O2 | 2.31 | 0.49 |
| 5:F:181:LEU:CD2 | 5:F:186:ILE:HD11 | 2.42 | 0.49 |
| 6:G:97:ASP:HA | 6:G:100:TRP:HD1 | 1.77 | 0.49 |
| 19:T:30:VAL:HG11 | 19:T:39:ILE:HD11 | 1.93 | 0.49 |
| 24:Y:47:ASN:O | 24:Y:49:LYS:N | 2.45 | 0.49 |
| 26:1:39:ARG:NH2 | 26:1:47:VAL:HG12 | 2.28 | 0.49 |
| 28:3:11:LEU:HD13 | 28:3:12:GLU:N | 2.28 | 0.49 |
| 1:A:2190:G:H2' | 1:A:2191:G:H8 | 1.78 | 0.49 |
| 1:A:2473:U:H2' | 1:A:2474:C:H6 | 1.77 | 0.49 |
| 1:A:1786:A:C2 | 1:A:2606:C:H1' | 2.48 | 0.49 |
| 1:A:2652:C:H2' | 1:A:2653:U:O4' | 2.13 | 0.49 |
| 1:A:2688:U:H1' | 1:A:2721:A:N6 | 2.28 | 0.49 |
| 1:A:932:G:H4' | 1:A:933:A:O5' | 2.12 | 0.49 |
| 5:F:184:TYR:CE2 | 5:F:188:ARG:HD2 | 2.48 | 0.49 |
| 8:I:127:VAL:HG12 | 8:I:141:LYS:HG3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 11:L:23:PRO:HB2 | 11:L:33:ARG:CD | 2.43 | 0.49 |
| 1:A:411:G:C2 | 11:L:71:VAL:HG11 | 2.48 | 0.49 |
| 11:L:95:VAL:HG22 | 11:L:125:VAL:HB | 1.94 | 0.49 |
| 12:M:127:ILE:HG22 | 12:M:128:LYS:O | 2.13 | 0.49 |
| 14:O:89:ARG:HD3 | 14:O:94:TYR:HB2 | 1.95 | 0.49 |
| 19:T:55:ASN:HB2 | 19:T:80:ILE:CG1 | 2.41 | 0.49 |
| 24:Y:37:PHE:O | 24:Y:41:ILE:HG23 | 2.12 | 0.49 |
| 27:2:25:LEU:HD12 | 27:2:25:LEU:N | 2.26 | 0.49 |
| 1:A:1045:A:H5' | 1:A:1047:G:C5' | 2.42 | 0.49 |
| 9:J:61:HIS:CD2 | 9:J:62:ARG:HG3 | 2.47 | 0.49 |
| 12:M:134:ARG:NH2 | 12:M:137:TYR:O | 2.46 | 0.49 |
| 12:M:83:MET:HG2 | 12:M:84:GLY:N | 2.28 | 0.49 |
| 13:N:11:ASN:CG | 13:N:12:ARG:H | 2.14 | 0.49 |
| 15:P:62:THR:HG22 | 15:P:75:ILE:HG13 | 1.94 | 0.49 |
| 17:R:22:VAL:CG1 | 17:R:23:GLU:N | 2.75 | 0.49 |
| 18:S:23:LEU:HD13 | 27:2:25:LEU:HD13 | 1.94 | 0.49 |
| 20:U:50:ARG:HG3 | 20:U:52:SER:O | 2.13 | 0.49 |
| 28:3:15:GLU:OE2 | 28:3:18:ARG:CZ | 2.61 | 0.48 |
| 30:5:22:VAL:CB | 30:5:54:GLU:HG3 | 2.30 | 0.48 |
| 1:A:1164:G:H2' | 1:A:1165:U:C6 | 2.48 | 0.48 |
| 1:A:973:A:O4' | 1:A:1188:U:C6 | 2.65 | 0.48 |
| 1:A:1385:G:H4' | 1:A:1386:C:OP1 | 2.11 | 0.48 |
| 1:A:1946:U:H2' | 1:A:1947:C:C6 | 2.48 | 0.48 |
| 1:A:444:C:H4' | 5:F:49:ALA:HB2 | 1.94 | 0.48 |
| 1:A:483:A:O3' | 20:U:49:VAL:HG22 | 2.13 | 0.48 |
| 3:D:168:ARG:N | 3:D:168:ARG:HD2 | 2.28 | 0.48 |
| 9:J:119:GLU:HB2 | 9:J:145:VAL:HG12 | 1.94 | 0.48 |
| 10:K:87:ILE:HG22 | 10:K:93:PRO:HA | 1.95 | 0.48 |
| 17:R:35:LEU:HB2 | 17:R:57:VAL:CG1 | 2.41 | 0.48 |
| 19:T:62:LYS:O | 19:T:63:LYS:HD3 | 2.13 | 0.48 |
| 1:A:1203:G:C6 | 1:A:1204:A:N6 | 2.81 | 0.48 |
| 1:A:1205:U:H4' | 1:A:1206:G:OP2 | 2.14 | 0.48 |
| 1:A:2176:A:H2' | 1:A:2177:C:C6 | 2.49 | 0.48 |
| 1:A:2892:A:H2' | 1:A:2893:G:O4' | 2.13 | 0.48 |
| 4:E:130:GLY:O | 4:E:131:ALA:HB3 | 2.13 | 0.48 |
| 4:E:154:LYS:O | 4:E:156:MET:HG3 | 2.14 | 0.48 |
| 11:L:38:GLN:CG | 11:L:39:LYS:H | 2.15 | 0.48 |
| 19:T:43:VAL:HG11 | 19:T:81:VAL:HG11 | 1.95 | 0.48 |
| 25:Z:7:LYS:O | 25:Z:9:VAL:HG23 | 2.13 | 0.48 |
| 1:A:1028:A:N6 | 1:A:1125:G:H2' | 2.28 | 0.48 |
| 1:A:1499:C:H2' | 1:A:1500:G:O4' | 2.13 | 0.48 |
| 1:A:1790:C:H4' | 3:D:209:ALA:CB | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:17:G:H2' | 1:A:18:C:C6 | 2.48 | 0.48 |
| 1:A:2250:G:H5'' | 1:A:2250:G:N3 | 2.27 | 0.48 |
| 1:A:228:A:H3' | 1:A:229:A:C5' | 2.43 | 0.48 |
| 1:A:1782:C:H1' | 1:A:2609:U:H5'' | 1.96 | 0.48 |
| 1:A:2647:U:H2' | 1:A:2648:C:C6 | 2.48 | 0.48 |
| 1:A:2691:C:C4 | 1:A:2719:G:N2 | 2.81 | 0.48 |
| 1:A:301:G:H4' | 1:A:301:G:OP1 | 2.13 | 0.48 |
| 1:A:1190:G:O3' | 11:L:35:HIS:HB3 | 2.12 | 0.48 |
| 11:L:55:ARG:HG3 | 11:L:56:SER:N | 2.28 | 0.48 |
| 1:A:2822:G:O6 | 13:N:4:LEU:HD12 | 2.14 | 0.48 |
| 14:O:90:GLY:O | 14:O:92:TYR:N | 2.47 | 0.48 |
| 17:R:35:LEU:O | 17:R:37:VAL:N | 2.46 | 0.48 |
| 1:A:2593:U:H2' | 1:A:2594:C:H6 | 1.75 | 0.48 |
| 1:A:2866:U:C6 | 1:A:2868:A:H1' | 2.49 | 0.48 |
| 1:A:833:U:H2' | 1:A:834:C:C6 | 2.48 | 0.48 |
| 1:A:952:G:C6 | 1:A:953:A:N7 | 2.81 | 0.48 |
| 11:L:39:LYS:NZ | 11:L:42:SER:OG | 2.46 | 0.48 |
| 12:M:20:ALA:HB2 | 12:M:99:PRO:HD2 | 1.96 | 0.48 |
| 13:N:53:HIS:HA | 13:N:56:LYS:HB2 | 1.96 | 0.48 |
| 24:Y:50:ILE:HD12 | 24:Y:51:ARG:H | 1.74 | 0.48 |
| 25:Z:29:ARG:HG3 | 25:Z:30:ARG:H | 1.77 | 0.48 |
| 1:A:1110:G:OP1 | 1:A:1110:G:H4' | 2.13 | 0.48 |
| 1:A:1468:C:H2' | 1:A:1469:A:C8 | 2.48 | 0.48 |
| 1:A:1532:C:C2 | 1:A:1540:G:N2 | 2.82 | 0.48 |
| 1:A:1568:G:O5' | 3:D:61:LEU:HD22 | 2.14 | 0.48 |
| 1:A:2037:G:C6 | 1:A:2038:G:C6 | 3.01 | 0.48 |
| 2:B:89(A):G:C6 | 2:B:89(B):A:N6 | 2.82 | 0.48 |
| 3:D:264:LYS:HG2 | 3:D:266:SER:H | 1.78 | 0.48 |
| 1:A:2050:C:H1' | 4:E:156:MET:CE | 2.44 | 0.48 |
| 5:F:101:LEU:O | 5:F:106:ARG:NH1 | 2.46 | 0.48 |
| 1:A:2312:U:H4' | 6:G:71:THR:CG2 | 2.43 | 0.48 |
| 7:H:92:ILE:HD12 | 7:H:92:ILE:N | 2.29 | 0.48 |
| 1:A:2414:G:H21 | 11:L:67:MET:HE1 | 1.78 | 0.48 |
| 16:Q:92:ARG:HG2 | 17:R:11:GLN:NE2 | 2.28 | 0.48 |
| 17:R:20:LEU:HG | 17:R:22:VAL:HG23 | 1.94 | 0.48 |
| 19:T:88:LYS:HZ3 | 19:T:90:GLU:HG2 | 1.78 | 0.48 |
| 20:U:4:LYS:H | 20:U:4:LYS:HD3 | 1.78 | 0.48 |
| 21:V:10:ARG:HH21 | 21:V:26:GLY:N | 2.11 | 0.48 |
| 23:X:58:ILE:HD12 | 23:X:90:ILE:HG22 | 1.95 | 0.48 |
| 1:A:101:G:O2' | 1:A:102:G:P | 2.71 | 0.48 |
| 1:A:1022:G:N2 | 1:A:1142(B):A:C2 | 2.77 | 0.48 |
| 1:A:1187:G:H8 | 1:A:1187:G:O5' | 1.97 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1417:C:H42 | 1:A:1581:G:H1 | 1.61 | 0.48 |
| 4:E:128:SER:O | 4:E:129:HIS:HB2 | 2.13 | 0.48 |
| 5:F:101:LEU:HB3 | 5:F:106:ARG:HD3 | 1.95 | 0.48 |
| 8:I:61:ARG:O | 8:I:61:ARG:HD2 | 2.14 | 0.48 |
| 11:L:101:VAL:HG13 | 11:L:102:ARG:N | 2.28 | 0.48 |
| 1:A:1434:A:H61 | 1:A:1558:A:N6 | 2.11 | 0.48 |
| 1:A:1754:C:OP1 | 15:P:96:ARG:NH1 | 2.41 | 0.48 |
| 3:D:220:HIS:HD2 | 3:D:221:VAL:N | 2.11 | 0.48 |
| 6:G:133:LEU:HD21 | 6:G:157:ILE:HB | 1.94 | 0.48 |
| 9:J:151:HIS:HB2 | 9:J:152:PRO:HD2 | 1.96 | 0.48 |
| 12:M:10:ARG:NH1 | 12:M:10:ARG:HA | 2.28 | 0.48 |
| 14:O:49:VAL:HG21 | 14:O:77:ALA:HA | 1.96 | 0.48 |
| 9:J:27:TYR:CD2 | 16:Q:100:VAL:HG11 | 2.48 | 0.48 |
| 23:X:13:ILE:CD1 | 23:X:14:VAL:N | 2.77 | 0.48 |
| 25:Z:4:LEU:O | 25:Z:36:VAL:HA | 2.12 | 0.48 |
| 1:A:643:A:N7 | 28:3:42:TRP:CH2 | 2.82 | 0.48 |
| 28:3:11:LEU:HD21 | 28:3:51:GLU:HG2 | 1.95 | 0.48 |
| 1:A:1106:G:H2' | 1:A:1107:G:H5' | 1.96 | 0.48 |
| 1:A:1175:U:H5 | 1:A:1177:A:C6 | 2.31 | 0.48 |
| 1:A:1951:U:O2 | 1:A:1953:A:H8 | 1.97 | 0.48 |
| 1:A:1999:C:H4' | 1:A:2723:C:O2 | 2.14 | 0.48 |
| 1:A:2285:C:OP1 | 28:3:30:THR:HG21 | 2.13 | 0.48 |
| 1:A:2747:G:C2 | 1:A:2756:U:C5 | 3.02 | 0.48 |
| 2:B:73:A:C4 | 2:B:104:A:C2 | 3.02 | 0.48 |
| 2:B:95:U:H2' | 2:B:96:G:H8 | 1.79 | 0.48 |
| 3:D:168:ARG:O | 3:D:169:GLU:HB2 | 2.12 | 0.48 |
| 20:U:10:GLY:HA2 | 20:U:27:VAL:HG22 | 1.96 | 0.48 |
| 23:X:48:LYS:HG3 | 23:X:61:ARG:HH11 | 1.78 | 0.48 |
| 25:Z:53:LEU:N | 25:Z:53:LEU:HD23 | 2.29 | 0.48 |
| 28:3:18:ARG:NH1 | 28:3:43:CYS:O | 2.46 | 0.48 |
| 30:5:57:ARG:NH1 | 30:5:57:ARG:HB2 | 2.28 | 0.48 |
| 1:A:1051:G:H1 | 1:A:1107:G:N2 | 2.06 | 0.48 |
| 1:A:1022:G:C5 | 1:A:1140:C:N4 | 2.81 | 0.48 |
| 1:A:1336:A:H2' | 1:A:1337:G:C8 | 2.48 | 0.48 |
| 1:A:1993:U:H2' | 1:A:1994:C:O4' | 2.14 | 0.48 |
| 1:A:480:A:O4' | 20:U:44:ILE:HG21 | 2.13 | 0.48 |
| 1:A:602:G:O5' | 1:A:602:G:H8 | 1.96 | 0.48 |
| 1:A:847:U:O2' | 1:A:848:G:H8 | 1.97 | 0.48 |
| 3:D:31:LYS:HE2 | 3:D:102:LYS:HD3 | 1.95 | 0.48 |
| 3:D:97:TYR:CE1 | 3:D:103:ARG:HD2 | 2.49 | 0.48 |
| 4:E:37:ARG:HA | 4:E:42:ASP:OD2 | 2.13 | 0.48 |
| 5:F:170:LEU:HD13 | 5:F:172:TRP:CZ2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:I:133:HIS:CE1 | 8:I:135:GLU:H | 2.32 | 0.48 |
| 1:A:637:A:OP2 | 11:L:115:LEU:HB2 | 2.13 | 0.48 |
| 2:B:50:G:OP2 | 14:O:62:LYS:HD2 | 2.14 | 0.48 |
| 15:P:100:TYR:CD1 | 15:P:100:TYR:N | 2.81 | 0.48 |
| 1:A:298:G:OP2 | 20:U:85:VAL:HG22 | 2.14 | 0.48 |
| 26:1:46:ASN:ND2 | 26:1:47:VAL:H | 2.10 | 0.48 |
| 29:4:29:LYS:O | 29:4:33:ARG:HB2 | 2.14 | 0.48 |
| 1:A:1478:G:O2' | 1:A:1558:A:C2 | 2.66 | 0.48 |
| 1:A:1973:G:H2' | 1:A:1974:C:H6 | 1.78 | 0.48 |
| 1:A:2873:A:C2 | 13:N:6:SER:HB2 | 2.48 | 0.48 |
| 1:A:288:C:H2' | 1:A:289:A:H8 | 1.79 | 0.48 |
| 1:A:478:A:C6 | 1:A:480:A:C6 | 3.01 | 0.48 |
| 1:A:804:A:H5'' | 1:A:805:G:OP1 | 2.14 | 0.48 |
| 3:D:172:TYR:HD1 | 3:D:185:VAL:C | 2.17 | 0.48 |
| 12:M:89:ASN:O | 12:M:92:GLY:N | 2.47 | 0.48 |
| 18:S:65:LEU:HB2 | 18:S:68:ARG:HB2 | 1.96 | 0.48 |
| 19:T:8:ILE:H | 19:T:8:ILE:HD12 | 1.78 | 0.48 |
| 23:X:9:GLY:O | 23:X:13:ILE:HD11 | 2.14 | 0.48 |
| 23:X:11:ARG:HB2 | 23:X:13:ILE:HG13 | 1.96 | 0.48 |
| 24:Y:46:GLN:HB2 | 24:Y:49:LYS:HZ1 | 1.78 | 0.48 |
| 6:G:112:PRO:HB3 | 26:1:62:CYS:HA | 1.96 | 0.47 |
| 1:A:1497:U:H5' | 1:A:1498:C:H5 | 1.79 | 0.47 |
| 1:A:528:A:C2 | 1:A:2042:A:H2' | 2.49 | 0.47 |
| 1:A:2050:C:H2' | 1:A:2051:A:O4' | 2.14 | 0.47 |
| 1:A:2182:G:H2' | 1:A:2183:C:C6 | 2.49 | 0.47 |
| 1:A:2207:C:H2' | 1:A:2208:U:O4' | 2.14 | 0.47 |
| 1:A:828:U:H3' | 1:A:828:U:O2 | 2.14 | 0.47 |
| 3:D:113:VAL:HG12 | 3:D:114:GLY:N | 2.29 | 0.47 |
| 12:M:9:TYR:HD2 | 12:M:10:ARG:HB2 | 1.77 | 0.47 |
| 12:M:76:LYS:N | 12:M:88:GLY:HA3 | 2.28 | 0.47 |
| 14:O:34:HIS:HA | 14:O:54:LEU:HD23 | 1.96 | 0.47 |
| 19:T:40:LYS:HG3 | 19:T:51:VAL:HG23 | 1.96 | 0.47 |
| 21:V:56:VAL:HG12 | 21:V:57:ILE:N | 2.29 | 0.47 |
| 1:A:1464:C:H2' | 1:A:1465:G:C8 | 2.49 | 0.47 |
| 1:A:2250:G:C8 | 1:A:2496:C:H5'' | 2.49 | 0.47 |
| 1:A:2063:C:O2 | 1:A:2450:A:N1 | 2.47 | 0.47 |
| 1:A:773:U:H5' | 3:D:47:GLY:HA3 | 1.96 | 0.47 |
| 1:A:792:G:H5'' | 1:A:793:A:H5' | 1.95 | 0.47 |
| 1:A:857:C:H4' | 22:W:23:VAL:HG21 | 1.96 | 0.47 |
| 2:B:9:G:H2' | 2:B:10:C:H6 | 1.80 | 0.47 |
| 3:D:25:THR:O | 3:D:26:LYS:C | 2.52 | 0.47 |
| 3:D:33:LEU:O | 3:D:35:LYS:N | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 9:J:70:ALA:HB2 | 9:J:135:LEU:HD11 | 1.96 | 0.47 |
| 12:M:19:GLY:C | 12:M:21:THR:H | 2.17 | 0.47 |
| 18:S:15:ARG:O | 18:S:19:LEU:HD23 | 2.14 | 0.47 |
| 1:A:1614:A:N6 | 18:S:88:ARG:H | 2.11 | 0.47 |
| 1:A:2261:C:C5 | 22:W:16:SER:HB3 | 2.49 | 0.47 |
| 1:A:1235:G:C6 | 1:A:1236:G:N1 | 2.82 | 0.47 |
| 1:A:140:A:C8 | 1:A:1408:C:O2' | 2.47 | 0.47 |
| 1:A:1538:G:O2' | 1:A:1539:G:H5' | 2.14 | 0.47 |
| 1:A:1902:C:H2' | 1:A:1903:G:O4' | 2.14 | 0.47 |
| 1:A:2015:A:H1' | 27:2:2:ALA:CA | 2.41 | 0.47 |
| 1:A:2128:C:H2' | 1:A:2129:C:C2 | 2.48 | 0.47 |
| 1:A:2498:C:O2' | 1:A:2499:C:H5' | 2.13 | 0.47 |
| 1:A:34:C:N4 | 1:A:447:A:H61 | 2.10 | 0.47 |
| 1:A:363(E):G:O2' | 1:A:363(F):U:H5' | 2.14 | 0.47 |
| 3:D:240:ALA:HB1 | 3:D:241:PRO:HD2 | 1.96 | 0.47 |
| 13:N:88:ARG:CA | 13:N:88:ARG:HH21 | 2.27 | 0.47 |
| 17:R:38:LEU:HD23 | 17:R:39:LEU:N | 2.27 | 0.47 |
| 18:S:19:LEU:O | 27:2:25:LEU:HD11 | 2.14 | 0.47 |
| 27:2:40:LYS:CE | 27:2:46:CYS:HB3 | 2.44 | 0.47 |
| 1:A:1577:C:H2' | 1:A:1578:U:C6 | 2.48 | 0.47 |
| 1:A:2165:G:C6 | 1:A:2166:G:H1' | 2.50 | 0.47 |
| 1:A:2391:G:O6 | 1:A:2425:A:H8 | 1.98 | 0.47 |
| 1:A:2601:C:O2' | 1:A:2602:A:H4' | 2.14 | 0.47 |
| 1:A:27:G:N2 | 1:A:512:G:H1' | 2.29 | 0.47 |
| 1:A:857:C:N4 | 1:A:858:U:O4 | 2.48 | 0.47 |
| 4:E:202:LYS:HZ2 | 4:E:202:LYS:N | 2.12 | 0.47 |
| 6:G:115:ARG:NH2 | 6:G:136:ARG:H | 2.12 | 0.47 |
| 7:H:23:ARG:HD3 | 7:H:23:ARG:N | 2.29 | 0.47 |
| 11:L:79:ARG:O | 11:L:111:ARG:HB2 | 2.14 | 0.47 |
| 14:O:93:LYS:CD | 14:O:95:HIS:HB2 | 2.45 | 0.47 |
| 24:Y:10:LEU:O | 24:Y:13:ALA:HB3 | 2.14 | 0.47 |
| 1:A:1040:C:O2' | 1:A:1041:C:H5' | 2.15 | 0.47 |
| 1:A:2389:G:H5'' | 1:A:2390:U:O4' | 2.15 | 0.47 |
| 1:A:2516:G:C6 | 1:A:2517:C:N4 | 2.82 | 0.47 |
| 1:A:2731:G:C6 | 1:A:2732:G:O6 | 2.67 | 0.47 |
| 1:A:84:A:H61 | 1:A:102:G:C2' | 2.27 | 0.47 |
| 1:A:1812:A:O2' | 3:D:45:ASN:HB3 | 2.15 | 0.47 |
| 4:E:131:ALA:HB1 | 4:E:134:ILE:HG12 | 1.96 | 0.47 |
| 10:K:36:GLY:HA2 | 10:K:106:LEU:HD23 | 1.97 | 0.47 |
| 14:O:12:PHE:C | 14:O:12:PHE:CD1 | 2.88 | 0.47 |
| 15:P:80:SER:HA | 15:P:81:PRO:HD3 | 1.78 | 0.47 |
| 21:V:91:LEU:HD22 | 21:V:96:VAL:HG11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 21:V:99:TYR:CE1 | 21:V:125:LEU:HB2 | 2.48 | 0.47 |
| 22:W:51:VAL:CG2 | 22:W:81:VAL:HG23 | 2.43 | 0.47 |
| 24:Y:46:GLN:HB2 | 24:Y:49:LYS:HZ3 | 1.78 | 0.47 |
| 1:A:1024:G:C3' | 1:A:1025:G:H5'' | 2.43 | 0.47 |
| 1:A:1042:G:C6 | 1:A:1043:C:C4 | 3.02 | 0.47 |
| 1:A:1496:A:H1' | 1:A:1577:C:O2' | 2.14 | 0.47 |
| 1:A:1973:G:H2' | 1:A:1974:C:C6 | 2.49 | 0.47 |
| 1:A:2630:G:H2' | 1:A:2631:G:C8 | 2.49 | 0.47 |
| 1:A:589:C:O3' | 5:F:95:ARG:NH1 | 2.47 | 0.47 |
| 6:G:52:ILE:HD12 | 6:G:52:ILE:H | 1.78 | 0.47 |
| 9:J:160:LYS:C | 9:J:161:LEU:HD23 | 2.35 | 0.47 |
| 11:L:61:ARG:CA | 11:L:62:LEU:HD13 | 2.45 | 0.47 |
| 12:M:34:LEU:HD13 | 12:M:131:ILE:HD13 | 1.96 | 0.47 |
| 30:5:53:PRO:O | 30:5:57:ARG:NH1 | 2.47 | 0.47 |
| 1:A:1824:G:O2' | 1:A:1825:A:H5' | 2.15 | 0.47 |
| 1:A:2290:G:C6 | 1:A:2291:U:C4 | 3.03 | 0.47 |
| 1:A:848:G:N9 | 1:A:933:A:H8 | 2.13 | 0.47 |
| 1:A:2050:C:H1' | 4:E:156:MET:HE2 | 1.97 | 0.47 |
| 1:A:663:G:OP1 | 11:L:21:ARG:HG2 | 2.15 | 0.47 |
| 14:O:61:ASN:O | 14:O:65:VAL:HG23 | 2.14 | 0.47 |
| 21:V:5:LEU:HD11 | 21:V:44:PHE:HA | 1.96 | 0.47 |
| 1:A:150:C:H2' | 1:A:151:C:C6 | 2.50 | 0.47 |
| 1:A:1858:G:O2' | 1:A:1859:A:C8 | 2.68 | 0.47 |
| 1:A:2811:G:C6 | 1:A:2891:G:N2 | 2.82 | 0.47 |
| 1:A:320:A:H4' | 1:A:322:A:N7 | 2.29 | 0.47 |
| 1:A:587:C:C6 | 1:A:671:C:H1' | 2.49 | 0.47 |
| 1:A:779:U:OP1 | 3:D:49:ILE:HG13 | 2.15 | 0.47 |
| 8:I:44:LEU:O | 8:I:48:GLU:HG2 | 2.15 | 0.47 |
| 9:J:59:GLY:C | 9:J:61:HIS:H | 2.17 | 0.47 |
| 16:Q:88:ILE:HG22 | 16:Q:90:VAL:CG1 | 2.45 | 0.47 |
| 18:S:19:LEU:HD12 | 27:2:25:LEU:HG | 1.96 | 0.47 |
| 19:T:56:THR:HB | 19:T:77:LYS:HE2 | 1.97 | 0.47 |
| 20:U:4:LYS:H | 20:U:4:LYS:CD | 2.28 | 0.47 |
| 28:3:9:LEU:HD13 | 28:3:28:ARG:HB2 | 1.96 | 0.47 |
| 1:A:1394:U:C4 | 1:A:1395:A:C5 | 3.02 | 0.47 |
| 1:A:1742:C:H2' | 1:A:1743:G:O4' | 2.14 | 0.47 |
| 1:A:1993:U:H5'' | 4:E:128:SER:HB3 | 1.96 | 0.47 |
| 1:A:2129:C:N3 | 1:A:2159:G:O6 | 2.48 | 0.47 |
| 1:A:2211:G:H2' | 1:A:2212:A:H5'' | 1.97 | 0.47 |
| 1:A:2389:G:H5'' | 1:A:2390:U:H5' | 1.97 | 0.47 |
| 1:A:2637:U:C4 | 1:A:2638:G:C6 | 3.02 | 0.47 |
| 1:A:363(A):G:N2 | 1:A:363(B):A:C4 | 2.83 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:414:C:H2' | 1:A:415:A:C8 | 2.50 | 0.47 |
| 4:E:188:VAL:CG2 | 4:E:189:PRO:HD2 | 2.44 | 0.47 |
| 6:G:101:ILE:HD12 | 6:G:102:PHE:N | 2.30 | 0.47 |
| 2:B:55:U:H4' | 6:G:27:ASN:HD21 | 1.80 | 0.47 |
| 11:L:57:THR:HG22 | 11:L:58:THR:H | 1.80 | 0.47 |
| 12:M:116:GLU:HA | 12:M:116:GLU:OE1 | 2.14 | 0.47 |
| 21:V:29:TYR:HA | 21:V:33:LEU:O | 2.14 | 0.47 |
| 22:W:72:ARG:HB2 | 22:W:75:LEU:HB2 | 1.97 | 0.47 |
| 30:5:53:PRO:HA | 30:5:56:GLU:HB2 | 1.96 | 0.47 |
| 30:5:6:THR:HG21 | 30:5:64:TYR:HD1 | 1.79 | 0.47 |
| 1:A:99:U:C4' | 1:A:102:G:H1' | 2.44 | 0.47 |
| 1:A:1044:G:N3 | 1:A:1111:A:H2 | 2.13 | 0.47 |
| 1:A:1110:G:H5' | 1:A:1111:A:OP1 | 2.14 | 0.47 |
| 1:A:1494:A:H2' | 1:A:1494:A:N3 | 2.30 | 0.47 |
| 1:A:2377:A:H2' | 1:A:2378:A:C8 | 2.50 | 0.47 |
| 1:A:2398:U:H2' | 1:A:2399:G:H8 | 1.78 | 0.47 |
| 3:D:103:ARG:CG | 3:D:103:ARG:NH1 | 2.70 | 0.47 |
| 3:D:158:ALA:HB3 | 3:D:161:THR:HG21 | 1.96 | 0.47 |
| 5:F:28:ILE:CD1 | 5:F:28:ILE:H | 2.25 | 0.47 |
| 6:G:167:GLU:CA | 6:G:170:ARG:HB3 | 2.39 | 0.47 |
| 6:G:77:ILE:O | 6:G:77:ILE:HG22 | 2.14 | 0.47 |
| 14:O:18:ILE:O | 14:O:21:THR:HB | 2.15 | 0.47 |
| 16:Q:44:ASN:HD22 | 16:Q:44:ASN:N | 2.12 | 0.47 |
| 19:T:63:LYS:HZ1 | 19:T:72:LYS:HB3 | 1.75 | 0.47 |
| 23:X:27:GLU:HB2 | 23:X:33:LYS:CA | 2.45 | 0.47 |
| 1:A:1487:G:H2' | 1:A:1488:G:H8 | 1.80 | 0.47 |
| 1:A:2327:A:H2' | 1:A:2328:A:C8 | 2.50 | 0.47 |
| 1:A:2561:A:H2' | 1:A:2562:U:O4' | 2.14 | 0.47 |
| 1:A:2815:C:H5' | 27:2:29:ILE:HG12 | 1.97 | 0.47 |
| 1:A:448:U:C4 | 1:A:583:G:H1' | 2.50 | 0.47 |
| 1:A:540:G:H2' | 1:A:541:C:C6 | 2.49 | 0.47 |
| 1:A:848:G:H2' | 1:A:849:A:C8 | 2.49 | 0.47 |
| 11:L:21:ARG:O | 11:L:23:PRO:HD3 | 2.15 | 0.47 |
| 12:M:89:ASN:C | 12:M:92:GLY:H | 2.19 | 0.47 |
| 18:S:65:LEU:HB2 | 18:S:68:ARG:HG3 | 1.95 | 0.47 |
| 12:M:63:LYS:HA | 21:V:178:GLU:HG2 | 1.97 | 0.47 |
| 22:W:71:ASP:C | 22:W:72:ARG:HG2 | 2.35 | 0.47 |
| 1:A:2019:A:H62 | 27:2:9:LYS:NZ | 2.13 | 0.46 |
| 1:A:1408:C:C2 | 1:A:1595:G:N2 | 2.84 | 0.46 |
| 1:A:2370:G:H2' | 1:A:2371:G:C8 | 2.50 | 0.46 |
| 1:A:603:A:C5 | 1:A:655:A:C2 | 3.03 | 0.46 |
| 6:G:146:TYR:O | 6:G:149:VAL:HG22 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 7:H:149:ARG:HA | 7:H:162:ILE:HB | 1.97 | 0.46 |
| 8:I:77:LEU:HB2 | 8:I:142:VAL:HG12 | 1.96 | 0.46 |
| 12:M:81:VAL:HG12 | 12:M:82:ARG:HB2 | 1.96 | 0.46 |
| 16:Q:36:ARG:HD3 | 16:Q:40:PHE:CZ | 2.50 | 0.46 |
| 20:U:90:LEU:HG | 20:U:91:GLU:H | 1.79 | 0.46 |
| 1:A:249:C:O2 | 30:5:12:LYS:HE3 | 2.15 | 0.46 |
| 1:A:1179:C:O2' | 1:A:1180:C:H5' | 2.15 | 0.46 |
| 1:A:2212:A:H1' | 1:A:2215:G:C5 | 2.50 | 0.46 |
| 1:A:2792:G:H1' | 1:A:2805:G:N2 | 2.29 | 0.46 |
| 1:A:881:G:H22 | 1:A:895:U:H3 | 1.63 | 0.46 |
| 3:D:106:ILE:H | 3:D:106:ILE:CD1 | 2.04 | 0.46 |
| 3:D:27:THR:HG23 | 3:D:83:GLU:HG2 | 1.95 | 0.46 |
| 5:F:93:LYS:HB3 | 5:F:94:PRO:HD2 | 1.96 | 0.46 |
| 1:A:1952:A:C2 | 10:K:22:ILE:HG13 | 2.50 | 0.46 |
| 11:L:57:THR:HB | 11:L:59:LEU:HB3 | 1.96 | 0.46 |
| 13:N:37:THR:OG1 | 13:N:40:LYS:HB2 | 2.15 | 0.46 |
| 14:O:90:GLY:C | 14:O:92:TYR:H | 2.18 | 0.46 |
| 18:S:14:PRO:O | 18:S:18:ARG:HB2 | 2.16 | 0.46 |
| 12:M:134:ARG:HG2 | 21:V:122:ARG:HH12 | 1.79 | 0.46 |
| 1:A:1009:A:H5' | 1:A:1009:A:H8 | 1.80 | 0.46 |
| 1:A:1048:A:H2 | 1:A:1112:G:N3 | 2.13 | 0.46 |
| 1:A:1025:G:C4 | 1:A:1135:C:H1' | 2.50 | 0.46 |
| 1:A:1716:U:O2 | 1:A:1746:G:C2 | 2.69 | 0.46 |
| 1:A:2472:G:H3' | 1:A:2473:U:C5' | 2.45 | 0.46 |
| 1:A:2789:C:O3' | 1:A:2790:A:H4' | 2.15 | 0.46 |
| 1:A:690:G:H2' | 1:A:691:C:C6 | 2.50 | 0.46 |
| 5:F:117:ARG:HD3 | 5:F:120:GLU:OE2 | 2.15 | 0.46 |
| 8:I:41:GLU:HA | 8:I:44:LEU:HB2 | 1.98 | 0.46 |
| 10:K:7:TYR:HE1 | 10:K:20:MET:HB2 | 1.78 | 0.46 |
| 11:L:112:LEU:H | 11:L:128:HIS:CD2 | 2.34 | 0.46 |
| 15:P:34:VAL:HG12 | 15:P:35:LYS:N | 2.31 | 0.46 |
| 20:U:75:ILE:HD12 | 20:U:76:CYS:H | 1.80 | 0.46 |
| 23:X:73:LEU:CD2 | 23:X:94:LEU:HD22 | 2.44 | 0.46 |
| 6:G:113:ARG:HD3 | 26:1:60:GLU:OE2 | 2.15 | 0.46 |
| 1:A:1035:U:H2' | 1:A:1036:G:C8 | 2.50 | 0.46 |
| 1:A:195:A:C8 | 1:A:197:A:OP1 | 2.69 | 0.46 |
| 1:A:2210:G:H21 | 1:A:2211:G:H5' | 1.80 | 0.46 |
| 1:A:262:A:H2' | 1:A:263:C:O4' | 2.14 | 0.46 |
| 1:A:2780:G:H4' | 1:A:2781:A:OP2 | 2.15 | 0.46 |
| 1:A:2893:G:H5'' | 1:A:2894:G:O4' | 2.16 | 0.46 |
| 1:A:589:C:H2' | 1:A:590:A:C8 | 2.50 | 0.46 |
| 1:A:844:C:O2' | 1:A:845:G:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:99:U:H4' | 1:A:102:G:H1' | 1.97 | 0.46 |
| 3:D:35:LYS:HB3 | 3:D:36:PRO:HD3 | 1.97 | 0.46 |
| 4:E:134:ILE:HA | 4:E:137:HIS:CD2 | 2.51 | 0.46 |
| 6:G:52:ILE:HD12 | 6:G:52:ILE:N | 2.30 | 0.46 |
| 15:P:19:LEU:HD23 | 15:P:86:ILE:HG21 | 1.98 | 0.46 |
| 17:R:52:VAL:HG13 | 17:R:52:VAL:O | 2.15 | 0.46 |
| 19:T:34:ALA:HA | 19:T:38:GLU:OE2 | 2.15 | 0.46 |
| 20:U:97:ARG:C | 20:U:97:ARG:HD3 | 2.36 | 0.46 |
| 30:5:50:LEU:O | 30:5:51:ALA:HB3 | 2.15 | 0.46 |
| 1:A:1657:C:H4' | 4:E:133:LYS:HG2 | 1.95 | 0.46 |
| 1:A:2224:G:H4' | 1:A:2226:C:C2 | 2.51 | 0.46 |
| 1:A:2243:U:H2' | 1:A:2244:U:C6 | 2.50 | 0.46 |
| 1:A:2315:G:C6 | 1:A:2316:C:C4 | 3.04 | 0.46 |
| 1:A:2781:A:H5'' | 1:A:2782:G:H5' | 1.98 | 0.46 |
| 1:A:886:C:C2' | 1:A:887:A:O4' | 2.58 | 0.46 |
| 4:E:169:ASN:OD1 | 4:E:201:THR:HG21 | 2.16 | 0.46 |
| 6:G:10:LYS:O | 6:G:15:VAL:HG23 | 2.15 | 0.46 |
| 6:G:36:LYS:HD3 | 6:G:160:VAL:HG21 | 1.96 | 0.46 |
| 8:I:3:VAL:HG22 | 8:I:36:ALA:HB1 | 1.97 | 0.46 |
| 9:J:119:GLU:CD | 9:J:119:GLU:H | 2.19 | 0.46 |
| 1:A:1665:A:H4' | 10:K:67:LYS:HB2 | 1.96 | 0.46 |
| 11:L:48:PRO:C | 11:L:50:ARG:N | 2.69 | 0.46 |
| 13:N:8:ARG:HG2 | 13:N:9:LYS:N | 2.31 | 0.46 |
| 13:N:90:ARG:O | 13:N:90:ARG:CG | 2.63 | 0.46 |
| 13:N:45:ARG:HA | 13:N:95:THR:HG21 | 1.96 | 0.46 |
| 15:P:100:TYR:HD2 | 15:P:103:ARG:NH2 | 2.13 | 0.46 |
| 30:5:39:LYS:HA | 30:5:42:ARG:NH2 | 2.31 | 0.46 |
| 1:A:1542:G:OP2 | 1:A:1543:A:OP1 | 2.33 | 0.46 |
| 1:A:2116:G:N2 | 1:A:2163:C:N4 | 2.62 | 0.46 |
| 1:A:1658:C:OP1 | 4:E:132:HIS:CE1 | 2.68 | 0.46 |
| 4:E:195:LEU:HG | 4:E:196:VAL:N | 2.30 | 0.46 |
| 4:E:98:PRO:HG3 | 4:E:175:VAL:HG12 | 1.96 | 0.46 |
| 6:G:107:LEU:HD23 | 6:G:111:LEU:CD1 | 2.45 | 0.46 |
| 9:J:89:LYS:O | 9:J:90:LEU:C | 2.53 | 0.46 |
| 11:L:122:PRO:HA | 11:L:141:ALA:O | 2.16 | 0.46 |
| 12:M:134:ARG:O | 12:M:135:ASP:C | 2.53 | 0.46 |
| 13:N:10:LEU:HB2 | 13:N:17:ARG:HE | 1.80 | 0.46 |
| 14:O:42:ASP:C | 14:O:44:LYS:H | 2.19 | 0.46 |
| 14:O:56:LEU:HB3 | 14:O:57:LYS:HZ2 | 1.81 | 0.46 |
| 18:S:75:TYR:CE2 | 18:S:104:THR:HB | 2.51 | 0.46 |
| 18:S:83:LYS:O | 18:S:84:ARG:HD2 | 2.15 | 0.46 |
| 23:X:19:GLN:HG2 | 23:X:41:ARG:HE | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1113:U:H2' | 1:A:1114:G:H8 | 1.77 | 0.46 |
| 1:A:2216:G:C4 | 1:A:2217:G:C8 | 3.03 | 0.46 |
| 1:A:2415:G:H4' | 11:L:66:GLY:C | 2.36 | 0.46 |
| 1:A:2807:G:N2 | 1:A:2893:G:H22 | 2.07 | 0.46 |
| 1:A:330:A:H2 | 1:A:1210:A:HO2' | 1.63 | 0.46 |
| 1:A:335:C:H2' | 1:A:336:C:H6 | 1.81 | 0.46 |
| 1:A:777:A:C2 | 1:A:778:G:C4 | 3.04 | 0.46 |
| 3:D:35:LYS:HG2 | 3:D:104:TYR:CD2 | 2.51 | 0.46 |
| 6:G:39:ILE:HD12 | 6:G:39:ILE:N | 2.29 | 0.46 |
| 23:X:27:GLU:CB | 23:X:33:LYS:HA | 2.44 | 0.46 |
| 23:X:93:GLU:C | 23:X:95:LEU:H | 2.19 | 0.46 |
| 1:A:1705:G:C6 | 1:A:1706:U:C4 | 3.04 | 0.46 |
| 1:A:1997:G:O2' | 1:A:1998:G:H5' | 2.16 | 0.46 |
| 1:A:2419:U:H2' | 1:A:2420:C:C6 | 2.51 | 0.46 |
| 1:A:245:G:H2' | 1:A:246:C:H6 | 1.80 | 0.46 |
| 1:A:675:A:N6 | 1:A:676:A:N6 | 2.63 | 0.46 |
| 2:B:30:C:C2' | 2:B:31:C:H5' | 2.45 | 0.46 |
| 2:B:82:G:O2' | 2:B:83:G:H5' | 2.16 | 0.46 |
| 4:E:9:VAL:HG13 | 4:E:25:VAL:C | 2.35 | 0.46 |
| 6:G:137:GLU:HB3 | 6:G:139:LEU:HD23 | 1.98 | 0.46 |
| 7:H:144:VAL:O | 7:H:148:ILE:HG12 | 2.15 | 0.46 |
| 13:N:33:ARG:N | 13:N:33:ARG:HD2 | 2.30 | 0.46 |
| 4:E:181:LEU:HD11 | 15:P:7:ILE:CG2 | 2.46 | 0.46 |
| 19:T:53:LYS:HZ2 | 19:T:55:ASN:HD21 | 1.63 | 0.46 |
| 20:U:13:VAL:HA | 20:U:75:ILE:HG22 | 1.97 | 0.46 |
| 20:U:27:VAL:HG22 | 20:U:27:VAL:O | 2.16 | 0.46 |
| 21:V:11:GLU:HG3 | 21:V:12:GLY:H | 1.80 | 0.46 |
| 30:5:32:LEU:HD23 | 30:5:33:ASN:H | 1.80 | 0.46 |
| 1:A:1011:G:H5'' | 16:Q:77:SER:HG | 1.81 | 0.46 |
| 1:A:1021:A:C3' | 1:A:1021:A:C8 | 2.97 | 0.46 |
| 1:A:139:G:N3 | 1:A:141(A):A:N1 | 2.63 | 0.46 |
| 1:A:1786:A:H4' | 1:A:1787:A:OP2 | 2.15 | 0.46 |
| 1:A:2219:G:H2' | 1:A:2224:G:H5' | 1.98 | 0.46 |
| 1:A:335:C:H2' | 1:A:336:C:C6 | 2.50 | 0.46 |
| 1:A:479:A:N3 | 1:A:481:G:H5'' | 2.31 | 0.46 |
| 1:A:773:U:H4' | 3:D:47:GLY:CA | 2.40 | 0.46 |
| 1:A:783:A:C4 | 1:A:785:G:H1' | 2.51 | 0.46 |
| 1:A:919:G:H4' | 2:B:81:G:O2' | 2.16 | 0.46 |
| 8:I:56:LYS:O | 8:I:56:LYS:HD2 | 2.16 | 0.46 |
| 11:L:113:LYS:HA | 11:L:129:ALA:O | 2.16 | 0.46 |
| 13:N:72:ASP:HB3 | 13:N:75:LEU:HB2 | 1.97 | 0.46 |
| 18:S:9:TYR:N | 18:S:9:TYR:CD2 | 2.84 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 21:V:63:ASP:C | 21:V:65:GLN:H | 2.19 | 0.46 |
| 1:A:1169:G:N2 | 1:A:1181:C:C2 | 2.84 | 0.46 |
| 1:A:2363:C:O2' | 1:A:2364:C:H5' | 2.16 | 0.46 |
| 1:A:2393:A:P | 30:5:28:GLY:H | 2.39 | 0.46 |
| 1:A:2547:U:H2' | 1:A:2548:G:C8 | 2.51 | 0.46 |
| 1:A:2748:A:N6 | 1:A:2749:A:C6 | 2.84 | 0.46 |
| 1:A:322:A:H2' | 5:F:169:ASN:ND2 | 2.30 | 0.46 |
| 1:A:309:G:N3 | 1:A:329:G:O2' | 2.49 | 0.46 |
| 1:A:523:C:H4' | 1:A:541:C:O2 | 2.15 | 0.46 |
| 1:A:751:A:C6 | 1:A:789:A:C5 | 3.04 | 0.46 |
| 3:D:62:TYR:HA | 3:D:87:ASN:ND2 | 2.31 | 0.46 |
| 6:G:41:GLN:HG2 | 6:G:155:MET:HG2 | 1.97 | 0.46 |
| 12:M:22:LYS:O | 12:M:24:GLY:N | 2.48 | 0.46 |
| 19:T:88:LYS:NZ | 19:T:90:GLU:HG2 | 2.30 | 0.46 |
| 20:U:81:LYS:CG | 20:U:97:ARG:HB3 | 2.46 | 0.46 |
| 22:W:32:ARG:HB3 | 22:W:32:ARG:HH11 | 1.80 | 0.46 |
| 1:A:1105:U:O2' | 1:A:1106:G:H5' | 2.16 | 0.45 |
| 1:A:1149:G:H2' | 1:A:1150:C:C6 | 2.51 | 0.45 |
| 1:A:1763:G:H2' | 1:A:1764:G:O5' | 2.16 | 0.45 |
| 1:A:1817:G:OP1 | 3:D:88:ARG:NH2 | 2.47 | 0.45 |
| 1:A:1998:G:H2' | 1:A:1999:C:C6 | 2.50 | 0.45 |
| 1:A:797:C:OP2 | 5:F:62:ARG:HG3 | 2.16 | 0.45 |
| 1:A:865:C:H4' | 1:A:866:A:N7 | 2.31 | 0.45 |
| 2:B:13:A:O2' | 2:B:14:U:H3' | 2.16 | 0.45 |
| 2:B:30:C:H2' | 2:B:31:C:H5' | 1.97 | 0.45 |
| 3:D:176:ARG:HA | 3:D:182:LEU:HD23 | 1.97 | 0.45 |
| 5:F:53:THR:C | 5:F:55:GLY:H | 2.18 | 0.45 |
| 5:F:63:LYS:NZ | 5:F:67:GLN:HE21 | 2.15 | 0.45 |
| 8:I:109:ILE:HD13 | 8:I:109:ILE:N | 2.31 | 0.45 |
| 1:A:956:G:OP2 | 12:M:14:ARG:NH2 | 2.50 | 0.45 |
| 17:R:61:VAL:HA | 17:R:94:LEU:HD23 | 1.97 | 0.45 |
| 21:V:125:LEU:CD1 | 21:V:164:ALA:HB3 | 2.45 | 0.45 |
| 21:V:9:TYR:CZ | 21:V:61:LEU:HD13 | 2.51 | 0.45 |
| 23:X:11:ARG:HD3 | 23:X:11:ARG:HA | 1.63 | 0.45 |
| 29:4:9:ARG:NE | 29:4:47:ARG:HB2 | 2.21 | 0.45 |
| 11:L:62:LEU:HD21 | 30:5:25:MET:HB2 | 1.96 | 0.45 |
| 30:5:37:SER:HB3 | 30:5:40:GLU:HG2 | 1.97 | 0.45 |
| 30:5:11:LYS:HE3 | 30:5:64:TYR:CE2 | 2.52 | 0.45 |
| 1:A:176:G:O2' | 1:A:177:G:H5' | 2.15 | 0.45 |
| 1:A:2599:G:C8 | 3:D:237:GLU:HG3 | 2.52 | 0.45 |
| 1:A:358:U:O2' | 1:A:359:A:H5' | 2.17 | 0.45 |
| 3:D:32:SER:O | 3:D:34:VAL:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:I:61:ARG:NH2 | 8:I:133:HIS:HD2 | 2.14 | 0.45 |
| 9:J:42:GLU:HA | 9:J:82:LYS:O | 2.16 | 0.45 |
| 14:O:49:VAL:HG13 | 14:O:76:LYS:NZ | 2.30 | 0.45 |
| 21:V:141:VAL:HG22 | 21:V:141:VAL:O | 2.16 | 0.45 |
| 1:A:197:A:H5' | 1:A:197:A:H8 | 1.82 | 0.45 |
| 1:A:2134:A:P | 1:A:2157:G:H22 | 2.39 | 0.45 |
| 1:A:2364:C:H2' | 1:A:2365:G:O4' | 2.17 | 0.45 |
| 1:A:2729:G:H2' | 1:A:2730:C:C6 | 2.51 | 0.45 |
| 1:A:500:G:N2 | 1:A:502:A:H3' | 2.30 | 0.45 |
| 3:D:245:PRO:HB2 | 3:D:255:LYS:CE | 2.46 | 0.45 |
| 12:M:43:THR:OG1 | 12:M:46:GLN:HG3 | 2.17 | 0.45 |
| 1:A:583:G:OP2 | 16:Q:10:ARG:HD2 | 2.16 | 0.45 |
| 17:R:47:VAL:HB | 17:R:50:PRO:O | 2.16 | 0.45 |
| 17:R:51:VAL:HG12 | 17:R:52:VAL:N | 2.31 | 0.45 |
| 20:U:12:THR:HA | 20:U:26:LYS:HA | 1.98 | 0.45 |
| 22:W:32:ARG:HB3 | 22:W:32:ARG:NH1 | 2.31 | 0.45 |
| 23:X:40:ARG:HH12 | 23:X:42:GLN:HG2 | 1.81 | 0.45 |
| 29:4:15:THR:HG22 | 29:4:16:HIS:CE1 | 2.52 | 0.45 |
| 1:A:1417:C:H2' | 1:A:1418:G:O4' | 2.16 | 0.45 |
| 1:A:1773:A:C5 | 1:A:1829:A:H1' | 2.52 | 0.45 |
| 1:A:1786:A:H1' | 1:A:1938:A:N6 | 2.32 | 0.45 |
| 1:A:2056:G:H2' | 1:A:2056:G:N3 | 2.31 | 0.45 |
| 1:A:2335:A:O2' | 1:A:2336:A:H5" | 2.16 | 0.45 |
| 1:A:2647:U:H2' | 1:A:2648:C:H6 | 1.80 | 0.45 |
| 1:A:390:A:C6 | 11:L:71:VAL:HG21 | 2.52 | 0.45 |
| 3:D:245:PRO:HB2 | 3:D:255:LYS:NZ | 2.32 | 0.45 |
| 4:E:196:VAL:HG22 | 4:E:197:ILE:N | 2.31 | 0.45 |
| 6:G:135:LEU:HD23 | 6:G:140:ILE:HD11 | 1.99 | 0.45 |
| 6:G:56:ALA:HB2 | 6:G:153:ARG:NE | 2.30 | 0.45 |
| 7:H:38:SER:OG | 7:H:40:GLU:HG2 | 2.16 | 0.45 |
| 7:H:72:ILE:O | 7:H:76:VAL:HG23 | 2.17 | 0.45 |
| 8:I:133:HIS:HE1 | 8:I:135:GLU:CB | 2.29 | 0.45 |
| 8:I:3:VAL:CG2 | 8:I:36:ALA:HB1 | 2.47 | 0.45 |
| 8:I:5:LEU:HD23 | 8:I:5:LEU:N | 2.16 | 0.45 |
| 15:P:105:LEU:CD2 | 15:P:109:GLU:HG3 | 2.47 | 0.45 |
| 18:S:18:ARG:HG3 | 18:S:76:VAL:CG1 | 2.47 | 0.45 |
| 21:V:151:HIS:NE2 | 21:V:170:THR:HG22 | 2.32 | 0.45 |
| 27:2:45:VAL:HG22 | 27:2:51:TYR:CE1 | 2.52 | 0.45 |
| 1:A:1001:A:H2' | 1:A:1002:G:O4' | 2.16 | 0.45 |
| 1:A:1142(B):A:C4 | 1:A:1144:G:N7 | 2.84 | 0.45 |
| 1:A:1394:U:C4 | 1:A:1395:A:C6 | 3.05 | 0.45 |
| 1:A:1472:A:N6 | 1:A:1521:G:H1' | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:188:G:C2' | 1:A:189:G:H5' | 2.45 | 0.45 |
| 1:A:228:A:H2' | 1:A:229:A:H5' | 1.99 | 0.45 |
| 1:A:2792:G:N2 | 1:A:2804:C:O2 | 2.49 | 0.45 |
| 1:A:34:C:HO2' | 1:A:35:G:H5' | 1.75 | 0.45 |
| 3:D:246:PRO:HB2 | 3:D:255:LYS:HG3 | 1.98 | 0.45 |
| 10:K:10:VAL:HG12 | 10:K:12:ASP:OD2 | 2.17 | 0.45 |
| 13:N:101:ALA:HB2 | 27:2:44:THR:OG1 | 2.17 | 0.45 |
| 13:N:97:VAL:HG22 | 13:N:114:VAL:HG23 | 1.99 | 0.45 |
| 14:O:100:ALA:HA | 14:O:103:GLU:HB3 | 1.99 | 0.45 |
| 17:R:55:ALA:HA | 17:R:101:GLY:HA2 | 1.99 | 0.45 |
| 18:S:4:LYS:HA | 18:S:106:ILE:HG22 | 1.97 | 0.45 |
| 26:1:54:LYS:HA | 26:1:55:PRO:HD3 | 1.76 | 0.45 |
| 27:2:40:LYS:HE2 | 27:2:46:CYS:SG | 2.57 | 0.45 |
| 1:A:1668:A:N3 | 1:A:1670:C:C4 | 2.84 | 0.45 |
| 1:A:2469:A:OP2 | 1:A:2476:A:H8 | 2.00 | 0.45 |
| 1:A:2480:C:H2' | 1:A:2481:G:H5' | 1.98 | 0.45 |
| 1:A:2784:C:H1' | 4:E:37:ARG:NH1 | 2.31 | 0.45 |
| 1:A:2790:A:H2' | 1:A:2791:C:C5' | 2.41 | 0.45 |
| 1:A:769:G:H5' | 1:A:1379:A:N6 | 2.31 | 0.45 |
| 3:D:154:LYS:HE2 | 3:D:154:LYS:HB3 | 1.73 | 0.45 |
| 5:F:127:GLU:HB2 | 5:F:196:LEU:HD12 | 1.99 | 0.45 |
| 5:F:65:TRP:CB | 5:F:66:PRO:HD2 | 2.45 | 0.45 |
| 7:H:109:PHE:C | 7:H:111:HIS:H | 2.19 | 0.45 |
| 9:J:90:LEU:HA | 9:J:110:LEU:HD12 | 1.99 | 0.45 |
| 10:K:73:ASP:HB2 | 15:P:82:LEU:HD11 | 1.99 | 0.45 |
| 11:L:47:ASP:OD1 | 11:L:49:ARG:N | 2.50 | 0.45 |
| 12:M:24:GLY:HA2 | 12:M:100:GLY:C | 2.37 | 0.45 |
| 16:Q:95:LEU:C | 16:Q:97:ASP:H | 2.19 | 0.45 |
| 17:R:78:LYS:HG2 | 17:R:79:VAL:HG13 | 1.98 | 0.45 |
| 18:S:70:TYR:CD2 | 18:S:70:TYR:N | 2.85 | 0.45 |
| 20:U:50:ARG:HD3 | 20:U:51:VAL:H | 1.81 | 0.45 |
| 23:X:31:GLY:O | 23:X:32:LYS:CB | 2.64 | 0.45 |
| 28:3:28:ARG:HG3 | 28:3:29:ASN:HD22 | 1.81 | 0.45 |
| 1:A:1517:G:H2' | 1:A:1518:C:C6 | 2.51 | 0.45 |
| 1:A:1899:G:H2' | 1:A:1900:A:OP2 | 2.17 | 0.45 |
| 1:A:2046:G:O5' | 27:2:19:ARG:HA | 2.17 | 0.45 |
| 1:A:2306:C:C5 | 1:A:2307:G:O4' | 2.69 | 0.45 |
| 1:A:2323:G:H2' | 1:A:2324:C:O4' | 2.17 | 0.45 |
| 1:A:2745:C:C4 | 1:A:2746:U:C4 | 3.04 | 0.45 |
| 1:A:380:U:H4' | 23:X:21:ARG:O | 2.16 | 0.45 |
| 1:A:729:G:O2' | 1:A:763:G:H4' | 2.17 | 0.45 |
| 1:A:1568:G:C5' | 3:D:61:LEU:HD22 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:E:144:ARG:HB3 | 4:E:145:LYS:H | 1.53 | 0.45 |
| 5:F:72:ARG:O | 5:F:73:ALA:O | 2.35 | 0.45 |
| 6:G:108:ASN:C | 6:G:112:PRO:HG2 | 2.37 | 0.45 |
| 6:G:70:VAL:HA | 6:G:88:ILE:HD11 | 1.98 | 0.45 |
| 8:I:69:LYS:HD2 | 8:I:73:GLU:HB2 | 1.98 | 0.45 |
| 8:I:83:ALA:CB | 8:I:88:ILE:HA | 2.47 | 0.45 |
| 14:O:67:ARG:HD3 | 14:O:103:GLU:OE1 | 2.16 | 0.45 |
| 14:O:15:ARG:O | 14:O:19:LYS:HG3 | 2.16 | 0.45 |
| 15:P:78:LEU:HD12 | 15:P:79:HIS:CD2 | 2.52 | 0.45 |
| 23:X:65:SER:OG | 23:X:66:HIS:HD2 | 2.00 | 0.45 |
| 23:X:58:ILE:HD12 | 23:X:90:ILE:CG2 | 2.46 | 0.45 |
| 24:Y:61:LEU:HD13 | 24:Y:61:LEU:HA | 1.62 | 0.45 |
| 1:A:78:A:H5' | 24:Y:7:ARG:HH12 | 1.81 | 0.45 |
| 1:A:1459:G:H5'' | 1:A:1460:A:OP2 | 2.17 | 0.45 |
| 1:A:1681:G:OP2 | 1:A:1681:G:H8 | 2.00 | 0.45 |
| 1:A:2134:A:H2 | 1:A:2159:G:H4' | 1.81 | 0.45 |
| 1:A:2305:A:H3' | 1:A:2306:C:H5'' | 1.99 | 0.45 |
| 1:A:2313:C:H5'' | 6:G:91:ARG:HD3 | 1.99 | 0.45 |
| 1:A:2443:C:O2' | 1:A:2444:G:H5' | 2.16 | 0.45 |
| 1:A:2517:C:C2 | 1:A:2542:A:N1 | 2.85 | 0.45 |
| 1:A:459:U:H4' | 29:4:40:TRP:CZ3 | 2.51 | 0.45 |
| 1:A:556:G:H2' | 1:A:557:U:C6 | 2.52 | 0.45 |
| 1:A:576:U:H2' | 1:A:577:G:C8 | 2.52 | 0.45 |
| 3:D:118:VAL:HG22 | 3:D:119:ALA:N | 2.32 | 0.45 |
| 1:A:1568:G:H5'' | 3:D:61:LEU:HD22 | 1.99 | 0.45 |
| 5:F:153:SER:OG | 5:F:190:GLU:HG3 | 2.17 | 0.45 |
| 6:G:98:ARG:HG2 | 6:G:98:ARG:H | 1.59 | 0.45 |
| 11:L:23:PRO:HD2 | 11:L:33:ARG:CZ | 2.45 | 0.45 |
| 13:N:2:ARG:HD3 | 13:N:5:LYS:NZ | 2.31 | 0.45 |
| 15:P:118:ARG:HB2 | 15:P:118:ARG:CZ | 2.46 | 0.45 |
| 15:P:51:ARG:CG | 15:P:98:LYS:HG3 | 2.47 | 0.45 |
| 16:Q:90:VAL:O | 16:Q:91:ASP:C | 2.55 | 0.45 |
| 17:R:49:THR:O | 17:R:50:PRO:C | 2.54 | 0.45 |
| 19:T:63:LYS:HD2 | 19:T:72:LYS:HA | 1.97 | 0.45 |
| 19:T:80:ILE:HD12 | 19:T:80:ILE:C | 2.36 | 0.45 |
| 19:T:27:THR:HB | 19:T:80:ILE:HG22 | 1.98 | 0.45 |
| 21:V:102:LEU:HD11 | 21:V:124:ILE:HD11 | 1.99 | 0.45 |
| 21:V:19:ARG:HH12 | 21:V:84:GLU:HA | 1.82 | 0.45 |
| 1:A:1185:C:H5'' | 1:A:1186:G:OP1 | 2.17 | 0.45 |
| 1:A:1726:G:C6 | 1:A:1727:U:C4 | 3.05 | 0.45 |
| 1:A:2019:A:H5'' | 16:Q:27:LEU:CD1 | 2.46 | 0.45 |
| 1:A:686:G:N2 | 1:A:788:A:H61 | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:D:264:LYS:CG | 3:D:266:SER:HB3 | 2.47 | 0.45 |
| 11:L:88:LEU:HD11 | 11:L:95:VAL:HG21 | 1.99 | 0.45 |
| 12:M:74:TYR:CD2 | 12:M:91:GLU:HB2 | 2.42 | 0.45 |
| 16:Q:27:LEU:HD22 | 16:Q:31:SER:CB | 2.47 | 0.45 |
| 19:T:30:VAL:HG21 | 19:T:79:ALA:HB3 | 1.99 | 0.45 |
| 29:4:30:VAL:O | 29:4:34:ARG:HG2 | 2.17 | 0.45 |
| 30:5:51:ALA:H | 30:5:54:GLU:CB | 2.30 | 0.45 |
| 1:A:1420:U:H2' | 1:A:1420:U:H6 | 1.36 | 0.45 |
| 1:A:1669:A:O3' | 1:A:2549:G:H5' | 2.16 | 0.45 |
| 1:A:2127:G:H2' | 1:A:2128:C:C2 | 2.52 | 0.45 |
| 1:A:2306:C:C6 | 1:A:2307:G:O4' | 2.70 | 0.45 |
| 1:A:2537:U:H2' | 1:A:2538:C:C6 | 2.52 | 0.45 |
| 1:A:409:C:O2' | 1:A:410:G:H5' | 2.16 | 0.45 |
| 1:A:498:G:O2' | 1:A:499:U:H5' | 2.17 | 0.45 |
| 1:A:775:G:H4' | 1:A:776:G:O5' | 2.17 | 0.45 |
| 3:D:269:PHE:HD1 | 3:D:269:PHE:N | 2.14 | 0.45 |
| 3:D:35:LYS:HZ2 | 3:D:35:LYS:HA | 1.82 | 0.45 |
| 6:G:128:ARG:HA | 6:G:164:GLU:O | 2.16 | 0.45 |
| 2:B:42:C:C4 | 6:G:91:ARG:NH2 | 2.85 | 0.45 |
| 8:I:7:GLU:HB3 | 8:I:35:LEU:HD13 | 1.97 | 0.45 |
| 9:J:90:LEU:HA | 9:J:110:LEU:HB3 | 1.99 | 0.45 |
| 11:L:38:GLN:HG3 | 11:L:39:LYS:N | 2.20 | 0.45 |
| 12:M:51:ARG:HB3 | 12:M:51:ARG:NH1 | 2.27 | 0.45 |
| 1:A:2820:A:C4' | 13:N:5:LYS:HG2 | 2.47 | 0.45 |
| 14:O:82:ILE:HG22 | 14:O:83:LYS:N | 2.32 | 0.45 |
| 18:S:64:MET:HA | 18:S:109:GLU:OE2 | 2.17 | 0.45 |
| 24:Y:15:LYS:HA | 24:Y:15:LYS:HE2 | 1.98 | 0.45 |
| 1:A:1049:C:N4 | 1:A:1050:A:H62 | 2.15 | 0.44 |
| 1:A:1105:U:C2 | 1:A:1106:G:N7 | 2.85 | 0.44 |
| 1:A:1105:U:H2' | 1:A:1106:G:C8 | 2.52 | 0.44 |
| 1:A:1543:A:H2' | 1:A:1545:A:H4' | 1.98 | 0.44 |
| 1:A:1557:C:H5'' | 1:A:1558:A:OP2 | 2.18 | 0.44 |
| 1:A:191:A:H2' | 1:A:192:C:C6 | 2.52 | 0.44 |
| 1:A:2846:G:H2' | 1:A:2847:U:O4' | 2.16 | 0.44 |
| 1:A:317:G:C2 | 1:A:318:C:C2 | 3.05 | 0.44 |
| 1:A:372:G:O2' | 1:A:373:U:OP2 | 2.33 | 0.44 |
| 1:A:851:U:O2' | 25:Z:45:GLY:HA3 | 2.18 | 0.44 |
| 1:A:924:C:H2' | 1:A:925:C:C6 | 2.52 | 0.44 |
| 1:A:974(B):C:OP2 | 1:A:974(B):C:H4' | 2.16 | 0.44 |
| 2:B:103:U:C2' | 2:B:104:A:H5' | 2.47 | 0.44 |
| 3:D:120:GLY:O | 3:D:131:LEU:HB3 | 2.17 | 0.44 |
| 5:F:47:GLY:HA3 | 5:F:95:ARG:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 6:G:86:MET:N | 6:G:87:PRO:CD | 2.80 | 0.44 |
| 9:J:154:GLN:CG | 9:J:155:ALA:N | 2.78 | 0.44 |
| 10:K:4:PRO:O | 10:K:5:GLN:CB | 2.61 | 0.44 |
| 11:L:146:VAL:HG13 | 11:L:147:LEU:N | 2.31 | 0.44 |
| 11:L:148:LEU:H | 11:L:148:LEU:CD1 | 2.23 | 0.44 |
| 11:L:39:LYS:HD2 | 11:L:39:LYS:HA | 1.83 | 0.44 |
| 1:A:871:U:OP1 | 12:M:6:ARG:HA | 2.17 | 0.44 |
| 14:O:19:LYS:O | 14:O:21:THR:N | 2.50 | 0.44 |
| 17:R:66:ARG:HB2 | 17:R:88:ARG:HD3 | 1.99 | 0.44 |
| 21:V:103:ARG:HD2 | 21:V:136:PHE:CD1 | 2.51 | 0.44 |
| 1:A:2353:G:H4' | 22:W:32:ARG:NH1 | 2.32 | 0.44 |
| 30:5:17:THR:HG23 | 30:5:21:LYS:O | 2.17 | 0.44 |
| 1:A:1459:G:H2' | 1:A:1461:G:O4' | 2.18 | 0.44 |
| 1:A:2022:U:O2' | 1:A:2617:C:H5' | 2.17 | 0.44 |
| 1:A:2411:A:O2' | 1:A:2412:A:H5' | 2.17 | 0.44 |
| 1:A:2694:G:C6 | 1:A:2695:C:C4 | 3.06 | 0.44 |
| 1:A:2884:U:C6 | 1:A:2885:C:C6 | 3.05 | 0.44 |
| 1:A:664:C:H4' | 1:A:941:A:OP1 | 2.17 | 0.44 |
| 1:A:674:G:C1' | 5:F:74:ARG:HD3 | 2.46 | 0.44 |
| 8:I:92:VAL:HG13 | 8:I:120:ILE:CG1 | 2.44 | 0.44 |
| 10:K:19:ILE:HB | 10:K:42:SER:O | 2.16 | 0.44 |
| 17:R:28:GLU:HB3 | 17:R:31:ALA:CB | 2.37 | 0.44 |
| 20:U:47:LYS:HE3 | 20:U:47:LYS:HB2 | 1.75 | 0.44 |
| 24:Y:17:SER:O | 24:Y:18:PRO:C | 2.56 | 0.44 |
| 24:Y:46:GLN:N | 24:Y:49:LYS:HE2 | 2.31 | 0.44 |
| 1:A:1047:G:HO2' | 1:A:1110:G:H1 | 1.64 | 0.44 |
| 1:A:2646:C:OP2 | 1:A:2732:G:O2' | 2.32 | 0.44 |
| 1:A:540:G:H2' | 1:A:541:C:H6 | 1.82 | 0.44 |
| 1:A:775:G:H1' | 1:A:776:G:OP2 | 2.18 | 0.44 |
| 1:A:1805:U:H5'' | 3:D:250:TRP:CE2 | 2.53 | 0.44 |
| 4:E:85:ASN:HA | 4:E:86:PRO:HD3 | 1.80 | 0.44 |
| 6:G:143:GLU:HB2 | 26:1:54:LYS:HE2 | 1.99 | 0.44 |
| 6:G:16:ARG:N | 6:G:17:PRO:HD2 | 2.33 | 0.44 |
| 9:J:101:TYR:CD1 | 9:J:101:TYR:N | 2.85 | 0.44 |
| 11:L:126:VAL:HG22 | 11:L:145:PRO:CG | 2.46 | 0.44 |
| 11:L:59:LEU:CA | 11:L:61:ARG:CZ | 2.95 | 0.44 |
| 11:L:59:LEU:HA | 11:L:61:ARG:HD2 | 1.99 | 0.44 |
| 12:M:40:ALA:CB | 12:M:127:ILE:HD11 | 2.47 | 0.44 |
| 30:5:52:LYS:CD | 30:5:52:LYS:N | 2.77 | 0.44 |
| 1:A:1045:A:C5' | 1:A:1046:A:H3' | 2.44 | 0.44 |
| 1:A:1317:A:H2' | 1:A:1318:C:C6 | 2.52 | 0.44 |
| 1:A:2633:G:O2' | 4:E:61:ARG:HD3 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:289:A:H2' | 1:A:290:G:O4' | 2.16 | 0.44 |
| 1:A:642:G:N2 | 1:A:645:C:OP2 | 2.50 | 0.44 |
| 1:A:643:A:C2 | 1:A:644:A:C4 | 3.05 | 0.44 |
| 1:A:664:C:H2' | 1:A:665:C:H6 | 1.83 | 0.44 |
| 8:I:15:VAL:HG12 | 8:I:16:GLY:N | 2.32 | 0.44 |
| 9:J:119:GLU:N | 9:J:119:GLU:CD | 2.70 | 0.44 |
| 9:J:157:ARG:N | 9:J:158:PRO:CD | 2.78 | 0.44 |
| 11:L:128:HIS:HB3 | 11:L:147:LEU:HD23 | 1.99 | 0.44 |
| 11:L:6:LEU:HD23 | 11:L:6:LEU:N | 2.31 | 0.44 |
| 15:P:36:GLU:O | 15:P:39:ARG:HG3 | 2.17 | 0.44 |
| 19:T:54:VAL:C | 19:T:55:ASN:HD22 | 2.19 | 0.44 |
| 22:W:82:ARG:O | 22:W:82:ARG:HG3 | 2.18 | 0.44 |
| 23:X:83:GLU:HB3 | 23:X:84:GLY:H | 1.58 | 0.44 |
| 25:Z:44:ARG:HB2 | 25:Z:44:ARG:HE | 1.43 | 0.44 |
| 28:3:28:ARG:HD2 | 28:3:28:ARG:HA | 1.86 | 0.44 |
| 1:A:161:U:H1' | 1:A:171:G:N2 | 2.32 | 0.44 |
| 1:A:1726:G:C5 | 1:A:1727:U:C5 | 3.05 | 0.44 |
| 1:A:1771:C:O2' | 1:A:1786:A:H8 | 2.01 | 0.44 |
| 1:A:2482:G:H21 | 12:M:56:ARG:HH21 | 1.64 | 0.44 |
| 1:A:675:A:H4' | 5:F:67:GLN:HE22 | 1.75 | 0.44 |
| 7:H:24:VAL:HG12 | 7:H:25:LYS:N | 2.32 | 0.44 |
| 16:Q:61:TRP:CD2 | 16:Q:94:ASN:HA | 2.52 | 0.44 |
| 17:R:64:HIS:CG | 17:R:92:THR:HG22 | 2.52 | 0.44 |
| 19:T:14:SER:O | 19:T:15:GLU:C | 2.56 | 0.44 |
| 21:V:56:VAL:HG12 | 21:V:57:ILE:H | 1.82 | 0.44 |
| 23:X:80:LEU:HD23 | 23:X:80:LEU:C | 2.37 | 0.44 |
| 28:3:44:ARG:HB3 | 28:3:45:LYS:H | 1.57 | 0.44 |
| 30:5:52:LYS:CA | 30:5:52:LYS:CE | 2.95 | 0.44 |
| 30:5:14:VAL:HG21 | 30:5:57:ARG:HD3 | 2.00 | 0.44 |
| 1:A:1504:C:H2' | 1:A:1505:C:C6 | 2.52 | 0.44 |
| 1:A:1543:A:H2' | 1:A:1545:A:C4' | 2.48 | 0.44 |
| 1:A:1639:U:C2' | 1:A:1640:C:H5'' | 2.46 | 0.44 |
| 1:A:2050:C:N4 | 1:A:2051:A:C6 | 2.86 | 0.44 |
| 1:A:2758:A:C2 | 1:A:2759:G:H1' | 2.53 | 0.44 |
| 1:A:649:G:H2' | 1:A:650:C:O4' | 2.17 | 0.44 |
| 1:A:747:U:C4 | 1:A:2613:U:C4 | 3.05 | 0.44 |
| 3:D:231:HIS:ND1 | 3:D:232:PRO:HD2 | 2.33 | 0.44 |
| 6:G:98:ARG:O | 6:G:101:ILE:HG13 | 2.17 | 0.44 |
| 6:G:111:LEU:HB2 | 6:G:112:PRO:HD3 | 1.99 | 0.44 |
| 6:G:173:LEU:HB3 | 6:G:178:PHE:CD2 | 2.52 | 0.44 |
| 10:K:39:ILE:HG13 | 10:K:39:ILE:O | 2.17 | 0.44 |
| 11:L:51:PHE:HE1 | 11:L:59:LEU:HD13 | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:389:G:N1 | 11:L:70:GLN:HG3 | 2.33 | 0.44 |
| 12:M:27:VAL:HA | 12:M:105:GLU:OE1 | 2.17 | 0.44 |
| 1:A:2839:G:H4' | 13:N:49:ASP:HB3 | 2.00 | 0.44 |
| 18:S:57:ASN:O | 18:S:61:ASN:HB2 | 2.17 | 0.44 |
| 21:V:144:LEU:HD21 | 21:V:150:LEU:HD11 | 2.00 | 0.44 |
| 23:X:13:ILE:CD1 | 23:X:14:VAL:H | 2.22 | 0.44 |
| 28:3:34:LEU:H | 28:3:34:LEU:HD22 | 1.82 | 0.44 |
| 29:4:13:ALA:O | 29:4:17:GLY:HA3 | 2.18 | 0.44 |
| 1:A:1232:G:H2' | 1:A:1233:C:H6 | 1.83 | 0.44 |
| 1:A:1471:A:C6 | 1:A:1522:G:C2 | 3.05 | 0.44 |
| 1:A:270(P):U:H4' | 1:A:270(Q):C:OP2 | 2.18 | 0.44 |
| 1:A:969:U:H2' | 1:A:970:C:C6 | 2.53 | 0.44 |
| 5:F:28:ILE:O | 5:F:30:PRO:HD3 | 2.18 | 0.44 |
| 1:A:2093:G:H4' | 8:I:25:TYR:N | 2.33 | 0.44 |
| 11:L:85:LEU:HB2 | 11:L:118:GLY:HA3 | 2.00 | 0.44 |
| 12:M:39:PRO:O | 12:M:40:ALA:HB2 | 2.18 | 0.44 |
| 12:M:82:ARG:HD3 | 12:M:82:ARG:HA | 1.74 | 0.44 |
| 14:O:12:PHE:C | 14:O:12:PHE:HD1 | 2.20 | 0.44 |
| 15:P:49:VAL:HG13 | 15:P:49:VAL:O | 2.17 | 0.44 |
| 20:U:50:ARG:CZ | 20:U:58:GLY:HA2 | 2.47 | 0.44 |
| 1:A:1327:C:H2' | 1:A:1328:G:O4' | 2.18 | 0.44 |
| 1:A:1444(B):A:OP2 | 1:A:1445:C:H5 | 2.01 | 0.44 |
| 1:A:1686:C:H2' | 1:A:1687:G:O4' | 2.18 | 0.44 |
| 4:E:181:LEU:HD11 | 15:P:7:ILE:HG23 | 1.99 | 0.44 |
| 6:G:77:ILE:HG22 | 6:G:80:PHE:N | 2.33 | 0.44 |
| 1:A:2747:G:O2' | 7:H:67:LEU:HD13 | 2.18 | 0.44 |
| 8:I:19:VAL:HG22 | 8:I:20:ASP:N | 2.33 | 0.44 |
| 9:J:118:PRO:C | 9:J:120:ARG:N | 2.71 | 0.44 |
| 11:L:132:LYS:O | 11:L:136:GLU:HG2 | 2.17 | 0.44 |
| 11:L:75:ILE:HD12 | 11:L:75:ILE:H | 1.82 | 0.44 |
| 15:P:100:TYR:HB3 | 15:P:103:ARG:NH1 | 2.33 | 0.44 |
| 16:Q:113:ALA:O | 16:Q:117:GLN:HG2 | 2.18 | 0.44 |
| 21:V:23:LYS:HB3 | 21:V:38:TYR:CD1 | 2.52 | 0.44 |
| 28:3:17:LYS:HA | 28:3:17:LYS:HD3 | 1.72 | 0.44 |
| 28:3:28:ARG:HG3 | 28:3:29:ASN:N | 2.33 | 0.44 |
| 29:4:9:ARG:NH2 | 29:4:47:ARG:HG3 | 2.25 | 0.44 |
| 30:5:35:GLN:O | 30:5:35:GLN:HG2 | 2.18 | 0.44 |
| 1:A:1108:U:C2 | 1:A:1109:C:N4 | 2.86 | 0.44 |
| 1:A:1241:A:O2' | 1:A:1242:A:H5' | 2.18 | 0.44 |
| 1:A:2124:G:H3' | 1:A:2125:G:C8 | 2.53 | 0.44 |
| 1:A:2315:G:H2' | 1:A:2316:C:C6 | 2.53 | 0.44 |
| 1:A:2469:A:OP2 | 1:A:2476:A:C8 | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:2704:C:H2' | 1:A:2705:A:O4' | 2.17 | 0.44 |
| 1:A:896:A:O4' | 21:V:146:ILE:HD12 | 2.17 | 0.44 |
| 3:D:131:LEU:N | 3:D:131:LEU:HD23 | 2.33 | 0.44 |
| 3:D:166:GLN:CA | 3:D:166:GLN:HE21 | 2.30 | 0.44 |
| 6:G:10:LYS:O | 6:G:14:GLU:HB3 | 2.17 | 0.44 |
| 6:G:139:LEU:HA | 6:G:144:ILE:HG21 | 2.00 | 0.44 |
| 7:H:94:TYR:CE1 | 7:H:160:LYS:HE2 | 2.52 | 0.44 |
| 13:N:10:LEU:HB3 | 13:N:17:ARG:HD3 | 1.98 | 0.44 |
| 14:O:90:GLY:C | 14:O:92:TYR:N | 2.70 | 0.44 |
| 20:U:35:TYR:CE1 | 20:U:69:ALA:HB3 | 2.53 | 0.44 |
| 24:Y:1:MET:O | 24:Y:1:MET:SD | 2.76 | 0.44 |
| 6:G:104:GLU:HB3 | 26:1:50:THR:HG21 | 1.99 | 0.43 |
| 1:A:1464:C:H2' | 1:A:1465:G:H8 | 1.84 | 0.43 |
| 1:A:1652:A:N6 | 1:A:1653:G:N1 | 2.65 | 0.43 |
| 1:A:2776:A:H4' | 1:A:2777:G:H5'' | 2.00 | 0.43 |
| 1:A:374:A:C2 | 1:A:401:A:C4 | 3.06 | 0.43 |
| 1:A:389:G:O6 | 11:L:71:VAL:HG23 | 2.18 | 0.43 |
| 1:A:518:G:H2' | 1:A:519:U:C6 | 2.53 | 0.43 |
| 1:A:663:G:C6 | 1:A:664:C:C4 | 3.05 | 0.43 |
| 1:A:930:U:O4' | 1:A:930:U:O2 | 2.36 | 0.43 |
| 4:E:196:VAL:CG2 | 4:E:197:ILE:N | 2.81 | 0.43 |
| 6:G:73:ALA:H | 6:G:85:GLY:HA2 | 1.83 | 0.43 |
| 11:L:95:VAL:CG2 | 11:L:125:VAL:HB | 2.48 | 0.43 |
| 11:L:17:LYS:C | 11:L:19:VAL:H | 2.20 | 0.43 |
| 1:A:587:C:C4 | 11:L:33:ARG:HG2 | 2.53 | 0.43 |
| 11:L:61:ARG:CD | 30:5:13:ARG:HD2 | 2.48 | 0.43 |
| 11:L:62:LEU:CD2 | 11:L:62:LEU:N | 2.74 | 0.43 |
| 1:A:2880:C:O2 | 13:N:93:GLY:HA3 | 2.18 | 0.43 |
| 14:O:78:LEU:HD13 | 14:O:78:LEU:O | 2.18 | 0.43 |
| 15:P:75:ILE:N | 15:P:75:ILE:HD12 | 2.32 | 0.43 |
| 16:Q:92:ARG:HD2 | 16:Q:94:ASN:HB3 | 1.95 | 0.43 |
| 1:A:488:G:O2' | 18:S:49:LYS:HE3 | 2.17 | 0.43 |
| 20:U:50:ARG:HD3 | 20:U:51:VAL:N | 2.33 | 0.43 |
| 19:T:11:PRO:HD3 | 24:Y:37:PHE:CD2 | 2.52 | 0.43 |
| 1:A:1523:U:H2' | 1:A:1524:G:C8 | 2.53 | 0.43 |
| 1:A:1676:A:H2' | 1:A:1677:A:O4' | 2.18 | 0.43 |
| 1:A:2262:U:O2' | 1:A:2263:C:H5' | 2.18 | 0.43 |
| 1:A:2068:U:N3 | 1:A:2430:A:C2 | 2.80 | 0.43 |
| 1:A:270(N):U:H1' | 1:A:270(O):G:N7 | 2.33 | 0.43 |
| 1:A:343:C:O2' | 1:A:344:G:H5' | 2.18 | 0.43 |
| 1:A:358:U:C2' | 1:A:359:A:H5' | 2.48 | 0.43 |
| 2:B:52:A:C6 | 2:B:53:A:C5 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 3:D:220:HIS:CD2 | 3:D:220:HIS:C | 2.91 | 0.43 |
| 5:F:175:THR:O | 5:F:176:LEU:HB2 | 2.18 | 0.43 |
| 1:A:2641:G:H5'' | 9:J:99:SER:HB2 | 2.00 | 0.43 |
| 10:K:22:ILE:HD12 | 10:K:22:ILE:HA | 1.73 | 0.43 |
| 1:A:389:G:N1 | 11:L:71:VAL:HG23 | 2.32 | 0.43 |
| 2:B:50:G:OP1 | 14:O:63:THR:HG23 | 2.18 | 0.43 |
| 30:5:11:LYS:HG3 | 30:5:64:TYR:CZ | 2.54 | 0.43 |
| 1:A:1022:G:N2 | 1:A:1142(B):A:H2 | 2.14 | 0.43 |
| 1:A:1494:A:H4' | 1:A:1494:A:OP1 | 2.17 | 0.43 |
| 1:A:2135:A:H4' | 1:A:2160:G:H5' | 2.00 | 0.43 |
| 1:A:2601:C:OP2 | 31:A:4001:BLS:H131 | 2.18 | 0.43 |
| 1:A:991:C:H2' | 1:A:992:C:H6 | 1.83 | 0.43 |
| 3:D:132:PRO:HB2 | 3:D:135:PHE:HD1 | 1.83 | 0.43 |
| 6:G:143:GLU:O | 6:G:144:ILE:HD13 | 2.18 | 0.43 |
| 9:J:49:LEU:O | 9:J:53:ILE:HG13 | 2.18 | 0.43 |
| 10:K:88:ASN:ND2 | 10:K:92:GLU:HB2 | 2.32 | 0.43 |
| 11:L:96:THR:HB | 11:L:97:PRO:HD2 | 1.99 | 0.43 |
| 12:M:81:VAL:HG12 | 12:M:82:ARG:N | 2.33 | 0.43 |
| 13:N:84:ALA:HB3 | 13:N:85:PRO:HD3 | 2.01 | 0.43 |
| 13:N:9:LYS:HG3 | 13:N:10:LEU:N | 2.34 | 0.43 |
| 14:O:59:LYS:NZ | 14:O:59:LYS:HB2 | 2.33 | 0.43 |
| 15:P:113:LYS:HD2 | 15:P:113:LYS:HA | 1.89 | 0.43 |
| 15:P:29:ARG:HA | 15:P:46:GLU:HA | 2.00 | 0.43 |
| 17:R:1:MET:HB3 | 17:R:42:GLY:HA3 | 1.98 | 0.43 |
| 21:V:138:GLU:HB2 | 21:V:156:LYS:HD3 | 1.99 | 0.43 |
| 23:X:51:VAL:HG22 | 23:X:53:VAL:HG23 | 2.00 | 0.43 |
| 1:A:2611:U:O2 | 27:2:3:LYS:HG3 | 2.19 | 0.43 |
| 28:3:44:ARG:O | 28:3:45:LYS:HG2 | 2.18 | 0.43 |
| 29:4:39:ARG:HD2 | 29:4:39:ARG:HA | 1.77 | 0.43 |
| 1:A:1026:U:H5' | 1:A:1027:A:OP2 | 2.18 | 0.43 |
| 1:A:1274:A:N3 | 1:A:1297:C:H1' | 2.34 | 0.43 |
| 1:A:184:C:H2' | 1:A:185:U:C6 | 2.53 | 0.43 |
| 1:A:1925:C:O2' | 1:A:1926:U:H5' | 2.18 | 0.43 |
| 1:A:2006:C:O2' | 1:A:2823:A:N3 | 2.49 | 0.43 |
| 1:A:317:G:N2 | 1:A:318:C:H1' | 2.33 | 0.43 |
| 1:A:311:A:C8 | 1:A:332:A:N7 | 2.86 | 0.43 |
| 1:A:481:G:C4 | 1:A:507:A:C2 | 3.06 | 0.43 |
| 1:A:582:G:H2' | 1:A:583:G:C8 | 2.52 | 0.43 |
| 3:D:155:LEU:HD23 | 3:D:177:LEU:CD2 | 2.48 | 0.43 |
| 6:G:131:TYR:HB3 | 6:G:159:VAL:CG1 | 2.48 | 0.43 |
| 6:G:60:LEU:O | 6:G:63:ILE:HG13 | 2.17 | 0.43 |
| 1:A:661:C:O2' | 11:L:18:ARG:HA | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:910:A:C6 | 12:M:13:GLN:HG3 | 2.52 | 0.43 |
| 1:A:2820:A:H4' | 13:N:5:LYS:HG2 | 1.99 | 0.43 |
| 1:A:1754:C:P | 15:P:96:ARG:HH12 | 2.41 | 0.43 |
| 17:R:18:LEU:CD1 | 17:R:20:LEU:HB2 | 2.48 | 0.43 |
| 17:R:61:VAL:O | 17:R:61:VAL:HG22 | 2.17 | 0.43 |
| 22:W:53:MET:HB3 | 22:W:59:LEU:CD2 | 2.46 | 0.43 |
| 1:A:1021:A:N6 | 1:A:1141:U:N3 | 2.66 | 0.43 |
| 1:A:1404:C:O2' | 1:A:1405:U:H5' | 2.19 | 0.43 |
| 1:A:1444:G:H2' | 1:A:1445:C:C5 | 2.54 | 0.43 |
| 1:A:273(F):U:C3' | 1:A:273(G):C:H5'' | 2.49 | 0.43 |
| 1:A:637:A:OP1 | 11:L:133:SER:HB2 | 2.18 | 0.43 |
| 1:A:687:C:H5' | 29:4:4:THR:O | 2.19 | 0.43 |
| 3:D:175:LEU:HD21 | 3:D:185:VAL:HG23 | 2.01 | 0.43 |
| 3:D:268:ARG:C | 3:D:269:PHE:HD1 | 2.21 | 0.43 |
| 4:E:174:ASP:O | 4:E:182:LEU:HD12 | 2.18 | 0.43 |
| 4:E:31:CYS:HA | 4:E:32:PRO:HD3 | 1.82 | 0.43 |
| 7:H:48:GLY:O | 7:H:49:VAL:HG13 | 2.19 | 0.43 |
| 13:N:87:TYR:OH | 13:N:116:LEU:HB3 | 2.19 | 0.43 |
| 14:O:65:VAL:O | 14:O:69:VAL:HG12 | 2.17 | 0.43 |
| 1:A:1048:A:C2 | 1:A:1112:G:N3 | 2.86 | 0.43 |
| 1:A:2340:G:O2' | 1:A:2341:G:H5' | 2.18 | 0.43 |
| 1:A:2419:U:H2' | 1:A:2420:C:H6 | 1.82 | 0.43 |
| 1:A:242:G:O5' | 30:5:3:LYS:HE3 | 2.17 | 0.43 |
| 1:A:2555:U:C5 | 1:A:2556:C:C2 | 3.06 | 0.43 |
| 1:A:2695:C:H2' | 1:A:2696:U:H6 | 1.84 | 0.43 |
| 1:A:1639:U:H4' | 1:A:2699:C:H4' | 2.01 | 0.43 |
| 1:A:2854:G:C2 | 1:A:2864:G:C2 | 3.06 | 0.43 |
| 1:A:681:G:H2' | 1:A:682:G:O4' | 2.19 | 0.43 |
| 1:A:712(B):A:H5'' | 1:A:2713:A:OP2 | 2.19 | 0.43 |
| 1:A:943:U:OP2 | 11:L:38:GLN:OE1 | 2.36 | 0.43 |
| 2:B:44:G:C2 | 2:B:48:A:C2 | 3.07 | 0.43 |
| 3:D:125:ILE:HD11 | 3:D:131:LEU:HD11 | 2.00 | 0.43 |
| 3:D:263:ARG:HB2 | 3:D:263:ARG:CZ | 2.48 | 0.43 |
| 3:D:35:LYS:HZ3 | 3:D:35:LYS:HB2 | 1.84 | 0.43 |
| 1:A:2563:U:H4' | 10:K:28:SER:HA | 1.99 | 0.43 |
| 11:L:27:HIS:CD2 | 11:L:28:GLY:N | 2.87 | 0.43 |
| 12:M:104:PHE:N | 12:M:104:PHE:CD1 | 2.86 | 0.43 |
| 12:M:78:PRO:O | 12:M:79:LEU:CB | 2.66 | 0.43 |
| 14:O:25:ARG:HD3 | 14:O:88:ASP:OD1 | 2.18 | 0.43 |
| 2:B:7:G:H4' | 14:O:29:PHE:CB | 2.49 | 0.43 |
| 14:O:40:ILE:HG22 | 14:O:47:THR:HG23 | 2.01 | 0.43 |
| 1:A:2875:C:O2' | 15:P:5:ALA:HB3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 17:R:35:LEU:H | 17:R:35:LEU:HD22 | 1.83 | 0.43 |
| 19:T:92:LEU:HA | 19:T:92:LEU:HD23 | 1.85 | 0.43 |
| 20:U:4:LYS:O | 20:U:5:MET:C | 2.56 | 0.43 |
| 21:V:62:PRO:C | 21:V:64:GLY:H | 2.21 | 0.43 |
| 23:X:9:GLY:O | 23:X:10:LYS:O | 2.37 | 0.43 |
| 25:Z:7:LYS:HE2 | 25:Z:32:GLN:HE21 | 1.82 | 0.43 |
| 1:A:458:G:O2' | 29:4:39:ARG:HD3 | 2.18 | 0.43 |
| 30:5:41:ILE:C | 30:5:41:ILE:HD12 | 2.39 | 0.43 |
| 1:A:1506:C:H2' | 1:A:1508:A:C8 | 2.54 | 0.43 |
| 1:A:1853:A:N1 | 1:A:2087:G:H1' | 2.34 | 0.43 |
| 1:A:2415:G:H2' | 1:A:2416:C:H6 | 1.83 | 0.43 |
| 1:A:2643:G:C2' | 1:A:2644:G:H5' | 2.48 | 0.43 |
| 1:A:603:A:C5 | 1:A:655:A:N3 | 2.86 | 0.43 |
| 1:A:856:C:O4' | 22:W:27:GLU:HB3 | 2.19 | 0.43 |
| 6:G:109:VAL:C | 6:G:112:PRO:HD2 | 2.39 | 0.43 |
| 1:A:2531:A:H4' | 7:H:157:TYR:CD2 | 2.53 | 0.43 |
| 12:M:54:MET:O | 12:M:57:HIS:HB3 | 2.19 | 0.43 |
| 14:O:66:ALA:O | 14:O:69:VAL:HG13 | 2.19 | 0.43 |
| 16:Q:90:VAL:HB | 17:R:39:LEU:HG | 2.00 | 0.43 |
| 1:A:1335:U:OP1 | 19:T:65:ARG:HG3 | 2.19 | 0.43 |
| 20:U:42:VAL:O | 20:U:42:VAL:HG12 | 2.19 | 0.43 |
| 21:V:16:SER:O | 21:V:20:ARG:HD2 | 2.18 | 0.43 |
| 21:V:81:ARG:O | 21:V:82:ARG:HB2 | 2.18 | 0.43 |
| 22:W:81:VAL:O | 22:W:83:PRO:HD3 | 2.17 | 0.43 |
| 30:5:8:LYS:HB3 | 30:5:12:LYS:HE2 | 2.00 | 0.43 |
| 1:A:1705:G:O2' | 1:A:1706:U:H5' | 2.18 | 0.43 |
| 1:A:1787:A:H2' | 1:A:1787:A:N3 | 2.32 | 0.43 |
| 1:A:1824:G:C2' | 1:A:1825:A:H5' | 2.49 | 0.43 |
| 1:A:2572:A:C5 | 4:E:144:ARG:NH2 | 2.84 | 0.43 |
| 1:A:2678:C:H2' | 1:A:2679:A:O4' | 2.18 | 0.43 |
| 1:A:593:G:C6 | 1:A:594:U:C4 | 3.07 | 0.43 |
| 1:A:744:G:H2' | 1:A:745:G:O4' | 2.19 | 0.43 |
| 3:D:106:ILE:N | 3:D:106:ILE:HD13 | 2.17 | 0.43 |
| 3:D:185:VAL:HG12 | 3:D:186:HIS:N | 2.34 | 0.43 |
| 6:G:107:LEU:HA | 6:G:111:LEU:HD12 | 2.01 | 0.43 |
| 9:J:36:TRP:O | 9:J:158:PRO:HG2 | 2.19 | 0.43 |
| 1:A:663:G:H5'' | 11:L:21:ARG:HD2 | 2.01 | 0.43 |
| 12:M:52:VAL:HG23 | 21:V:183:LEU:HD13 | 1.99 | 0.43 |
| 13:N:47:PHE:HE2 | 13:N:51:LEU:HD11 | 1.83 | 0.43 |
| 20:U:56:PRO:HB2 | 20:U:57:GLN:H | 1.52 | 0.43 |
| 20:U:88:LYS:N | 20:U:88:LYS:HD3 | 2.33 | 0.43 |
| 20:U:90:LEU:HD23 | 20:U:90:LEU:N | 2.28 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 22:W:46:LYS:HB3 | 22:W:47:PRO:HD2 | 2.00 | 0.43 |
| 24:Y:2:LYS:HA | 24:Y:5:GLU:OE2 | 2.18 | 0.43 |
| 28:3:30:THR:O | 28:3:32:ASN:N | 2.52 | 0.43 |
| 11:L:49:ARG:HB2 | 30:5:60:LEU:HD21 | 2.00 | 0.43 |
| 1:A:1021:A:H2' | 1:A:1023:U:H5' | 2.01 | 0.43 |
| 1:A:119:A:H4' | 1:A:120:U:OP1 | 2.19 | 0.43 |
| 1:A:1356:G:C5 | 1:A:1357:U:C5 | 3.07 | 0.43 |
| 1:A:1540:G:H2' | 1:A:1541:U:O4' | 2.19 | 0.43 |
| 1:A:1543:A:C5' | 1:A:1544:C:OP2 | 2.67 | 0.43 |
| 1:A:1680:U:N3 | 1:A:1764:G:OP2 | 2.51 | 0.43 |
| 1:A:1788:C:H2' | 1:A:1789:A:O4' | 2.19 | 0.43 |
| 1:A:2208:U:O4' | 3:D:151:LYS:HE2 | 2.18 | 0.43 |
| 1:A:2359:C:H2' | 1:A:2360:A:O4' | 2.19 | 0.43 |
| 1:A:2395:C:O2' | 23:X:32:LYS:HE3 | 2.18 | 0.43 |
| 1:A:2773:C:H2' | 1:A:2774:C:C6 | 2.54 | 0.43 |
| 1:A:2884:U:H5 | 1:A:2885:C:N1 | 2.16 | 0.43 |
| 1:A:610:C:H2' | 1:A:611:C:C6 | 2.53 | 0.43 |
| 1:A:646:A:N3 | 1:A:646:A:H5' | 2.34 | 0.43 |
| 2:B:51:G:H21 | 2:B:52:A:N6 | 2.16 | 0.43 |
| 3:D:130:ALA:HB2 | 3:D:192:THR:HB | 2.01 | 0.43 |
| 1:A:2787:C:H1' | 4:E:62:PRO:CG | 2.49 | 0.43 |
| 5:F:31:HIS:O | 5:F:34:TRP:HB3 | 2.18 | 0.43 |
| 11:L:139:LYS:NZ | 11:L:139:LYS:HB2 | 2.34 | 0.43 |
| 11:L:58:THR:C | 11:L:60:MET:H | 2.21 | 0.43 |
| 1:A:2393:A:H5' | 11:L:62:LEU:HB3 | 2.01 | 0.43 |
| 11:L:66:GLY:O | 11:L:67:MET:HB3 | 2.18 | 0.43 |
| 12:M:41:TRP:HB3 | 12:M:94:VAL:HG21 | 2.01 | 0.43 |
| 15:P:64:ARG:HD2 | 15:P:73:GLU:HG2 | 2.00 | 0.43 |
| 21:V:13:GLU:HB3 | 21:V:18:LEU:HD11 | 2.00 | 0.43 |
| 1:A:1210:A:H4' | 1:A:1211:U:O5' | 2.19 | 0.43 |
| 1:A:1483:G:C2 | 1:A:1508:A:C2 | 3.06 | 0.43 |
| 1:A:1854:A:N6 | 1:A:1888:G:C8 | 2.83 | 0.43 |
| 1:A:2219:G:C2' | 1:A:2224:G:H5' | 2.49 | 0.43 |
| 1:A:2579:C:H4' | 4:E:134:ILE:HG21 | 2.00 | 0.43 |
| 1:A:2748:A:C6 | 1:A:2749:A:C5 | 3.07 | 0.43 |
| 1:A:869:G:C4 | 1:A:870:A:C8 | 3.06 | 0.43 |
| 2:B:5:C:C2 | 2:B:116:G:N2 | 2.87 | 0.43 |
| 3:D:18:VAL:HG22 | 3:D:19:ALA:N | 2.34 | 0.43 |
| 4:E:134:ILE:HG13 | 4:E:134:ILE:O | 2.19 | 0.43 |
| 5:F:53:THR:C | 5:F:55:GLY:N | 2.72 | 0.43 |
| 11:L:51:PHE:N | 11:L:57:THR:HG23 | 2.31 | 0.43 |
| 16:Q:16:LYS:HE2 | 16:Q:16:LYS:HB3 | 1.77 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 21:V:134:PRO:HG3 | 21:V:161:VAL:HG21 | 2.00 | 0.43 |
| 1:A:2395:C:O2' | 23:X:32:LYS:HG3 | 2.19 | 0.43 |
| 24:Y:12:GLU:C | 24:Y:14:ARG:H | 2.23 | 0.43 |
| 24:Y:60:LEU:HD23 | 24:Y:60:LEU:HA | 1.87 | 0.43 |
| 30:5:23:VAL:HA | 30:5:48:PHE:O | 2.18 | 0.42 |
| 1:A:102:G:OP1 | 1:A:102:G:C4' | 2.67 | 0.42 |
| 1:A:1291:C:H2' | 1:A:1292:U:C6 | 2.54 | 0.42 |
| 1:A:165:U:H3' | 1:A:165:U:O2 | 2.19 | 0.42 |
| 1:A:2156:G:C6 | 1:A:2157:G:C2 | 3.07 | 0.42 |
| 1:A:2212:A:N3 | 1:A:2215:G:C2 | 2.87 | 0.42 |
| 1:A:2294:C:H2' | 1:A:2295:C:C6 | 2.53 | 0.42 |
| 1:A:2370:G:C6 | 1:A:2371:G:C6 | 3.07 | 0.42 |
| 1:A:2815:C:O2' | 27:2:42:PRO:HB2 | 2.19 | 0.42 |
| 1:A:363(E):G:C6 | 1:A:363(F):U:C4 | 3.07 | 0.42 |
| 1:A:433:C:C4 | 1:A:434:U:O4 | 2.71 | 0.42 |
| 1:A:926:A:H2' | 1:A:928:G:C8 | 2.52 | 0.42 |
| 1:A:963:U:H2' | 1:A:964:C:C6 | 2.54 | 0.42 |
| 1:A:729:G:C8 | 3:D:208:LYS:HD2 | 2.53 | 0.42 |
| 3:D:37:LEU:O | 3:D:38:LYS:HG3 | 2.18 | 0.42 |
| 5:F:114:VAL:HG21 | 5:F:202:PHE:CE1 | 2.54 | 0.42 |
| 5:F:65:TRP:HB2 | 5:F:66:PRO:HD2 | 2.01 | 0.42 |
| 6:G:148:MET:CE | 6:G:148:MET:HA | 2.49 | 0.42 |
| 6:G:50:ALA:O | 6:G:53:LEU:HB3 | 2.19 | 0.42 |
| 7:H:121:ILE:N | 7:H:121:ILE:HD12 | 2.33 | 0.42 |
| 21:V:23:LYS:HB3 | 21:V:38:TYR:HD1 | 1.84 | 0.42 |
| 29:4:3:ARG:HG3 | 29:4:4:THR:H | 1.83 | 0.42 |
| 1:A:106:C:H2' | 1:A:107:C:C6 | 2.53 | 0.42 |
| 1:A:1106:G:C2' | 1:A:1107:G:H5' | 2.49 | 0.42 |
| 1:A:1167:U:C2 | 1:A:1183:G:N2 | 2.87 | 0.42 |
| 1:A:1607:C:H4' | 1:A:1608:A:C5' | 2.49 | 0.42 |
| 1:A:1919:A:H2' | 1:A:1919:A:N3 | 2.34 | 0.42 |
| 1:A:1952:A:C5 | 1:A:1953:A:C6 | 3.07 | 0.42 |
| 1:A:2134:A:C6 | 1:A:2157:G:O2' | 2.72 | 0.42 |
| 1:A:2116:G:H21 | 1:A:2163:C:H41 | 1.64 | 0.42 |
| 1:A:2287:A:N6 | 1:A:2344:U:N3 | 2.57 | 0.42 |
| 1:A:2308:G:O2' | 1:A:2309:A:P | 2.77 | 0.42 |
| 1:A:2473:U:HO2' | 1:A:2474:C:H5' | 1.79 | 0.42 |
| 1:A:864:G:H1' | 1:A:914:C:H42 | 1.84 | 0.42 |
| 5:F:155:LEU:HD23 | 5:F:186:ILE:HD13 | 2.01 | 0.42 |
| 10:K:89:ASN:O | 10:K:91:LEU:HD22 | 2.18 | 0.42 |
| 11:L:25:SER:O | 11:L:30:THR:HG23 | 2.18 | 0.42 |
| 2:B:50:G:OP2 | 14:O:62:LYS:HB2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 15:P:105:LEU:HG | 15:P:109:GLU:HB2 | 2.01 | 0.42 |
| 16:Q:104:GLN:OE1 | 16:Q:105:VAL:HG23 | 2.19 | 0.42 |
| 1:A:1252:G:H21 | 16:Q:33:ARG:NH1 | 2.16 | 0.42 |
| 16:Q:47:TYR:C | 16:Q:47:TYR:CD2 | 2.92 | 0.42 |
| 17:R:47:VAL:HG12 | 17:R:52:VAL:CA | 2.49 | 0.42 |
| 1:A:1309:G:H3' | 29:4:9:ARG:NH1 | 2.34 | 0.42 |
| 1:A:1666:G:C2' | 1:A:1667:G:H5' | 2.49 | 0.42 |
| 1:A:2258:C:H4' | 1:A:2259:G:OP2 | 2.20 | 0.42 |
| 1:A:2475:C:H2' | 1:A:2477:C:OP1 | 2.19 | 0.42 |
| 1:A:251:A:C5 | 1:A:252:G:H1' | 2.54 | 0.42 |
| 1:A:2646:C:H2' | 1:A:2647:U:O4' | 2.18 | 0.42 |
| 1:A:603:A:C8 | 1:A:655:A:H2 | 2.37 | 0.42 |
| 1:A:839:U:H2' | 1:A:840:C:C6 | 2.54 | 0.42 |
| 2:B:83:G:H4' | 25:Z:52:HIS:CG | 2.54 | 0.42 |
| 6:G:32:PRO:HB2 | 6:G:172:LEU:HD22 | 2.00 | 0.42 |
| 7:H:94:TYR:CE2 | 7:H:107:VAL:O | 2.72 | 0.42 |
| 8:I:26:ALA:HB1 | 8:I:31:LEU:CD2 | 2.49 | 0.42 |
| 9:J:65:TRP:O | 16:Q:64:ARG:HD3 | 2.18 | 0.42 |
| 12:M:133:ARG:HB3 | 12:M:134:ARG:H | 1.44 | 0.42 |
| 14:O:26:LEU:HG | 14:O:39:ILE:CD1 | 2.48 | 0.42 |
| 1:A:2012:G:O3' | 18:S:96:ILE:HG13 | 2.19 | 0.42 |
| 20:U:87:LYS:HE2 | 20:U:87:LYS:HB3 | 1.82 | 0.42 |
| 20:U:98:VAL:HG13 | 20:U:99:CYS:N | 2.31 | 0.42 |
| 24:Y:29:LYS:HG2 | 24:Y:57:ILE:HD13 | 2.01 | 0.42 |
| 1:A:1218:C:O2' | 1:A:1219:G:H5' | 2.19 | 0.42 |
| 1:A:2019:A:H62 | 27:2:9:LYS:HZ3 | 1.67 | 0.42 |
| 1:A:2161:C:H2' | 1:A:2162:G:O4' | 2.19 | 0.42 |
| 1:A:2415:G:C5 | 1:A:2416:C:C5 | 3.07 | 0.42 |
| 1:A:2592:G:C5 | 1:A:2593:U:C5 | 3.07 | 0.42 |
| 1:A:2688:U:H3' | 1:A:2688:U:O2 | 2.19 | 0.42 |
| 1:A:699:A:H2' | 1:A:700:G:O4' | 2.19 | 0.42 |
| 1:A:786:C:O2' | 1:A:787:U:H5' | 2.20 | 0.42 |
| 1:A:848:G:C4 | 1:A:933:A:H8 | 2.38 | 0.42 |
| 3:D:206:LEU:HD23 | 3:D:206:LEU:HA | 1.78 | 0.42 |
| 5:F:117:ARG:HA | 5:F:117:ARG:HD3 | 1.82 | 0.42 |
| 6:G:56:ALA:HB2 | 6:G:153:ARG:HE | 1.84 | 0.42 |
| 7:H:20:ALA:HB3 | 7:H:23:ARG:O | 2.18 | 0.42 |
| 9:J:81:ASP:OD1 | 9:J:147:ALA:O | 2.37 | 0.42 |
| 15:P:9:LEU:HA | 15:P:9:LEU:HD23 | 1.76 | 0.42 |
| 20:U:95:LYS:HA | 20:U:101:LYS:H | 1.84 | 0.42 |
| 20:U:95:LYS:HG2 | 20:U:96:ILE:O | 2.18 | 0.42 |
| 28:3:25:LYS:HD3 | 30:5:34:TRP:HZ3 | 1.80 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 30:5:17:THR:HG23 | 30:5:21:LYS:C | 2.40 | 0.42 |
| 1:A:1108:U:H2' | 1:A:1109:C:C6 | 2.54 | 0.42 |
| 1:A:1590:U:H2' | 1:A:1591:G:H8 | 1.85 | 0.42 |
| 1:A:2516:G:C4 | 1:A:2569:G:N2 | 2.88 | 0.42 |
| 1:A:2648:C:H2' | 1:A:2649:U:C6 | 2.55 | 0.42 |
| 1:A:679:C:O2' | 1:A:680:G:H5' | 2.20 | 0.42 |
| 1:A:1812:A:O2' | 3:D:45:ASN:N | 2.51 | 0.42 |
| 6:G:111:LEU:O | 6:G:117:PHE:HD2 | 2.02 | 0.42 |
| 7:H:86:GLU:N | 7:H:86:GLU:CD | 2.72 | 0.42 |
| 9:J:151:HIS:HE1 | 9:J:157:ARG:HE | 1.68 | 0.42 |
| 9:J:85:VAL:HG13 | 9:J:85:VAL:O | 2.19 | 0.42 |
| 12:M:24:GLY:HA2 | 12:M:101:ARG:CA | 2.47 | 0.42 |
| 15:P:107:ASP:HB2 | 15:P:108:ARG:H | 1.60 | 0.42 |
| 16:Q:92:ARG:O | 16:Q:94:ASN:N | 2.53 | 0.42 |
| 17:R:47:VAL:HG12 | 17:R:52:VAL:CB | 2.49 | 0.42 |
| 1:A:2815:C:O2 | 27:2:43:HIS:HE1 | 2.02 | 0.42 |
| 1:A:1379:A:C4' | 1:A:1380:G:OP2 | 2.61 | 0.42 |
| 1:A:1796:U:H2' | 1:A:1797:C:H6 | 1.83 | 0.42 |
| 1:A:1798:U:H5' | 3:D:259:THR:OG1 | 2.20 | 0.42 |
| 1:A:2078:C:H2' | 1:A:2079:U:C6 | 2.54 | 0.42 |
| 1:A:221:A:H4' | 1:A:222:A:O5' | 2.19 | 0.42 |
| 1:A:2685:G:O2' | 1:A:2726:U:H5 | 2.03 | 0.42 |
| 1:A:2742:C:O2' | 1:A:2743:C:H5' | 2.20 | 0.42 |
| 1:A:2820:A:O3' | 13:N:5:LYS:HE3 | 2.19 | 0.42 |
| 1:A:303:U:C2 | 1:A:304:G:C8 | 3.07 | 0.42 |
| 1:A:445:C:O2' | 1:A:446:G:H5' | 2.19 | 0.42 |
| 1:A:719:C:H6 | 1:A:719:C:O5' | 2.02 | 0.42 |
| 1:A:994:C:OP2 | 16:Q:50:ARG:HG2 | 2.20 | 0.42 |
| 3:D:146:GLU:HB2 | 3:D:189:CYS:HB3 | 2.00 | 0.42 |
| 5:F:164:ARG:CD | 5:F:175:THR:HB | 2.50 | 0.42 |
| 6:G:55:LYS:O | 6:G:58:GLN:HG2 | 2.20 | 0.42 |
| 10:K:22:ILE:H | 10:K:41:ALA:HA | 1.85 | 0.42 |
| 13:N:55:ALA:HB3 | 13:N:79:LEU:HD13 | 2.01 | 0.42 |
| 21:V:28:MET:O | 21:V:34:ASN:HA | 2.20 | 0.42 |
| 22:W:50:ASN:C | 22:W:62:LEU:HD12 | 2.40 | 0.42 |
| 1:A:1024:G:C6 | 1:A:1025:G:C6 | 3.07 | 0.42 |
| 1:A:1232:G:H2' | 1:A:1233:C:C6 | 2.55 | 0.42 |
| 1:A:1569:A:H2' | 1:A:1570:A:O4' | 2.20 | 0.42 |
| 1:A:2023:G:H4' | 1:A:2617:C:O3' | 2.20 | 0.42 |
| 1:A:2127:G:C6 | 1:A:2160:G:O6 | 2.72 | 0.42 |
| 1:A:2480:C:N4 | 1:A:2481:G:C6 | 2.88 | 0.42 |
| 1:A:610:C:H2' | 1:A:611:C:H6 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:612:G:C2 | 1:A:617:G:C6 | 3.07 | 0.42 |
| 1:A:78:A:H2' | 1:A:79:G:H8 | 1.85 | 0.42 |
| 7:H:13:LYS:CD | 7:H:14:GLY:N | 2.83 | 0.42 |
| 7:H:17:VAL:HG21 | 7:H:50:VAL:CG2 | 2.49 | 0.42 |
| 1:A:863:A:OP1 | 12:M:21:THR:HB | 2.20 | 0.42 |
| 12:M:39:PRO:HB3 | 12:M:99:PRO:HD3 | 2.01 | 0.42 |
| 13:N:10:LEU:C | 13:N:10:LEU:HD12 | 2.39 | 0.42 |
| 14:O:61:ASN:ND2 | 14:O:64:GLU:HG3 | 2.35 | 0.42 |
| 15:P:26:ASP:HB2 | 15:P:90:GLN:O | 2.19 | 0.42 |
| 20:U:73:ARG:HH21 | 20:U:82:PRO:HD3 | 1.83 | 0.42 |
| 21:V:24:LEU:HD12 | 21:V:24:LEU:C | 2.39 | 0.42 |
| 22:W:53:MET:HE1 | 22:W:57:PHE:CD1 | 2.55 | 0.42 |
| 24:Y:9:GLN:O | 24:Y:13:ALA:N | 2.53 | 0.42 |
| 24:Y:17:SER:HB3 | 24:Y:18:PRO:CD | 2.45 | 0.42 |
| 24:Y:7:ARG:C | 24:Y:7:ARG:HD3 | 2.39 | 0.42 |
| 26:1:38:ALA:O | 26:1:49:GLU:HG2 | 2.20 | 0.42 |
| 1:A:1144:G:H2' | 1:A:1145:C:C6 | 2.54 | 0.42 |
| 1:A:1477:A:C4 | 1:A:1517:G:N2 | 2.87 | 0.42 |
| 1:A:1763:G:C2' | 1:A:1764:G:O5' | 2.67 | 0.42 |
| 1:A:2039:C:H2' | 1:A:2040:C:C6 | 2.49 | 0.42 |
| 1:A:2543:G:H2' | 1:A:2544:G:H8 | 1.82 | 0.42 |
| 1:A:2869:G:H2' | 1:A:2870:C:O4' | 2.19 | 0.42 |
| 1:A:322:A:O4' | 1:A:340:A:H1' | 2.20 | 0.42 |
| 1:A:422:A:C6 | 1:A:423:A:C6 | 3.07 | 0.42 |
| 1:A:861:A:H2' | 1:A:862:G:O4' | 2.20 | 0.42 |
| 1:A:995:C:OP2 | 16:Q:54:LYS:HE3 | 2.20 | 0.42 |
| 3:D:27:THR:HG21 | 3:D:83:GLU:HG2 | 2.02 | 0.42 |
| 7:H:101:ARG:H | 7:H:101:ARG:NE | 2.17 | 0.42 |
| 7:H:127:GLU:CD | 7:H:128:PRO:HD2 | 2.39 | 0.42 |
| 8:I:69:LYS:HG3 | 8:I:70:GLU:N | 2.35 | 0.42 |
| 10:K:64:ARG:HG2 | 10:K:79:PHE:CD1 | 2.54 | 0.42 |
| 15:P:115:ARG:HD3 | 15:P:115:ARG:N | 2.30 | 0.42 |
| 21:V:151:HIS:HD2 | 21:V:168:GLU:O | 2.02 | 0.42 |
| 24:Y:49:LYS:H | 24:Y:49:LYS:HD2 | 1.83 | 0.42 |
| 1:A:1517:G:H2' | 1:A:1518:C:H6 | 1.84 | 0.42 |
| 1:A:17:G:H2' | 1:A:18:C:H6 | 1.83 | 0.42 |
| 1:A:2068:U:C2 | 1:A:2430:A:H2 | 2.37 | 0.42 |
| 1:A:2467:C:H2' | 1:A:2468:G:O4' | 2.20 | 0.42 |
| 1:A:2839:G:H4' | 13:N:49:ASP:CB | 2.50 | 0.42 |
| 1:A:2862:G:H2' | 1:A:2863:C:H6 | 1.84 | 0.42 |
| 1:A:41:C:H2' | 1:A:43:G:O4' | 2.20 | 0.42 |
| 1:A:443:A:C5 | 5:F:45:ARG:HD2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:666:G:OP1 | 11:L:47:ASP:O | 2.38 | 0.42 |
| 1:A:953:A:O2' | 1:A:954:G:H5' | 2.20 | 0.42 |
| 3:D:20:ASP:C | 3:D:22:SER:H | 2.23 | 0.42 |
| 6:G:108:ASN:O | 26:1:62:CYS:HB2 | 2.20 | 0.42 |
| 6:G:64:THR:HG23 | 6:G:66:GLN:H | 1.85 | 0.42 |
| 6:G:77:ILE:HG22 | 6:G:80:PHE:H | 1.84 | 0.42 |
| 6:G:81:LYS:N | 6:G:81:LYS:HD3 | 2.34 | 0.42 |
| 7:H:127:GLU:C | 7:H:129:THR:H | 2.23 | 0.42 |
| 9:J:33:GLU:OE1 | 9:J:33:GLU:HA | 2.20 | 0.42 |
| 9:J:88:LYS:O | 9:J:89:LYS:C | 2.58 | 0.42 |
| 13:N:13:HIS:CE1 | 13:N:16:HIS:H | 2.37 | 0.42 |
| 19:T:56:THR:HG22 | 19:T:79:ALA:HB2 | 2.02 | 0.42 |
| 20:U:59:GLY:C | 20:U:61:ILE:H | 2.22 | 0.42 |
| 20:U:13:VAL:HG21 | 20:U:72:VAL:HB | 2.02 | 0.42 |
| 1:A:336:C:H5'' | 20:U:7:VAL:HG11 | 2.01 | 0.42 |
| 22:W:71:ASP:O | 22:W:72:ARG:HG2 | 2.20 | 0.42 |
| 30:5:29:LYS:NZ | 30:5:45:GLY:HA2 | 2.35 | 0.42 |
| 1:A:110:G:O2' | 1:A:111:A:H5' | 2.19 | 0.42 |
| 1:A:1414:G:O2' | 1:A:1415:U:H5' | 2.20 | 0.42 |
| 1:A:1840:G:H1 | 1:A:1902:C:N4 | 2.15 | 0.42 |
| 1:A:2113:U:H2' | 1:A:2114:A:O4' | 2.20 | 0.42 |
| 1:A:2134:A:C2 | 1:A:2159:G:H4' | 2.55 | 0.42 |
| 1:A:2129:C:O2 | 1:A:2160:G:C2 | 2.73 | 0.42 |
| 1:A:2164:C:C6 | 1:A:2165:G:H5' | 2.54 | 0.42 |
| 1:A:69:C:O2' | 1:A:70:G:H5' | 2.20 | 0.42 |
| 1:A:1798:U:H5'' | 3:D:260:ARG:HB2 | 2.01 | 0.42 |
| 4:E:35:GLN:HB3 | 4:E:48:GLN:HE21 | 1.85 | 0.42 |
| 1:A:322:A:C3' | 5:F:169:ASN:HD21 | 2.33 | 0.42 |
| 6:G:106:LEU:HD12 | 6:G:110:ALA:HB3 | 2.01 | 0.42 |
| 6:G:90:LEU:CD2 | 6:G:90:LEU:H | 2.30 | 0.42 |
| 8:I:33:ARG:HB3 | 8:I:35:LEU:HD23 | 2.01 | 0.42 |
| 9:J:61:HIS:O | 16:Q:67:ALA:HB1 | 2.20 | 0.42 |
| 9:J:92:GLN:O | 9:J:93:LYS:O | 2.38 | 0.42 |
| 13:N:104:ARG:HH12 | 13:N:109:ALA:HB3 | 1.82 | 0.42 |
| 2:B:7:G:H4' | 14:O:29:PHE:CG | 2.55 | 0.42 |
| 14:O:25:ARG:O | 14:O:39:ILE:HA | 2.19 | 0.42 |
| 16:Q:106:PHE:O | 16:Q:110:VAL:HG23 | 2.19 | 0.42 |
| 17:R:13:ARG:HD3 | 17:R:13:ARG:C | 2.40 | 0.42 |
| 17:R:39:LEU:CD1 | 17:R:51:VAL:HA | 2.50 | 0.42 |
| 16:Q:95:LEU:HD13 | 17:R:4:ILE:HG23 | 2.02 | 0.42 |
| 19:T:57:LEU:CD1 | 19:T:78:LYS:HB3 | 2.50 | 0.42 |
| 20:U:85:VAL:HA | 20:U:94:LYS:HA | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 21:V:103:ARG:HD2 | 21:V:136:PHE:CE1 | 2.55 | 0.42 |
| 23:X:37:ILE:CG1 | 23:X:38:SER:N | 2.81 | 0.42 |
| 23:X:56:GLN:HE22 | 23:X:86:SER:H | 1.67 | 0.42 |
| 24:Y:15:LYS:C | 24:Y:16:LEU:HD22 | 2.39 | 0.42 |
| 24:Y:2:LYS:NZ | 24:Y:2:LYS:H | 2.18 | 0.42 |
| 1:A:1047:G:H4' | 1:A:1048:A:O4' | 2.20 | 0.41 |
| 1:A:1107:G:H2' | 1:A:1107:G:N3 | 2.35 | 0.41 |
| 1:A:1331:A:O2' | 1:A:1332:G:H8 | 2.02 | 0.41 |
| 1:A:1546:A:C2' | 1:A:1546(B):C:H5' | 2.50 | 0.41 |
| 1:A:1693:U:H4' | 1:A:1694:C:OP2 | 2.20 | 0.41 |
| 1:A:1767:C:C2' | 1:A:1768:U:H5' | 2.50 | 0.41 |
| 1:A:1971:A:N3 | 3:D:241:PRO:HD3 | 2.35 | 0.41 |
| 1:A:2287:A:O2' | 1:A:2288:A:H5'' | 2.20 | 0.41 |
| 1:A:2784:C:H2' | 1:A:2785:C:C6 | 2.55 | 0.41 |
| 1:A:2808:U:H2' | 1:A:2809:A:C5' | 2.50 | 0.41 |
| 1:A:280:C:N3 | 1:A:361:G:N2 | 2.68 | 0.41 |
| 1:A:882:G:N2 | 1:A:883:G:C6 | 2.88 | 0.41 |
| 1:A:979:G:C4 | 1:A:982:C:N4 | 2.88 | 0.41 |
| 2:B:88:C:H2' | 2:B:89(A):G:O4' | 2.20 | 0.41 |
| 1:A:1902:C:H5'' | 3:D:246:PRO:HD3 | 2.02 | 0.41 |
| 3:D:77:ALA:HB2 | 3:D:97:TYR:HA | 2.01 | 0.41 |
| 4:E:188:VAL:HG23 | 4:E:189:PRO:HD2 | 2.02 | 0.41 |
| 6:G:32:PRO:HB3 | 6:G:163:ALA:HB2 | 2.02 | 0.41 |
| 7:H:20:ALA:HB1 | 7:H:21:PRO:CD | 2.49 | 0.41 |
| 8:I:76:THR:HG22 | 8:I:141:LYS:HB2 | 2.01 | 0.41 |
| 11:L:6:LEU:CG | 11:L:8:PRO:HD2 | 2.50 | 0.41 |
| 15:P:112:ARG:HG3 | 15:P:112:ARG:H | 1.69 | 0.41 |
| 19:T:38:GLU:O | 19:T:42:ALA:HB2 | 2.19 | 0.41 |
| 20:U:13:VAL:HG22 | 20:U:14:LEU:N | 2.35 | 0.41 |
| 1:A:1443:G:O2' | 1:A:1444:G:H5' | 2.20 | 0.41 |
| 1:A:2031:A:C6 | 1:A:2498:C:H1' | 2.54 | 0.41 |
| 1:A:322:A:C6 | 1:A:340:A:C2 | 3.08 | 0.41 |
| 1:A:479:A:HO2' | 1:A:481:G:H8 | 1.63 | 0.41 |
| 1:A:603:A:C8 | 1:A:655:A:C2 | 3.08 | 0.41 |
| 4:E:55:ASN:O | 4:E:57:LYS:N | 2.51 | 0.41 |
| 5:F:122:LYS:HE2 | 5:F:190:GLU:O | 2.20 | 0.41 |
| 6:G:143:GLU:H | 6:G:143:GLU:CD | 2.23 | 0.41 |
| 6:G:82:LEU:HD22 | 6:G:87:PRO:HG2 | 2.02 | 0.41 |
| 7:H:118:PRO:HG2 | 7:H:121:ILE:CD1 | 2.48 | 0.41 |
| 8:I:6:LEU:N | 8:I:6:LEU:HD23 | 2.35 | 0.41 |
| 12:M:68:ILE:HD13 | 12:M:68:ILE:N | 2.33 | 0.41 |
| 19:T:71:GLY:O | 19:T:72:LYS:HG3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 20:U:42:VAL:HG21 | 20:U:67:LEU:HG | 2.02 | 0.41 |
| 30:5:32:LEU:HD23 | 30:5:33:ASN:N | 2.35 | 0.41 |
| 1:A:1273:U:O2' | 1:A:1275:A:OP1 | 2.35 | 0.41 |
| 1:A:1459:G:O3' | 1:A:1460:A:H3' | 2.21 | 0.41 |
| 1:A:1592:C:H2' | 1:A:1593:G:C8 | 2.55 | 0.41 |
| 1:A:1864:U:H5'' | 1:A:2410:G:O2' | 2.20 | 0.41 |
| 1:A:2777:G:H5' | 1:A:2778:A:H5' | 2.03 | 0.41 |
| 1:A:404:C:C4' | 1:A:405:U:H5' | 2.49 | 0.41 |
| 1:A:729:G:H5' | 1:A:730:C:H5'' | 2.02 | 0.41 |
| 3:D:256:GLY:O | 3:D:257:LEU:HB3 | 2.21 | 0.41 |
| 3:D:53:PHE:HE1 | 3:D:221:VAL:HG12 | 1.85 | 0.41 |
| 8:I:133:HIS:CE1 | 8:I:135:GLU:CB | 3.03 | 0.41 |
| 8:I:7:GLU:CD | 8:I:8:PRO:HD2 | 2.40 | 0.41 |
| 9:J:93:LYS:HE2 | 9:J:95:TYR:CE2 | 2.56 | 0.41 |
| 10:K:53:LYS:HD2 | 10:K:53:LYS:N | 2.34 | 0.41 |
| 11:L:101:VAL:HG13 | 11:L:102:ARG:H | 1.84 | 0.41 |
| 11:L:9:ASN:C | 11:L:11:GLY:N | 2.73 | 0.41 |
| 16:Q:28:ARG:CG | 16:Q:38:THR:OG1 | 2.68 | 0.41 |
| 19:T:40:LYS:HG3 | 19:T:51:VAL:CG2 | 2.50 | 0.41 |
| 19:T:62:LYS:C | 19:T:63:LYS:HD3 | 2.40 | 0.41 |
| 1:A:1142(B):A:C4 | 1:A:1144:G:C8 | 3.07 | 0.41 |
| 1:A:125:G:H4' | 1:A:126:A:OP2 | 2.20 | 0.41 |
| 1:A:1939:U:H3' | 1:A:1940:U:C5' | 2.49 | 0.41 |
| 1:A:2298:A:H2' | 1:A:2299:G:O4' | 2.20 | 0.41 |
| 1:A:2516:G:C6 | 1:A:2517:C:C4 | 3.08 | 0.41 |
| 1:A:2607:G:H2' | 1:A:2608:G:O4' | 2.20 | 0.41 |
| 1:A:2821:A:O2' | 1:A:2822:G:H5' | 2.21 | 0.41 |
| 1:A:274:G:O6 | 1:A:363(A):G:C2 | 2.73 | 0.41 |
| 1:A:579:G:H2' | 1:A:580:C:C6 | 2.55 | 0.41 |
| 3:D:107:ALA:HA | 3:D:108:PRO:HD2 | 1.97 | 0.41 |
| 6:G:167:GLU:HA | 6:G:170:ARG:CB | 2.43 | 0.41 |
| 8:I:110:ASP:OD2 | 8:I:113:ARG:HG2 | 2.20 | 0.41 |
| 9:J:89:LYS:O | 9:J:92:GLN:N | 2.53 | 0.41 |
| 10:K:105:GLU:OE1 | 10:K:105:GLU:N | 2.52 | 0.41 |
| 11:L:27:HIS:CG | 11:L:28:GLY:N | 2.80 | 0.41 |
| 11:L:66:GLY:O | 11:L:67:MET:CB | 2.68 | 0.41 |
| 11:L:84:ASN:HB3 | 11:L:117:GLU:O | 2.20 | 0.41 |
| 12:M:43:THR:HG1 | 12:M:45:GLN:HG2 | 1.85 | 0.41 |
| 16:Q:48:ALA:O | 16:Q:52:ARG:HG3 | 2.20 | 0.41 |
| 17:R:6:LYS:HB3 | 17:R:11:GLN:HG2 | 2.02 | 0.41 |
| 20:U:67:LEU:N | 20:U:67:LEU:HD12 | 2.36 | 0.41 |
| 21:V:108:PRO:HD2 | 21:V:111:VAL:HB | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1204:A:N1 | 1:A:1241:A:N1 | 2.68 | 0.41 |
| 1:A:164:U:C5 | 1:A:165:U:C4 | 3.08 | 0.41 |
| 1:A:2464:C:C2 | 1:A:2487:G:N2 | 2.89 | 0.41 |
| 1:A:315:G:C5 | 1:A:316:C:C4 | 3.08 | 0.41 |
| 1:A:883:G:H22 | 1:A:894:C:H1' | 1.85 | 0.41 |
| 1:A:569:U:O2' | 1:A:983:A:N1 | 2.47 | 0.41 |
| 2:B:74:U:C4 | 2:B:75:G:C5 | 3.09 | 0.41 |
| 4:E:13:ARG:HA | 4:E:23:VAL:HG23 | 2.02 | 0.41 |
| 4:E:78:LEU:HD23 | 4:E:78:LEU:N | 2.35 | 0.41 |
| 6:G:91:ARG:NH1 | 6:G:91:ARG:HB3 | 2.35 | 0.41 |
| 8:I:133:HIS:CD2 | 8:I:134:PRO:HD2 | 2.54 | 0.41 |
| 8:I:21:VAL:HG21 | 8:I:26:ALA:HB2 | 2.03 | 0.41 |
| 1:A:250:G:O3' | 11:L:51:PHE:CZ | 2.73 | 0.41 |
| 12:M:43:THR:HG23 | 12:M:46:GLN:CD | 2.41 | 0.41 |
| 13:N:99:LYS:HA | 13:N:112:ALA:CB | 2.51 | 0.41 |
| 20:U:39:VAL:O | 20:U:40:GLU:CD | 2.58 | 0.41 |
| 1:A:297:C:H5'' | 20:U:85:VAL:HG21 | 2.02 | 0.41 |
| 21:V:94:GLU:CD | 21:V:94:GLU:N | 2.73 | 0.41 |
| 24:Y:6:VAL:HG12 | 24:Y:10:LEU:HD11 | 2.02 | 0.41 |
| 1:A:1025:G:OP1 | 1:A:1025:G:C8 | 2.70 | 0.41 |
| 1:A:1105:U:C2' | 1:A:1106:G:H5' | 2.51 | 0.41 |
| 1:A:1493:C:O2 | 1:A:1493:C:C2' | 2.68 | 0.41 |
| 1:A:1748:G:O2' | 1:A:1749:A:H5' | 2.20 | 0.41 |
| 1:A:2334:G:H4' | 1:A:2335:A:OP2 | 2.21 | 0.41 |
| 1:A:2862:G:H2' | 1:A:2863:C:C6 | 2.56 | 0.41 |
| 1:A:728:G:C6 | 1:A:730:C:C4 | 3.09 | 0.41 |
| 1:A:883:G:N1 | 1:A:894:C:O2 | 2.54 | 0.41 |
| 1:A:910:A:C6 | 1:A:911:A:C6 | 3.09 | 0.41 |
| 2:B:16:G:N2 | 2:B:69:G:H1' | 2.35 | 0.41 |
| 3:D:31:LYS:CE | 3:D:102:LYS:HZ2 | 2.33 | 0.41 |
| 5:F:150:GLY:HA2 | 5:F:172:TRP:CE3 | 2.56 | 0.41 |
| 5:F:206:ILE:N | 5:F:206:ILE:HD13 | 2.35 | 0.41 |
| 1:A:2094:G:OP1 | 8:I:22:LYS:HG3 | 2.20 | 0.41 |
| 8:I:9:LEU:HD11 | 8:I:12:LEU:HD23 | 2.03 | 0.41 |
| 10:K:104:ARG:O | 10:K:107:ARG:HB3 | 2.21 | 0.41 |
| 11:L:16:ARG:O | 11:L:17:LYS:C | 2.58 | 0.41 |
| 12:M:40:ALA:HB3 | 12:M:127:ILE:HD11 | 2.02 | 0.41 |
| 14:O:69:VAL:HA | 14:O:72:ALA:HB3 | 2.02 | 0.41 |
| 17:R:75:PHE:C | 17:R:75:PHE:CD1 | 2.94 | 0.41 |
| 19:T:57:LEU:O | 19:T:57:LEU:HD12 | 2.21 | 0.41 |
| 12:M:62:GLY:O | 21:V:178:GLU:HG2 | 2.20 | 0.41 |
| 21:V:99:TYR:N | 21:V:99:TYR:CD1 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 24:Y:25:VAL:HG22 | 24:Y:60:LEU:HB3 | 2.02 | 0.41 |
| 24:Y:9:GLN:O | 24:Y:9:GLN:HG2 | 2.21 | 0.41 |
| 28:3:24:GLU:CD | 28:3:25:LYS:H | 2.23 | 0.41 |
| 30:5:61:LEU:O | 30:5:62:LEU:CB | 2.69 | 0.41 |
| 1:A:1416:G:N2 | 1:A:1582:C:O2 | 2.49 | 0.41 |
| 1:A:2117:A:N6 | 1:A:2172:U:N1 | 2.69 | 0.41 |
| 1:A:2126:A:O3' | 1:A:2127:G:C4' | 2.68 | 0.41 |
| 1:A:2392:A:H2' | 1:A:2393:A:O4' | 2.21 | 0.41 |
| 1:A:302:C:C2 | 1:A:303:U:C5 | 3.08 | 0.41 |
| 1:A:828:U:H4' | 1:A:831:G:N1 | 2.36 | 0.41 |
| 4:E:183:LEU:HD12 | 4:E:183:LEU:N | 2.35 | 0.41 |
| 5:F:160:ASN:ND2 | 5:F:163:VAL:HG23 | 2.36 | 0.41 |
| 5:F:206:ILE:HD13 | 5:F:206:ILE:H | 1.86 | 0.41 |
| 1:A:2305:A:O2' | 6:G:136:ARG:NE | 2.53 | 0.41 |
| 6:G:32:PRO:CB | 6:G:172:LEU:HD22 | 2.51 | 0.41 |
| 6:G:77:ILE:HB | 6:G:82:LEU:CD1 | 2.49 | 0.41 |
| 6:G:82:LEU:HD22 | 6:G:87:PRO:CG | 2.50 | 0.41 |
| 7:H:137:ASP:HB3 | 7:H:140:LYS:CG | 2.49 | 0.41 |
| 8:I:109:ILE:HB | 8:I:130:TYR:CZ | 2.55 | 0.41 |
| 11:L:9:ASN:C | 11:L:11:GLY:H | 2.22 | 0.41 |
| 14:O:24:LEU:HD12 | 14:O:84:GLN:HB3 | 2.03 | 0.41 |
| 15:P:41:ARG:O | 15:P:42:ILE:HG23 | 2.21 | 0.41 |
| 18:S:13:SER:HB3 | 18:S:16:LYS:HD2 | 2.02 | 0.41 |
| 20:U:92:ASN:OD1 | 20:U:93:GLY:N | 2.54 | 0.41 |
| 20:U:96:ILE:HG12 | 20:U:99:CYS:O | 2.20 | 0.41 |
| 23:X:47:GLN:N | 23:X:62:VAL:O | 2.53 | 0.41 |
| 1:A:1389:G:C2 | 1:A:1390:U:C2 | 3.09 | 0.41 |
| 1:A:1570:A:H4' | 3:D:38:LYS:HZ3 | 1.84 | 0.41 |
| 1:A:1790:C:H2' | 1:A:1791:A:C5 | 2.56 | 0.41 |
| 1:A:1799:G:OP1 | 3:D:260:ARG:NE | 2.51 | 0.41 |
| 1:A:1493:C:N4 | 1:A:2210:G:H1' | 2.35 | 0.41 |
| 1:A:2315:G:C6 | 1:A:2316:C:N4 | 2.89 | 0.41 |
| 1:A:2711:A:OP1 | 1:A:712(B):A:P | 2.79 | 0.41 |
| 1:A:2777:G:H5'' | 1:A:2778:A:OP1 | 2.21 | 0.41 |
| 1:A:2787:C:H2' | 1:A:2788:C:C6 | 2.56 | 0.41 |
| 1:A:390:A:C6 | 11:L:71:VAL:CG2 | 3.03 | 0.41 |
| 1:A:587:C:OP2 | 11:L:33:ARG:NH1 | 2.54 | 0.41 |
| 3:D:53:PHE:CE1 | 3:D:221:VAL:HG12 | 2.56 | 0.41 |
| 6:G:117:PHE:HD1 | 6:G:119:GLY:H | 1.68 | 0.41 |
| 8:I:71:ILE:HG13 | 8:I:72:LEU:CD2 | 2.48 | 0.41 |
| 9:J:79:ASN:HA | 9:J:147:ALA:O | 2.20 | 0.41 |
| 10:K:64:ARG:O | 10:K:82:ASN:HA | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 10:K:73:ASP:OD1 | 10:K:73:ASP:C | 2.59 | 0.41 |
| 13:N:63:ARG:O | 13:N:67:LEU:HB2 | 2.21 | 0.41 |
| 17:R:99:ILE:HD13 | 17:R:99:ILE:H | 1.85 | 0.41 |
| 1:A:64:A:H5' | 19:T:64:LYS:HE3 | 2.03 | 0.41 |
| 20:U:45:VAL:HG12 | 20:U:47:LYS:HG3 | 2.02 | 0.41 |
| 20:U:4:LYS:N | 20:U:4:LYS:CD | 2.83 | 0.41 |
| 21:V:53:ILE:HD12 | 21:V:53:ILE:C | 2.41 | 0.41 |
| 23:X:27:GLU:HG3 | 23:X:33:LYS:HD2 | 2.03 | 0.41 |
| 28:3:34:LEU:HD13 | 28:3:34:LEU:N | 2.36 | 0.41 |
| 1:A:459:U:H5' | 29:4:40:TRP:CD2 | 2.56 | 0.41 |
| 30:5:2:PRO:O | 30:5:3:LYS:HB3 | 2.20 | 0.41 |
| 1:A:1952:A:N3 | 10:K:22:ILE:HG13 | 2.35 | 0.41 |
| 1:A:2070:G:C2 | 1:A:2442:C:C2 | 3.09 | 0.41 |
| 1:A:746:A:HO2' | 1:A:2611:U:HO2' | 1.67 | 0.41 |
| 1:A:2564:A:OP1 | 1:A:2648:C:H4' | 2.21 | 0.41 |
| 1:A:319:C:H2' | 1:A:320:A:O4' | 2.21 | 0.41 |
| 1:A:373:U:O2 | 1:A:423:A:H2 | 2.04 | 0.41 |
| 1:A:483:A:H4' | 20:U:49:VAL:CG2 | 2.51 | 0.41 |
| 1:A:58:G:OP1 | 19:T:74:PRO:HA | 2.21 | 0.41 |
| 1:A:620:G:H8 | 1:A:622:G:O6 | 2.02 | 0.41 |
| 1:A:817:C:H4' | 1:A:932:G:C6 | 2.56 | 0.41 |
| 3:D:33:LEU:C | 3:D:35:LYS:N | 2.75 | 0.41 |
| 4:E:36:ARG:HH21 | 4:E:88:GLY:HA2 | 1.85 | 0.41 |
| 5:F:170:LEU:HD13 | 5:F:172:TRP:CE2 | 2.56 | 0.41 |
| 5:F:20:LEU:HD12 | 5:F:125:LEU:HD12 | 2.03 | 0.41 |
| 6:G:120:LEU:HB3 | 6:G:131:TYR:OH | 2.21 | 0.41 |
| 7:H:23:ARG:HG2 | 7:H:23:ARG:O | 2.20 | 0.41 |
| 9:J:143:LEU:CD1 | 9:J:145:VAL:HG23 | 2.50 | 0.41 |
| 11:L:96:THR:O | 11:L:100:LEU:HD23 | 2.21 | 0.41 |
| 11:L:138:LEU:HD23 | 11:L:144:GLU:HG2 | 2.03 | 0.41 |
| 13:N:98:LEU:HB2 | 13:N:113:LEU:HD23 | 2.03 | 0.41 |
| 23:X:19:GLN:CG | 23:X:41:ARG:HE | 2.34 | 0.41 |
| 24:Y:9:GLN:C | 24:Y:12:GLU:HB3 | 2.41 | 0.41 |
| 24:Y:60:LEU:C | 24:Y:62:THR:H | 2.23 | 0.41 |
| 1:A:850:C:H5' | 25:Z:17:LYS:HZ3 | 1.86 | 0.41 |
| 27:2:51:TYR:HD2 | 27:2:51:TYR:HA | 1.78 | 0.41 |
| 1:A:81:G:C2 | 1:A:106:C:C2 | 3.08 | 0.41 |
| 1:A:1110:G:H2' | 1:A:1111:A:C8 | 2.56 | 0.41 |
| 1:A:2079:U:H2' | 1:A:2080:G:O4' | 2.21 | 0.41 |
| 1:A:2415:G:H2' | 1:A:2416:C:C6 | 2.56 | 0.41 |
| 1:A:2660:A:H2' | 1:A:2661:G:O4' | 2.21 | 0.41 |
| 1:A:270(I):C:H2' | 1:A:270(J):G:C8 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2740:A:C6 | 1:A:2741:A:C6 | 3.08 | 0.41 |
| 1:A:2850:A:OP2 | 1:A:2866:U:C5 | 2.71 | 0.41 |
| 1:A:528:A:C8 | 1:A:528:A:H3' | 2.56 | 0.41 |
| 1:A:622:G:H2' | 1:A:623:G:H8 | 1.86 | 0.41 |
| 1:A:966:G:C6 | 1:A:967:C:N4 | 2.88 | 0.41 |
| 1:A:96:G:O5' | 24:Y:48:HIS:CE1 | 2.74 | 0.41 |
| 3:D:16:MET:HG3 | 3:D:211:ARG:HH21 | 1.86 | 0.41 |
| 6:G:41:GLN:HA | 6:G:155:MET:HB3 | 2.03 | 0.41 |
| 8:I:114:LEU:HD12 | 8:I:115:ALA:H | 1.86 | 0.41 |
| 9:J:151:HIS:CE1 | 9:J:157:ARG:HE | 2.39 | 0.41 |
| 13:N:47:PHE:CE2 | 13:N:51:LEU:HD11 | 2.55 | 0.41 |
| 14:O:34:HIS:ND1 | 14:O:54:LEU:HB2 | 2.36 | 0.41 |
| 17:R:98:GLU:OE1 | 17:R:100:ARG:HD3 | 2.20 | 0.41 |
| 17:R:4:ILE:HG22 | 17:R:39:LEU:HD23 | 2.03 | 0.41 |
| 21:V:128:VAL:CG1 | 21:V:132:ASN:HB2 | 2.51 | 0.41 |
| 23:X:26:ARG:O | 23:X:27:GLU:HB3 | 2.20 | 0.41 |
| 23:X:56:GLN:NE2 | 23:X:85:LEU:HA | 2.36 | 0.41 |
| 1:A:1162:G:O2' | 17:R:90:PRO:HG2 | 2.21 | 0.41 |
| 1:A:1230:C:H2' | 1:A:1231:G:C8 | 2.55 | 0.41 |
| 1:A:1788:C:H5'' | 3:D:225:ALA:HB1 | 2.02 | 0.41 |
| 1:A:2120:G:N2 | 1:A:2179:C:C2 | 2.89 | 0.41 |
| 1:A:2306:C:H4' | 6:G:136:ARG:CZ | 2.51 | 0.41 |
| 1:A:2643:G:H2' | 1:A:2644:G:O4' | 2.21 | 0.41 |
| 1:A:508:G:H2' | 1:A:509:C:OP2 | 2.21 | 0.41 |
| 1:A:78:A:H2' | 1:A:79:G:C8 | 2.55 | 0.41 |
| 3:D:79:VAL:O | 3:D:113:VAL:HG13 | 2.21 | 0.41 |
| 3:D:197:GLY:O | 3:D:198:ASN:C | 2.60 | 0.41 |
| 5:F:11:VAL:HA | 5:F:125:LEU:O | 2.20 | 0.41 |
| 6:G:16:ARG:HH12 | 6:G:28:VAL:CG1 | 2.33 | 0.41 |
| 7:H:137:ASP:HB3 | 7:H:140:LYS:CD | 2.51 | 0.41 |
| 8:I:104:GLN:HG2 | 8:I:105:HIS:CE1 | 2.56 | 0.41 |
| 9:J:90:LEU:O | 9:J:111:GLU:HG3 | 2.21 | 0.41 |
| 9:J:94:ILE:HD11 | 9:J:107:LYS:HE2 | 2.03 | 0.41 |
| 10:K:1:MET:HB2 | 10:K:32:TYR:HB3 | 2.03 | 0.41 |
| 12:M:111:GLU:O | 12:M:115:MET:HG2 | 2.20 | 0.41 |
| 13:N:28:LEU:HD12 | 13:N:48:VAL:HG21 | 2.02 | 0.41 |
| 17:R:81:TYR:C | 17:R:82:ARG:HD2 | 2.41 | 0.41 |
| 20:U:43:ASN:O | 20:U:44:ILE:HD13 | 2.21 | 0.41 |
| 20:U:2:ARG:C | 20:U:4:LYS:H | 2.24 | 0.41 |
| 30:5:30:ARG:HA | 30:5:30:ARG:NE | 2.29 | 0.40 |
| 1:A:1299:G:N2 | 1:A:1640:C:H5' | 2.35 | 0.40 |
| 1:A:137(B):G:O6 | 1:A:139:G:O2' | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1413:G:C4 | 1:A:1414:G:C8 | 3.09 | 0.40 |
| 1:A:1472:A:H61 | 1:A:1521:G:H1' | 1.86 | 0.40 |
| 1:A:155:C:H2' | 1:A:161:U:H5' | 2.03 | 0.40 |
| 1:A:1930:G:N2 | 1:A:1968:G:H2' | 2.36 | 0.40 |
| 1:A:1952:A:C6 | 1:A:1953:A:C6 | 3.08 | 0.40 |
| 1:A:2114:A:N1 | 1:A:2171:A:N1 | 2.69 | 0.40 |
| 1:A:2061:G:H5'' | 1:A:2503:A:C2 | 2.56 | 0.40 |
| 1:A:2729:G:H2' | 1:A:2730:C:H6 | 1.86 | 0.40 |
| 1:A:2760:C:O2' | 1:A:2761:G:H5' | 2.21 | 0.40 |
| 1:A:809:G:H4' | 1:A:1254:A:O4' | 2.21 | 0.40 |
| 3:D:125:ILE:HG12 | 3:D:137:PRO:HD3 | 1.99 | 0.40 |
| 4:E:87:GLU:O | 4:E:89:ASP:N | 2.54 | 0.40 |
| 6:G:77:ILE:HD12 | 6:G:77:ILE:N | 2.36 | 0.40 |
| 10:K:117:LEU:HD12 | 10:K:117:LEU:N | 2.36 | 0.40 |
| 13:N:88:ARG:HD3 | 13:N:88:ARG:HA | 1.87 | 0.40 |
| 19:T:12:VAL:O | 19:T:13:LEU:HD23 | 2.21 | 0.40 |
| 26:1:56:GLU:OE1 | 26:1:56:GLU:HA | 2.21 | 0.40 |
| 1:A:1153:C:H2' | 1:A:1154:G:O4' | 2.22 | 0.40 |
| 1:A:1831:G:H2' | 1:A:1832:C:C6 | 2.55 | 0.40 |
| 1:A:2319:G:C2 | 1:A:2320:A:N1 | 2.89 | 0.40 |
| 1:A:2562:U:C2' | 1:A:2563:U:H5' | 2.50 | 0.40 |
| 1:A:2626:C:H2' | 1:A:2627:G:O4' | 2.21 | 0.40 |
| 1:A:673:C:C2' | 1:A:674:G:H5' | 2.50 | 0.40 |
| 5:F:117:ARG:HA | 5:F:120:GLU:OE2 | 2.21 | 0.40 |
| 8:I:9:LEU:CD1 | 8:I:12:LEU:HD23 | 2.52 | 0.40 |
| 10:K:96:THR:O | 10:K:97:ARG:HB3 | 2.21 | 0.40 |
| 11:L:10:PRO:O | 11:L:11:GLY:C | 2.60 | 0.40 |
| 11:L:46:LYS:HG2 | 11:L:52:GLU:CD | 2.41 | 0.40 |
| 12:M:20:ALA:HB1 | 12:M:99:PRO:O | 2.21 | 0.40 |
| 12:M:80:GLU:OE2 | 12:M:80:GLU:CA | 2.68 | 0.40 |
| 13:N:100:LEU:HA | 13:N:100:LEU:HD13 | 1.87 | 0.40 |
| 13:N:70:LEU:H | 13:N:70:LEU:CD1 | 2.32 | 0.40 |
| 15:P:6:LEU:O | 15:P:10:VAL:HG23 | 2.21 | 0.40 |
| 15:P:61:PHE:CD2 | 15:P:78:LEU:HD23 | 2.57 | 0.40 |
| 20:U:60:PHE:O | 20:U:61:ILE:C | 2.59 | 0.40 |
| 21:V:107:THR:HA | 21:V:108:PRO:HD3 | 1.87 | 0.40 |
| 21:V:128:VAL:HG22 | 21:V:161:VAL:HA | 2.02 | 0.40 |
| 24:Y:41:ILE:O | 24:Y:41:ILE:HD12 | 2.21 | 0.40 |
| 19:T:60:ARG:NH2 | 29:4:47:ARG:CZ | 2.75 | 0.40 |
| 1:A:2419:U:O4 | 30:5:30:ARG:CZ | 2.69 | 0.40 |
| 1:A:1115:G:O2' | 1:A:1116:C:H5' | 2.21 | 0.40 |
| 1:A:1366:A:H2' | 1:A:1367:A:O4' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2344:U:H4' | 1:A:2345:G:OP1 | 2.21 | 0.40 |
| 1:A:2506:U:C6 | 1:A:2506:U:H3' | 2.55 | 0.40 |
| 1:A:2529:G:H5'' | 1:A:2530:A:C5' | 2.52 | 0.40 |
| 1:A:372:G:O2' | 1:A:373:U:P | 2.80 | 0.40 |
| 1:A:612:G:N2 | 1:A:617:G:C5 | 2.90 | 0.40 |
| 1:A:655:A:C2' | 1:A:656:G:C5' | 3.00 | 0.40 |
| 1:A:783:A:H3' | 1:A:783:A:C8 | 2.56 | 0.40 |
| 1:A:797:C:H2' | 1:A:798:G:O4' | 2.21 | 0.40 |
| 1:A:824:A:H1' | 1:A:2358:G:N7 | 2.36 | 0.40 |
| 1:A:993:G:OP1 | 16:Q:50:ARG:NH2 | 2.52 | 0.40 |
| 3:D:174:ILE:N | 3:D:174:ILE:CD1 | 2.84 | 0.40 |
| 1:A:322:A:C2' | 5:F:169:ASN:HD21 | 2.35 | 0.40 |
| 5:F:164:ARG:HD3 | 5:F:175:THR:HB | 2.03 | 0.40 |
| 5:F:197:ASP:O | 5:F:200:GLU:HB3 | 2.21 | 0.40 |
| 7:H:87:LEU:O | 7:H:130:ARG:HA | 2.21 | 0.40 |
| 14:O:89:ARG:HD2 | 14:O:94:TYR:H | 1.86 | 0.40 |
| 14:O:95:HIS:O | 14:O:98:VAL:HG23 | 2.21 | 0.40 |
| 19:T:63:LYS:HD2 | 19:T:72:LYS:CB | 2.50 | 0.40 |
| 20:U:75:ILE:HD12 | 20:U:76:CYS:N | 2.35 | 0.40 |
| 20:U:7:VAL:O | 20:U:8:LYS:HG3 | 2.21 | 0.40 |
| 21:V:63:ASP:CB | 21:V:65:GLN:HG3 | 2.51 | 0.40 |
| 21:V:70:LEU:HA | 21:V:70:LEU:HD23 | 1.99 | 0.40 |
| 24:Y:9:GLN:CA | 24:Y:12:GLU:HB3 | 2.49 | 0.40 |
| 27:2:18:ALA:O | 27:2:21:SER:HB2 | 2.21 | 0.40 |
| 27:2:48:GLU:O | 27:2:48:GLU:HG2 | 2.21 | 0.40 |
| 1:A:2286:A:H61 | 28:3:24:GLU:CD | 2.24 | 0.40 |
| 29:4:3:ARG:HD3 | 29:4:3:ARG:HA | 1.90 | 0.40 |
| 1:A:1731:G:O2' | 1:A:1732:A:C8 | 2.66 | 0.40 |
| 1:A:2114:A:C2 | 1:A:2168:G:O4' | 2.74 | 0.40 |
| 1:A:2320:A:C2 | 1:A:2333:A:C8 | 3.10 | 0.40 |
| 1:A:2555:U:C4 | 1:A:2556:C:C2 | 3.10 | 0.40 |
| 1:A:2867:G:OP2 | 15:P:119:LYS:HD3 | 2.21 | 0.40 |
| 1:A:2881:C:H2' | 1:A:2882:A:O4' | 2.21 | 0.40 |
| 1:A:619:G:H5'' | 1:A:620:G:OP2 | 2.21 | 0.40 |
| 1:A:864:G:C6 | 1:A:865:C:N4 | 2.89 | 0.40 |
| 2:B:35:U:O2' | 2:B:36:C:H5' | 2.21 | 0.40 |
| 3:D:142:VAL:HG23 | 3:D:193:VAL:HA | 2.03 | 0.40 |
| 5:F:140:LEU:CD2 | 5:F:170:LEU:HD11 | 2.52 | 0.40 |
| 9:J:118:PRO:HD2 | 9:J:119:GLU:H | 1.87 | 0.40 |
| 9:J:158:PRO:O | 9:J:159:GLU:C | 2.60 | 0.40 |
| 11:L:107:LYS:HD2 | 11:L:107:LYS:HA | 1.91 | 0.40 |
| 1:A:662:G:P | 11:L:18:ARG:HG2 | 2.61 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 12:M:54:MET:CE | 12:M:64:ILE:HG23 | 2.51 | 0.40 |
| 13:N:18:LEU:HD13 | 13:N:18:LEU:C | 2.41 | 0.40 |
| 17:R:33:VAL:O | 17:R:33:VAL:HG23 | 2.21 | 0.40 |
| 19:T:31:HIS:HA | 19:T:32:PRO:HD3 | 1.93 | 0.40 |
| 2:B:11:C:OP1 | 22:W:72:ARG:HD2 | 2.22 | 0.40 |
| 23:X:27:GLU:HG3 | 23:X:33:LYS:NZ | 2.36 | 0.40 |
| 1:A:1050:A:H3' | 1:A:1051:G:C8 | 2.57 | 0.40 |
| 1:A:1171:G:H2' | 1:A:1173:G:O4' | 2.22 | 0.40 |
| 1:A:1204:A:N3 | 1:A:1204:A:O4' | 2.54 | 0.40 |
| 1:A:1448(B):A:C4 | 1:A:1529:A:C2 | 3.09 | 0.40 |
| 1:A:1594:G:H2' | 1:A:1595:G:O4' | 2.22 | 0.40 |
| 1:A:2041:U:H2' | 1:A:2042:A:C8 | 2.57 | 0.40 |
| 1:A:2320:A:C2' | 1:A:2320:A:N3 | 2.83 | 0.40 |
| 1:A:2505:G:O6 | 1:A:2576:G:H2' | 2.22 | 0.40 |
| 1:A:310:A:N1 | 1:A:312:G:H1' | 2.37 | 0.40 |
| 1:A:30:G:H2' | 1:A:31:C:C6 | 2.56 | 0.40 |
| 1:A:414:C:H4' | 1:A:1879:C:O2 | 2.21 | 0.40 |
| 1:A:492:A:H2' | 1:A:493:G:O4' | 2.22 | 0.40 |
| 1:A:620:G:N3 | 1:A:620:G:H5'' | 2.36 | 0.40 |
| 1:A:896:A:H5'' | 21:V:146:ILE:HG13 | 2.02 | 0.40 |
| 3:D:243:GLY:O | 3:D:244:ARG:HB3 | 2.20 | 0.40 |
| 6:G:41:GLN:HG2 | 6:G:155:MET:CB | 2.52 | 0.40 |
| 8:I:110:ASP:HA | 8:I:111:PRO:HD2 | 1.88 | 0.40 |
| 11:L:32:THR:O | 11:L:33:ARG:O | 2.40 | 0.40 |
| 2:B:7:G:H4' | 14:O:29:PHE:HB2 | 2.03 | 0.40 |
| 14:O:62:LYS:HB3 | 14:O:97:ARG:NE | 2.36 | 0.40 |
| 22:W:36:ILE:HG23 | 22:W:58:THR:HG23 | 2.04 | 0.40 |
| 23:X:67:ILE:N | 23:X:68:PRO:CD | 2.85 | 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 |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 3 | D | 269/271 (99%) | 220 (82%) | 35 (13%) | 14 (5%) | 3 32 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 4 | E | 202/204 (99%) | 164 (81%) | 27 (13%) | 11 (5%) | 3 | 31 |
| 5 | F | 200/202 (99%) | 168 (84%) | 24 (12%) | 8 (4%) | 5 | 43 |
| 6 | G | 179/181 (99%) | 128 (72%) | 38 (21%) | 13 (7%) | 2 | 22 |
| 7 | H | 157/159 (99%) | 122 (78%) | 29 (18%) | 6 (4%) | 5 | 45 |
| 8 | I | 143/145 (99%) | 120 (84%) | 22 (15%) | 1 (1%) | 30 | 83 |
| 9 | J | 135/137 (98%) | 104 (77%) | 21 (16%) | 10 (7%) | 2 | 22 |
| 10 | K | 120/122 (98%) | 107 (89%) | 10 (8%) | 3 (2%) | 9 | 57 |
| 11 | L | 144/146 (99%) | 89 (62%) | 35 (24%) | 20 (14%) | 0 | 6 |
| 12 | M | 132/134 (98%) | 96 (73%) | 21 (16%) | 15 (11%) | 1 | 9 |
| 13 | N | 115/117 (98%) | 92 (80%) | 15 (13%) | 8 (7%) | 2 | 23 |
| 14 | O | 96/98 (98%) | 65 (68%) | 23 (24%) | 8 (8%) | 1 | 18 |
| 15 | P | 135/137 (98%) | 105 (78%) | 22 (16%) | 8 (6%) | 2 | 29 |
| 16 | Q | 115/117 (98%) | 102 (89%) | 10 (9%) | 3 (3%) | 8 | 56 |
| 17 | R | 99/101 (98%) | 79 (80%) | 16 (16%) | 4 (4%) | 5 | 43 |
| 18 | S | 110/112 (98%) | 102 (93%) | 8 (7%) | 0 | 100 | 100 |
| 19 | T | 90/92 (98%) | 76 (84%) | 12 (13%) | 2 (2%) | 10 | 60 |
| 20 | U | 98/100 (98%) | 63 (64%) | 23 (24%) | 12 (12%) | 1 | 8 |
| 21 | V | 185/187 (99%) | 159 (86%) | 19 (10%) | 7 (4%) | 5 | 45 |
| 22 | W | 74/76 (97%) | 59 (80%) | 13 (18%) | 2 (3%) | 8 | 55 |
| 23 | X | 86/88 (98%) | 56 (65%) | 19 (22%) | 11 (13%) | 0 | 7 |
| 24 | Y | 60/62 (97%) | 47 (78%) | 8 (13%) | 5 (8%) | 1 | 18 |
| 25 | Z | 57/59 (97%) | 52 (91%) | 4 (7%) | 1 (2%) | 13 | 65 |
| 26 | 1 | 28/30 (93%) | 13 (46%) | 13 (46%) | 2 (7%) | 2 | 23 |
| 27 | 2 | 50/52 (96%) | 45 (90%) | 3 (6%) | 2 (4%) | 5 | 43 |
| 28 | 3 | 42/44 (96%) | 26 (62%) | 12 (29%) | 4 (10%) | 1 | 14 |
| 29 | 4 | 46/48 (96%) | 44 (96%) | 1 (2%) | 1 (2%) | 10 | 60 |
| 30 | 5 | 61/63 (97%) | 46 (75%) | 9 (15%) | 6 (10%) | 1 | 13 |
| All | All | 3228/3284 (98%) | 2549 (79%) | 492 (15%) | 187 (6%) | 3 | 29 |

All (187) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 33 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 40 | THR |
| 3 | D | 59 | LYS |
| 3 | D | 239 | ARG |
| 4 | E | 86 | PRO |
| 4 | E | 89 | ASP |
| 4 | E | 132 | HIS |
| 5 | F | 73 | ALA |
| 5 | F | 133 | ASN |
| 6 | G | 75 | LYS |
| 9 | J | 60 | LYS |
| 9 | J | 93 | LYS |
| 10 | K | 26 | LYS |
| 11 | L | 31 | ALA |
| 11 | L | 65 | ARG |
| 11 | L | 141 | ALA |
| 11 | L | 148 | LEU |
| 12 | M | 8 | LYS |
| 12 | M | 21 | THR |
| 12 | M | 135 | ASP |
| 12 | M | 136 | ALA |
| 13 | N | 6 | SER |
| 14 | O | 59 | LYS |
| 15 | P | 3 | ARG |
| 15 | P | 97 | ALA |
| 15 | P | 115 | ARG |
| 16 | Q | 90 | VAL |
| 17 | R | 46 | VAL |
| 20 | U | 3 | VAL |
| 20 | U | 17 | SER |
| 20 | U | 49 | VAL |
| 20 | U | 56 | PRO |
| 20 | U | 77 | PRO |
| 20 | U | 78 | ALA |
| 22 | W | 47 | PRO |
| 22 | W | 84 | LEU |
| 23 | X | 10 | LYS |
| 23 | X | 11 | ARG |
| 23 | X | 32 | LYS |
| 23 | X | 58 | ILE |
| 24 | Y | 43 | GLN |
| 24 | Y | 45 | SER |
| 25 | Z | 2 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | 2 | 4 | HIS |
| 28 | 3 | 31 | PRO |
| 29 | 4 | 47 | ARG |
| 30 | 5 | 34 | TRP |
| 30 | 5 | 51 | ALA |
| 30 | 5 | 62 | LEU |
| 3 | D | 24 | ILE |
| 3 | D | 26 | LYS |
| 3 | D | 57 | GLY |
| 3 | D | 58 | HIS |
| 3 | D | 237 | GLU |
| 4 | E | 88 | GLY |
| 5 | F | 127 | GLU |
| 5 | F | 146 | ALA |
| 6 | G | 14 | GLU |
| 6 | G | 115 | ARG |
| 6 | G | 129 | GLY |
| 6 | G | 142 | PRO |
| 7 | H | 92 | ILE |
| 9 | J | 86 | THR |
| 9 | J | 89 | LYS |
| 9 | J | 154 | GLN |
| 11 | L | 11 | GLY |
| 11 | L | 15 | ARG |
| 11 | L | 17 | LYS |
| 11 | L | 33 | ARG |
| 11 | L | 47 | ASP |
| 11 | L | 56 | SER |
| 11 | L | 59 | LEU |
| 11 | L | 111 | ARG |
| 12 | M | 23 | GLY |
| 12 | M | 57 | HIS |
| 12 | M | 62 | GLY |
| 13 | N | 82 | GLU |
| 13 | N | 107 | ASP |
| 14 | O | 57 | LYS |
| 15 | P | 42 | ILE |
| 15 | P | 107 | ASP |
| 21 | V | 93 | ASP |
| 21 | V | 120 | ILE |
| 23 | X | 14 | VAL |
| 23 | X | 84 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | 1 | 54 | LYS |
| 26 | 1 | 64 | LYS |
| 27 | 2 | 49 | CYS |
| 30 | 5 | 28 | GLY |
| 30 | 5 | 35 | GLN |
| 3 | D | 169 | GLU |
| 3 | D | 236 | GLY |
| 4 | E | 4 | ILE |
| 4 | E | 56 | PRO |
| 6 | G | 4 | ASP |
| 6 | G | 35 | GLU |
| 6 | G | 87 | PRO |
| 9 | J | 92 | GLN |
| 10 | K | 29 | ASN |
| 11 | L | 43 | GLY |
| 11 | L | 50 | ARG |
| 11 | L | 74 | GLU |
| 12 | M | 7 | MET |
| 12 | M | 18 | LYS |
| 12 | M | 79 | LEU |
| 12 | M | 133 | ARG |
| 13 | N | 14 | SER |
| 13 | N | 93 | GLY |
| 14 | O | 42 | ASP |
| 15 | P | 86 | ILE |
| 16 | Q | 91 | ASP |
| 20 | U | 8 | LYS |
| 23 | X | 31 | GLY |
| 23 | X | 53 | VAL |
| 28 | 3 | 18 | ARG |
| 28 | 3 | 26 | ASN |
| 28 | 3 | 46 | HIS |
| 4 | E | 19 | ARG |
| 4 | E | 52 | LEU |
| 4 | E | 203 | LYS |
| 5 | F | 132 | VAL |
| 6 | G | 6 | ALA |
| 6 | G | 48 | GLU |
| 6 | G | 112 | PRO |
| 9 | J | 46 | LEU |
| 11 | L | 9 | ASN |
| 12 | M | 19 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | M | 20 | ALA |
| 12 | M | 82 | ARG |
| 14 | O | 83 | LYS |
| 14 | O | 89 | ARG |
| 15 | P | 116 | ALA |
| 17 | R | 78 | LYS |
| 21 | V | 11 | GLU |
| 21 | V | 114 | GLY |
| 23 | X | 94 | LEU |
| 24 | Y | 48 | HIS |
| 24 | Y | 61 | LEU |
| 3 | D | 34 | VAL |
| 4 | E | 185 | LYS |
| 5 | F | 66 | PRO |
| 7 | H | 49 | VAL |
| 7 | H | 97 | ARG |
| 10 | K | 94 | ARG |
| 11 | L | 35 | HIS |
| 13 | N | 4 | LEU |
| 13 | N | 10 | LEU |
| 14 | O | 85 | VAL |
| 17 | R | 35 | LEU |
| 19 | T | 4 | ALA |
| 19 | T | 93 | GLU |
| 20 | U | 39 | VAL |
| 20 | U | 88 | LYS |
| 21 | V | 37 | VAL |
| 21 | V | 141 | VAL |
| 23 | X | 83 | GLU |
| 24 | Y | 17 | SER |
| 30 | 5 | 29 | LYS |
| 3 | D | 234 | GLY |
| 6 | G | 24 | GLY |
| 7 | H | 110 | SER |
| 8 | I | 3 | VAL |
| 9 | J | 152 | PRO |
| 11 | L | 46 | LYS |
| 12 | M | 134 | ARG |
| 14 | O | 90 | GLY |
| 15 | P | 2 | ASN |
| 23 | X | 9 | GLY |
| 3 | D | 244 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | J | 59 | GLY |
| 9 | J | 118 | PRO |
| 11 | L | 125 | VAL |
| 14 | O | 91 | PRO |
| 20 | U | 18 | GLY |
| 4 | E | 29 | GLY |
| 5 | F | 134 | GLY |
| 7 | H | 48 | GLY |
| 20 | U | 10 | GLY |
| 20 | U | 61 | ILE |
| 5 | F | 89 | VAL |
| 6 | G | 89 | GLY |
| 13 | N | 7 | GLY |
| 17 | R | 36 | PRO |
| 21 | V | 165 | VAL |
| 7 | H | 22 | GLY |
| 11 | L | 19 | VAL |
| 16 | Q | 88 | ILE |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | D | 213/213 (100%) | 187 (88%) | 26 (12%) | 7 | 34 |
| 4 | E | 165/165 (100%) | 147 (89%) | 18 (11%) | 9 | 42 |
| 5 | F | 161/161 (100%) | 143 (89%) | 18 (11%) | 9 | 39 |
| 6 | G | 155/155 (100%) | 138 (89%) | 17 (11%) | 9 | 41 |
| 7 | H | 132/132 (100%) | 119 (90%) | 13 (10%) | 12 | 48 |
| 8 | I | 122/122 (100%) | 107 (88%) | 15 (12%) | 7 | 34 |
| 9 | J | 116/116 (100%) | 103 (89%) | 13 (11%) | 9 | 39 |
| 10 | K | 100/100 (100%) | 91 (91%) | 9 (9%) | 14 | 54 |
| 11 | L | 112/112 (100%) | 86 (77%) | 26 (23%) | 1 | 6 |
| 12 | M | 105/105 (100%) | 92 (88%) | 13 (12%) | 7 | 34 |
| 13 | N | 100/100 (100%) | 86 (86%) | 14 (14%) | 5 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|-------------|----|
| 14 | O | 77/77 (100%) | 64 (83%) | 13 (17%) | 3 | 18 |
| 15 | P | 121/121 (100%) | 102 (84%) | 19 (16%) | 4 | 23 |
| 16 | Q | 93/93 (100%) | 84 (90%) | 9 (10%) | 12 | 49 |
| 17 | R | 82/82 (100%) | 67 (82%) | 15 (18%) | 2 | 13 |
| 18 | S | 91/91 (100%) | 82 (90%) | 9 (10%) | 11 | 47 |
| 19 | T | 74/74 (100%) | 66 (89%) | 8 (11%) | 9 | 42 |
| 20 | U | 84/84 (100%) | 70 (83%) | 14 (17%) | 3 | 19 |
| 21 | V | 162/162 (100%) | 152 (94%) | 10 (6%) | 26 | 72 |
| 22 | W | 61/61 (100%) | 55 (90%) | 6 (10%) | 12 | 48 |
| 23 | X | 73/73 (100%) | 65 (89%) | 8 (11%) | 9 | 41 |
| 24 | Y | 58/58 (100%) | 51 (88%) | 7 (12%) | 7 | 35 |
| 25 | Z | 51/51 (100%) | 45 (88%) | 6 (12%) | 8 | 36 |
| 26 | 1 | 27/27 (100%) | 24 (89%) | 3 (11%) | 9 | 40 |
| 27 | 2 | 45/45 (100%) | 40 (89%) | 5 (11%) | 9 | 40 |
| 28 | 3 | 43/43 (100%) | 40 (93%) | 3 (7%) | 21 | 68 |
| 29 | 4 | 41/41 (100%) | 33 (80%) | 8 (20%) | 2 | 10 |
| 30 | 5 | 53/53 (100%) | 49 (92%) | 4 (8%) | 19 | 64 |
| All | All | 2717/2717 (100%) | 2388 (88%) | 329 (12%) | 7 | 35 |

All (329) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 25 | THR |
| 3 | D | 33 | LEU |
| 3 | D | 35 | LYS |
| 3 | D | 38 | LYS |
| 3 | D | 61 | LEU |
| 3 | D | 69 | ARG |
| 3 | D | 94 | LEU |
| 3 | D | 95 | LEU |
| 3 | D | 106 | ILE |
| 3 | D | 111 | LEU |
| 3 | D | 112 | GLN |
| 3 | D | 138 | VAL |
| 3 | D | 150 | LYS |
| 3 | D | 166 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 169 | GLU |
| 3 | D | 175 | LEU |
| 3 | D | 192 | THR |
| 3 | D | 198 | ASN |
| 3 | D | 204 | ILE |
| 3 | D | 211 | ARG |
| 3 | D | 212 | SER |
| 3 | D | 237 | GLU |
| 3 | D | 244 | ARG |
| 3 | D | 255 | LYS |
| 3 | D | 270 | ILE |
| 3 | D | 271 | ILE |
| 4 | E | 23 | VAL |
| 4 | E | 25 | VAL |
| 4 | E | 38 | THR |
| 4 | E | 41 | LYS |
| 4 | E | 54 | GLN |
| 4 | E | 73 | GLU |
| 4 | E | 78 | LEU |
| 4 | E | 79 | ARG |
| 4 | E | 82 | ARG |
| 4 | E | 87 | GLU |
| 4 | E | 93 | VAL |
| 4 | E | 113 | PHE |
| 4 | E | 119 | ARG |
| 4 | E | 175 | VAL |
| 4 | E | 192 | ASN |
| 4 | E | 195 | LEU |
| 4 | E | 202 | LYS |
| 4 | E | 203 | LYS |
| 5 | F | 6 | MET |
| 5 | F | 8 | GLN |
| 5 | F | 20 | LEU |
| 5 | F | 28 | ILE |
| 5 | F | 45 | ARG |
| 5 | F | 46 | ARG |
| 5 | F | 65 | TRP |
| 5 | F | 67 | GLN |
| 5 | F | 78 | ILE |
| 5 | F | 82 | ILE |
| 5 | F | 88 | VAL |
| 5 | F | 116 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | F | 165 | ARG |
| 5 | F | 181 | LEU |
| 5 | F | 183 | VAL |
| 5 | F | 191 | ARG |
| 5 | F | 192 | LEU |
| 5 | F | 206 | ILE |
| 6 | G | 16 | ARG |
| 6 | G | 26 | GLN |
| 6 | G | 34 | LEU |
| 6 | G | 35 | GLU |
| 6 | G | 43 | LEU |
| 6 | G | 47 | LYS |
| 6 | G | 86 | MET |
| 6 | G | 88 | ILE |
| 6 | G | 97 | ASP |
| 6 | G | 115 | ARG |
| 6 | G | 117 | PHE |
| 6 | G | 118 | ARG |
| 6 | G | 128 | ARG |
| 6 | G | 138 | GLN |
| 6 | G | 155 | MET |
| 6 | G | 159 | VAL |
| 6 | G | 167 | GLU |
| 7 | H | 23 | ARG |
| 7 | H | 41 | MET |
| 7 | H | 43 | VAL |
| 7 | H | 47 | GLU |
| 7 | H | 71 | LEU |
| 7 | H | 94 | TYR |
| 7 | H | 101 | ARG |
| 7 | H | 123 | PHE |
| 7 | H | 124 | GLU |
| 7 | H | 127 | GLU |
| 7 | H | 149 | ARG |
| 7 | H | 167 | GLU |
| 7 | H | 170 | ARG |
| 8 | I | 4 | ILE |
| 8 | I | 5 | LEU |
| 8 | I | 9 | LEU |
| 8 | I | 10 | GLU |
| 8 | I | 45 | LYS |
| 8 | I | 56 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | I | 67 | ARG |
| 8 | I | 69 | LYS |
| 8 | I | 92 | VAL |
| 8 | I | 96 | ASP |
| 8 | I | 107 | ILE |
| 8 | I | 109 | ILE |
| 8 | I | 118 | LYS |
| 8 | I | 126 | TYR |
| 8 | I | 142 | VAL |
| 9 | J | 56 | LEU |
| 9 | J | 57 | LEU |
| 9 | J | 68 | ASN |
| 9 | J | 90 | LEU |
| 9 | J | 91 | GLU |
| 9 | J | 107 | LYS |
| 9 | J | 117 | HIS |
| 9 | J | 119 | GLU |
| 9 | J | 129 | MET |
| 9 | J | 132 | LYS |
| 9 | J | 150 | ASP |
| 9 | J | 160 | LYS |
| 9 | J | 161 | LEU |
| 10 | K | 8 | LEU |
| 10 | K | 9 | GLU |
| 10 | K | 19 | ILE |
| 10 | K | 22 | ILE |
| 10 | K | 47 | ILE |
| 10 | K | 52 | VAL |
| 10 | K | 94 | ARG |
| 10 | K | 98 | VAL |
| 10 | K | 120 | GLU |
| 11 | L | 13 | ASN |
| 11 | L | 16 | ARG |
| 11 | L | 19 | VAL |
| 11 | L | 27 | HIS |
| 11 | L | 29 | LYS |
| 11 | L | 32 | THR |
| 11 | L | 35 | HIS |
| 11 | L | 41 | ARG |
| 11 | L | 42 | SER |
| 11 | L | 49 | ARG |
| 11 | L | 50 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | L | 51 | PHE |
| 11 | L | 57 | THR |
| 11 | L | 59 | LEU |
| 11 | L | 61 | ARG |
| 11 | L | 62 | LEU |
| 11 | L | 67 | MET |
| 11 | L | 75 | ILE |
| 11 | L | 91 | PHE |
| 11 | L | 115 | LEU |
| 11 | L | 123 | LEU |
| 11 | L | 125 | VAL |
| 11 | L | 135 | LEU |
| 11 | L | 144 | GLU |
| 11 | L | 146 | VAL |
| 11 | L | 148 | LEU |
| 12 | M | 9 | TYR |
| 12 | M | 10 | ARG |
| 12 | M | 16 | ARG |
| 12 | M | 22 | LYS |
| 12 | M | 45 | GLN |
| 12 | M | 51 | ARG |
| 12 | M | 55 | VAL |
| 12 | M | 58 | PHE |
| 12 | M | 68 | ILE |
| 12 | M | 83 | MET |
| 12 | M | 103 | MET |
| 12 | M | 111 | GLU |
| 12 | M | 133 | ARG |
| 13 | N | 2 | ARG |
| 13 | N | 18 | LEU |
| 13 | N | 28 | LEU |
| 13 | N | 49 | ASP |
| 13 | N | 60 | LEU |
| 13 | N | 67 | LEU |
| 13 | N | 75 | LEU |
| 13 | N | 79 | LEU |
| 13 | N | 88 | ARG |
| 13 | N | 95 | THR |
| 13 | N | 99 | LYS |
| 13 | N | 102 | GLU |
| 13 | N | 104 | ARG |
| 13 | N | 115 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | O | 12 | PHE |
| 14 | O | 30 | ARG |
| 14 | O | 35 | ILE |
| 14 | O | 44 | LYS |
| 14 | O | 57 | LYS |
| 14 | O | 59 | LYS |
| 14 | O | 68 | GLN |
| 14 | O | 69 | VAL |
| 14 | O | 73 | LEU |
| 14 | O | 76 | LYS |
| 14 | O | 92 | TYR |
| 14 | O | 98 | VAL |
| 14 | O | 101 | LEU |
| 15 | P | 15 | VAL |
| 15 | P | 18 | ASP |
| 15 | P | 27 | THR |
| 15 | P | 36 | GLU |
| 15 | P | 42 | ILE |
| 15 | P | 50 | ILE |
| 15 | P | 58 | ASN |
| 15 | P | 59 | THR |
| 15 | P | 85 | LYS |
| 15 | P | 86 | ILE |
| 15 | P | 87 | ASP |
| 15 | P | 88 | ILE |
| 15 | P | 99 | LEU |
| 15 | P | 100 | TYR |
| 15 | P | 107 | ASP |
| 15 | P | 110 | ILE |
| 15 | P | 112 | ARG |
| 15 | P | 115 | ARG |
| 15 | P | 124 | ASP |
| 16 | Q | 18 | LEU |
| 16 | Q | 64 | ARG |
| 16 | Q | 70 | ARG |
| 16 | Q | 72 | HIS |
| 16 | Q | 75 | ASN |
| 16 | Q | 88 | ILE |
| 16 | Q | 92 | ARG |
| 16 | Q | 97 | ASP |
| 16 | Q | 104 | GLN |
| 17 | R | 13 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | R | 24 | LYS |
| 17 | R | 37 | VAL |
| 17 | R | 38 | LEU |
| 17 | R | 39 | LEU |
| 17 | R | 44 | LYS |
| 17 | R | 49 | THR |
| 17 | R | 61 | VAL |
| 17 | R | 62 | LEU |
| 17 | R | 66 | ARG |
| 17 | R | 73 | SER |
| 17 | R | 80 | GLN |
| 17 | R | 88 | ARG |
| 17 | R | 95 | LEU |
| 17 | R | 99 | ILE |
| 18 | S | 8 | ARG |
| 18 | S | 11 | ARG |
| 18 | S | 27 | LYS |
| 18 | S | 67 | ASP |
| 18 | S | 70 | TYR |
| 18 | S | 78 | GLU |
| 18 | S | 88 | ARG |
| 18 | S | 96 | ILE |
| 18 | S | 107 | LEU |
| 19 | T | 27 | THR |
| 19 | T | 60 | ARG |
| 19 | T | 65 | ARG |
| 19 | T | 68 | ARG |
| 19 | T | 76 | ARG |
| 19 | T | 80 | ILE |
| 19 | T | 81 | VAL |
| 19 | T | 88 | LYS |
| 20 | U | 2 | ARG |
| 20 | U | 4 | LYS |
| 20 | U | 8 | LYS |
| 20 | U | 9 | LYS |
| 20 | U | 14 | LEU |
| 20 | U | 27 | VAL |
| 20 | U | 71 | LYS |
| 20 | U | 75 | ILE |
| 20 | U | 76 | CYS |
| 20 | U | 88 | LYS |
| 20 | U | 90 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | U | 96 | ILE |
| 20 | U | 97 | ARG |
| 20 | U | 101 | LYS |
| 21 | V | 24 | LEU |
| 21 | V | 30 | ASN |
| 21 | V | 33 | LEU |
| 21 | V | 34 | ASN |
| 21 | V | 67 | LEU |
| 21 | V | 72 | ARG |
| 21 | V | 77 | ASP |
| 21 | V | 94 | GLU |
| 21 | V | 97 | GLU |
| 21 | V | 133 | ILE |
| 22 | W | 19 | LYS |
| 22 | W | 20 | ARG |
| 22 | W | 25 | ARG |
| 22 | W | 55 | ARG |
| 22 | W | 64 | ASP |
| 22 | W | 84 | LEU |
| 23 | X | 11 | ARG |
| 23 | X | 13 | ILE |
| 23 | X | 16 | ASN |
| 23 | X | 37 | ILE |
| 23 | X | 45 | ASN |
| 23 | X | 75 | GLU |
| 23 | X | 76 | ARG |
| 23 | X | 83 | GLU |
| 24 | Y | 7 | ARG |
| 24 | Y | 17 | SER |
| 24 | Y | 24 | LEU |
| 24 | Y | 49 | LYS |
| 24 | Y | 53 | LEU |
| 24 | Y | 61 | LEU |
| 24 | Y | 62 | THR |
| 25 | Z | 31 | LEU |
| 25 | Z | 37 | LEU |
| 25 | Z | 40 | THR |
| 25 | Z | 44 | ARG |
| 25 | Z | 53 | LEU |
| 25 | Z | 56 | VAL |
| 26 | 1 | 39 | ARG |
| 26 | 1 | 46 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | 1 | 60 | GLU |
| 27 | 2 | 6 | VAL |
| 27 | 2 | 25 | LEU |
| 27 | 2 | 46 | CYS |
| 27 | 2 | 49 | CYS |
| 27 | 2 | 51 | TYR |
| 28 | 3 | 11 | LEU |
| 28 | 3 | 34 | LEU |
| 28 | 3 | 42 | TRP |
| 29 | 4 | 4 | THR |
| 29 | 4 | 8 | ASN |
| 29 | 4 | 10 | ARG |
| 29 | 4 | 19 | ARG |
| 29 | 4 | 24 | THR |
| 29 | 4 | 31 | LEU |
| 29 | 4 | 39 | ARG |
| 29 | 4 | 41 | ARG |
| 30 | 5 | 22 | VAL |
| 30 | 5 | 52 | LYS |
| 30 | 5 | 57 | ARG |
| 30 | 5 | 59 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 87 | ASN |
| 3 | D | 96 | HIS |
| 3 | D | 166 | GLN |
| 3 | D | 186 | HIS |
| 3 | D | 198 | ASN |
| 3 | D | 220 | HIS |
| 4 | E | 66 | HIS |
| 4 | E | 132 | HIS |
| 4 | E | 192 | ASN |
| 5 | F | 40 | GLN |
| 5 | F | 67 | GLN |
| 5 | F | 69 | HIS |
| 5 | F | 75 | HIS |
| 5 | F | 169 | ASN |
| 6 | G | 58 | GLN |
| 6 | G | 123 | ASN |
| 7 | H | 61 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | I | 54 | GLN |
| 9 | J | 68 | ASN |
| 9 | J | 79 | ASN |
| 9 | J | 151 | HIS |
| 9 | J | 154 | GLN |
| 10 | K | 29 | ASN |
| 11 | L | 13 | ASN |
| 11 | L | 27 | HIS |
| 11 | L | 35 | HIS |
| 11 | L | 68 | GLN |
| 11 | L | 128 | HIS |
| 12 | M | 13 | GLN |
| 13 | N | 13 | HIS |
| 13 | N | 16 | HIS |
| 13 | N | 53 | HIS |
| 13 | N | 61 | HIS |
| 14 | O | 61 | ASN |
| 15 | P | 79 | HIS |
| 16 | Q | 44 | ASN |
| 16 | Q | 49 | HIS |
| 16 | Q | 71 | GLN |
| 16 | Q | 75 | ASN |
| 16 | Q | 81 | HIS |
| 17 | R | 11 | GLN |
| 18 | S | 34 | ASN |
| 18 | S | 57 | ASN |
| 18 | S | 61 | ASN |
| 19 | T | 41 | ASN |
| 19 | T | 55 | ASN |
| 19 | T | 87 | GLN |
| 20 | U | 43 | ASN |
| 21 | V | 30 | ASN |
| 21 | V | 54 | HIS |
| 21 | V | 65 | GLN |
| 21 | V | 73 | GLN |
| 21 | V | 75 | ASN |
| 21 | V | 132 | ASN |
| 22 | W | 50 | ASN |
| 22 | W | 70 | GLN |
| 23 | X | 45 | ASN |
| 23 | X | 56 | GLN |
| 23 | X | 66 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | Z | 19 | GLN |
| 25 | Z | 46 | ASN |
| 25 | Z | 52 | HIS |
| 26 | 1 | 46 | ASN |
| 28 | 3 | 26 | ASN |
| 28 | 3 | 29 | ASN |
| 29 | 4 | 8 | ASN |
| 30 | 5 | 33 | ASN |
| 30 | 5 | 35 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2830/2879 (98%) | 442 (15%) | 0 |
| 2 | B | 118/119 (99%) | 9 (7%) | 0 |
| All | All | 2948/2998 (98%) | 451 (15%) | 0 |

All (451) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | G |
| 1 | A | 34 | C |
| 1 | A | 35 | G |
| 1 | A | 46 | C |
| 1 | A | 49 | A |
| 1 | A | 64 | A |
| 1 | A | 71 | A |
| 1 | A | 74 | A |
| 1 | A | 75 | G |
| 1 | A | 84 | A |
| 1 | A | 99 | U |
| 1 | A | 101 | G |
| 1 | A | 102 | G |
| 1 | A | 114 | U |
| 1 | A | 118 | A |
| 1 | A | 119 | A |
| 1 | A | 120 | U |
| 1 | A | 138 | G |
| 1 | A | 139 | G |
| 1 | A | 140 | A |
| 1 | A | 155 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 163 | U |
| 1 | A | 181 | A |
| 1 | A | 196 | A |
| 1 | A | 197 | A |
| 1 | A | 199 | A |
| 1 | A | 204 | A |
| 1 | A | 205 | G |
| 1 | A | 215 | G |
| 1 | A | 216 | A |
| 1 | A | 221 | A |
| 1 | A | 222 | A |
| 1 | A | 228 | A |
| 1 | A | 229 | A |
| 1 | A | 241 | A |
| 1 | A | 245 | G |
| 1 | A | 248 | G |
| 1 | A | 252 | G |
| 1 | A | 266 | G |
| 1 | A | 270(N) | U |
| 1 | A | 270(O) | G |
| 1 | A | 270(P) | U |
| 1 | A | 270(R) | C |
| 1 | A | 271(B) | C |
| 1 | A | 271(C) | G |
| 1 | A | 271 | G |
| 1 | A | 273(G) | C |
| 1 | A | 275 | G |
| 1 | A | 276 | C |
| 1 | A | 278 | A |
| 1 | A | 301 | G |
| 1 | A | 302 | C |
| 1 | A | 311 | A |
| 1 | A | 324 | A |
| 1 | A | 329 | G |
| 1 | A | 330 | A |
| 1 | A | 333 | G |
| 1 | A | 352 | G |
| 1 | A | 353 | G |
| 1 | A | 363(A) | G |
| 1 | A | 363(G) | A |
| 1 | A | 372 | G |
| 1 | A | 386 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 396 | G |
| 1 | A | 405 | U |
| 1 | A | 406 | G |
| 1 | A | 411 | G |
| 1 | A | 412 | A |
| 1 | A | 444 | C |
| 1 | A | 470 | A |
| 1 | A | 475 | U |
| 1 | A | 480 | A |
| 1 | A | 481 | G |
| 1 | A | 505 | A |
| 1 | A | 508 | G |
| 1 | A | 509 | C |
| 1 | A | 528 | A |
| 1 | A | 530 | G |
| 1 | A | 531 | C |
| 1 | A | 532 | A |
| 1 | A | 533 | G |
| 1 | A | 544 | C |
| 1 | A | 546 | C |
| 1 | A | 548 | A |
| 1 | A | 556 | G |
| 1 | A | 563 | G |
| 1 | A | 573 | G |
| 1 | A | 575 | A |
| 1 | A | 599 | G |
| 1 | A | 603 | A |
| 1 | A | 614 | U |
| 1 | A | 615 | G |
| 1 | A | 617 | G |
| 1 | A | 620 | G |
| 1 | A | 621 | A |
| 1 | A | 627 | A |
| 1 | A | 637 | A |
| 1 | A | 645 | C |
| 1 | A | 646 | A |
| 1 | A | 654 | U |
| 1 | A | 655 | A |
| 1 | A | 668 | G |
| 1 | A | 686 | G |
| 1 | A | 730 | C |
| 1 | A | 764 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 775 | G |
| 1 | A | 776 | G |
| 1 | A | 782 | A |
| 1 | A | 784 | A |
| 1 | A | 785 | G |
| 1 | A | 787 | U |
| 1 | A | 805 | G |
| 1 | A | 812 | C |
| 1 | A | 819 | A |
| 1 | A | 827 | U |
| 1 | A | 828 | U |
| 1 | A | 831 | G |
| 1 | A | 847 | U |
| 1 | A | 859 | G |
| 1 | A | 869 | G |
| 1 | A | 882 | G |
| 1 | A | 885 | C |
| 1 | A | 886 | C |
| 1 | A | 888 | C |
| 1 | A | 889 | C |
| 1 | A | 890 | A |
| 1 | A | 896 | A |
| 1 | A | 897 | C |
| 1 | A | 910 | A |
| 1 | A | 914 | C |
| 1 | A | 915 | C |
| 1 | A | 917 | A |
| 1 | A | 919 | G |
| 1 | A | 931 | G |
| 1 | A | 932 | G |
| 1 | A | 933 | A |
| 1 | A | 938 | G |
| 1 | A | 941 | A |
| 1 | A | 946 | G |
| 1 | A | 959 | A |
| 1 | A | 961 | C |
| 1 | A | 965 | C |
| 1 | A | 974(A) | G |
| 1 | A | 974(B) | C |
| 1 | A | 975 | G |
| 1 | A | 983 | A |
| 1 | A | 996 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1005 | C |
| 1 | A | 1009 | A |
| 1 | A | 1012 | U |
| 1 | A | 1013 | C |
| 1 | A | 1022 | G |
| 1 | A | 1023 | U |
| 1 | A | 1025 | G |
| 1 | A | 1026 | U |
| 1 | A | 1027 | A |
| 1 | A | 1033 | U |
| 1 | A | 1047 | G |
| 1 | A | 1048 | A |
| 1 | A | 1049 | C |
| 1 | A | 1101 | U |
| 1 | A | 1105 | U |
| 1 | A | 1106 | G |
| 1 | A | 1108 | U |
| 1 | A | 1110 | G |
| 1 | A | 1111 | A |
| 1 | A | 1112 | G |
| 1 | A | 1122 | G |
| 1 | A | 1126 | A |
| 1 | A | 1128 | A |
| 1 | A | 1129 | A |
| 1 | A | 1130 | U |
| 1 | A | 1135 | C |
| 1 | A | 1136 | G |
| 1 | A | 1139 | G |
| 1 | A | 1142(B) | A |
| 1 | A | 1155 | A |
| 1 | A | 1171 | G |
| 1 | A | 1174 | A |
| 1 | A | 1175 | U |
| 1 | A | 1176 | G |
| 1 | A | 1205 | U |
| 1 | A | 1211 | U |
| 1 | A | 1220 | A |
| 1 | A | 1221 | C |
| 1 | A | 1253 | A |
| 1 | A | 1256 | G |
| 1 | A | 1271 | G |
| 1 | A | 1272 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1273 | U |
| 1 | A | 1300 | U |
| 1 | A | 1301 | A |
| 1 | A | 1314 | C |
| 1 | A | 1329 | U |
| 1 | A | 1332 | G |
| 1 | A | 1345 | C |
| 1 | A | 1349 | A |
| 1 | A | 1352 | U |
| 1 | A | 1359 | A |
| 1 | A | 1360 | A |
| 1 | A | 1365 | A |
| 1 | A | 1380 | G |
| 1 | A | 1384 | A |
| 1 | A | 1385 | G |
| 1 | A | 1386 | C |
| 1 | A | 1396 | U |
| 1 | A | 1416 | G |
| 1 | A | 1420 | U |
| 1 | A | 1421 | G |
| 1 | A | 1428 | C |
| 1 | A | 1444(B) | A |
| 1 | A | 1455 | G |
| 1 | A | 1460 | A |
| 1 | A | 1467 | C |
| 1 | A | 1478 | G |
| 1 | A | 1483 | G |
| 1 | A | 1490 | A |
| 1 | A | 1493 | C |
| 1 | A | 1494 | A |
| 1 | A | 1495 | A |
| 1 | A | 1497 | U |
| 1 | A | 1509 | A |
| 1 | A | 1510 | A |
| 1 | A | 1535 | U |
| 1 | A | 1542 | G |
| 1 | A | 1543 | A |
| 1 | A | 1544 | C |
| 1 | A | 1545 | A |
| 1 | A | 1554 | A |
| 1 | A | 1558 | A |
| 1 | A | 1559 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1560 | G |
| 1 | A | 1566 | A |
| 1 | A | 1569 | A |
| 1 | A | 1578 | U |
| 1 | A | 1579 | A |
| 1 | A | 1585 | C |
| 1 | A | 1598 | C |
| 1 | A | 1603 | A |
| 1 | A | 1608 | A |
| 1 | A | 1609 | A |
| 1 | A | 1618 | A |
| 1 | A | 1639 | U |
| 1 | A | 1640 | C |
| 1 | A | 1646 | C |
| 1 | A | 1647 | G |
| 1 | A | 1648 | C |
| 1 | A | 1654 | A |
| 1 | A | 1674 | G |
| 1 | A | 1681 | G |
| 1 | A | 1703 | G |
| 1 | A | 1729 | A |
| 1 | A | 1732 | A |
| 1 | A | 1756 | G |
| 1 | A | 1761 | C |
| 1 | A | 1763 | G |
| 1 | A | 1764 | G |
| 1 | A | 1773 | A |
| 1 | A | 1776 | G |
| 1 | A | 1787 | A |
| 1 | A | 1791 | A |
| 1 | A | 1800 | C |
| 1 | A | 1801 | G |
| 1 | A | 1811 | G |
| 1 | A | 1816 | G |
| 1 | A | 1829 | A |
| 1 | A | 1833 | U |
| 1 | A | 1847 | A |
| 1 | A | 1900 | A |
| 1 | A | 1903 | G |
| 1 | A | 1906 | G |
| 1 | A | 1913 | A |
| 1 | A | 1914 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1929 | G |
| 1 | A | 1930 | G |
| 1 | A | 1936 | A |
| 1 | A | 1937 | A |
| 1 | A | 1938 | A |
| 1 | A | 1939 | U |
| 1 | A | 1955 | U |
| 1 | A | 1961 | C |
| 1 | A | 1963 | U |
| 1 | A | 1967 | C |
| 1 | A | 1970 | A |
| 1 | A | 1971 | A |
| 1 | A | 1972 | A |
| 1 | A | 1982 | C |
| 1 | A | 1992 | G |
| 1 | A | 1993 | U |
| 1 | A | 1997 | G |
| 1 | A | 2023 | G |
| 1 | A | 2030 | A |
| 1 | A | 2031 | A |
| 1 | A | 2032 | G |
| 1 | A | 2033 | A |
| 1 | A | 2036 | C |
| 1 | A | 2043 | C |
| 1 | A | 2055 | C |
| 1 | A | 2056 | G |
| 1 | A | 2060 | A |
| 1 | A | 2061 | G |
| 1 | A | 2069 | G |
| 1 | A | 2080 | G |
| 1 | A | 2093 | G |
| 1 | A | 2118 | U |
| 1 | A | 2120 | G |
| 1 | A | 2126 | A |
| 1 | A | 2127 | G |
| 1 | A | 2130 | U |
| 1 | A | 2131 | G |
| 1 | A | 2132 | U |
| 1 | A | 2133 | G |
| 1 | A | 2134 | A |
| 1 | A | 2136 | C |
| 1 | A | 2148 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2156 | G |
| 1 | A | 2158 | A |
| 1 | A | 2161 | C |
| 1 | A | 2164 | C |
| 1 | A | 2165 | G |
| 1 | A | 2167 | U |
| 1 | A | 2168 | G |
| 1 | A | 2170 | A |
| 1 | A | 2172 | U |
| 1 | A | 2173 | A |
| 1 | A | 2181 | G |
| 1 | A | 2198 | A |
| 1 | A | 2210 | G |
| 1 | A | 2211 | G |
| 1 | A | 2212 | A |
| 1 | A | 2213 | U |
| 1 | A | 2215 | G |
| 1 | A | 2225 | A |
| 1 | A | 2226 | C |
| 1 | A | 2234 | G |
| 1 | A | 2238 | G |
| 1 | A | 2239 | G |
| 1 | A | 2250 | G |
| 1 | A | 2273 | A |
| 1 | A | 2275 | C |
| 1 | A | 2279 | G |
| 1 | A | 2283 | C |
| 1 | A | 2287 | A |
| 1 | A | 2288 | A |
| 1 | A | 2304 | G |
| 1 | A | 2305 | A |
| 1 | A | 2306 | C |
| 1 | A | 2307 | G |
| 1 | A | 2308 | G |
| 1 | A | 2309 | A |
| 1 | A | 2319 | G |
| 1 | A | 2320 | A |
| 1 | A | 2321 | G |
| 1 | A | 2325 | G |
| 1 | A | 2334 | G |
| 1 | A | 2336 | A |
| 1 | A | 2345 | G |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2346 | A |
| 1 | A | 2347 | C |
| 1 | A | 2350 | C |
| 1 | A | 2361 | A |
| 1 | A | 2379 | G |
| 1 | A | 2383 | G |
| 1 | A | 2385 | C |
| 1 | A | 2392 | A |
| 1 | A | 2393 | A |
| 1 | A | 2394 | C |
| 1 | A | 2402 | C |
| 1 | A | 2422 | A |
| 1 | A | 2424 | C |
| 1 | A | 2425 | A |
| 1 | A | 2428 | G |
| 1 | A | 2429 | G |
| 1 | A | 2430 | A |
| 1 | A | 2431 | U |
| 1 | A | 2434 | A |
| 1 | A | 2439 | A |
| 1 | A | 2441 | C |
| 1 | A | 2447 | G |
| 1 | A | 2448 | A |
| 1 | A | 2470 | G |
| 1 | A | 2473 | U |
| 1 | A | 2474 | C |
| 1 | A | 2476 | A |
| 1 | A | 2477 | C |
| 1 | A | 2478 | A |
| 1 | A | 2484 | G |
| 1 | A | 2502 | G |
| 1 | A | 2503 | A |
| 1 | A | 2505 | G |
| 1 | A | 2506 | U |
| 1 | A | 2518 | A |
| 1 | A | 2525 | G |
| 1 | A | 2529 | G |
| 1 | A | 2542 | A |
| 1 | A | 2543 | G |
| 1 | A | 2554 | U |
| 1 | A | 2566 | A |
| 1 | A | 2567 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 2572 | A |
| 1 | A | 2602 | A |
| 1 | A | 2603 | G |
| 1 | A | 2610 | C |
| 1 | A | 2611 | U |
| 1 | A | 2612 | C |
| 1 | A | 2615 | U |
| 1 | A | 2630 | G |
| 1 | A | 2646 | C |
| 1 | A | 2663 | G |
| 1 | A | 2665 | A |
| 1 | A | 2689 | U |
| 1 | A | 2690 | C |
| 1 | A | 2691 | C |
| 1 | A | 2702 | U |
| 1 | A | 2703 | C |
| 1 | A | 2707 | G |
| 1 | A | 712(B) | A |
| 1 | A | 2713 | A |
| 1 | A | 2714 | G |
| 1 | A | 2726 | U |
| 1 | A | 2733 | A |
| 1 | A | 2751 | G |
| 1 | A | 2758 | A |
| 1 | A | 2764 | A |
| 1 | A | 2765 | A |
| 1 | A | 2766 | G |
| 1 | A | 2777 | G |
| 1 | A | 2778 | A |
| 1 | A | 2779 | U |
| 1 | A | 2790 | A |
| 1 | A | 2791 | C |
| 1 | A | 2792 | G |
| 1 | A | 2797 | U |
| 1 | A | 2798 | C |
| 1 | A | 2808 | U |
| 1 | A | 2820 | A |
| 1 | A | 2821 | A |
| 1 | A | 2823 | A |
| 1 | A | 2833 | G |
| 1 | A | 2835 | A |
| 1 | A | 2849 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2872 | G |
| 2 | B | 13 | A |
| 2 | B | 15 | A |
| 2 | B | 35 | U |
| 2 | B | 41 | U |
| 2 | B | 44 | G |
| 2 | B | 52 | A |
| 2 | B | 73 | A |
| 2 | B | 87 | G |
| 2 | B | 109 | G |

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4364 ligands modelled in this entry, 4363 are monoatomic - leaving 1 for Mogul analysis.

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$ |
| 31 | BLS | A | 4001 | - | 31,31,31 | 2.86 | 11 (35%) | 40,43,43 | 2.42 | 14 (35%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 31 | BLS | A | 4001 | - | - | 0/22/38/38 | 0/2/2/2 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31 | A | 4001 | BLS | C7-N6 | 7.46 | 1.49 | 1.34 |
| 31 | A | 4001 | BLS | C14-N12 | 7.35 | 1.54 | 1.35 |
| 31 | A | 4001 | BLS | O5'-C5' | 4.61 | 1.51 | 1.43 |
| 31 | A | 4001 | BLS | C11-N12 | 4.53 | 1.56 | 1.47 |
| 31 | A | 4001 | BLS | C3'-C2' | 4.42 | 1.47 | 1.33 |
| 31 | A | 4001 | BLS | C13-N12 | 4.29 | 1.61 | 1.45 |
| 31 | A | 4001 | BLS | C4-N4 | 4.12 | 1.47 | 1.35 |
| 31 | A | 4001 | BLS | C4'-N6 | 3.45 | 1.50 | 1.46 |
| 31 | A | 4001 | BLS | C2-N1 | -2.65 | 1.35 | 1.38 |
| 31 | A | 4001 | BLS | C5'-C6' | -2.31 | 1.48 | 1.53 |
| 31 | A | 4001 | BLS | C4'-C5' | -2.16 | 1.48 | 1.54 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31 | A | 4001 | BLS | C1'-C2'-C3' | -8.07 | 111.48 | 122.69 |
| 31 | A | 4001 | BLS | O5'-C1'-C2' | -4.70 | 110.48 | 113.13 |
| 31 | A | 4001 | BLS | C10-C11-N12 | 4.36 | 116.19 | 112.58 |
| 31 | A | 4001 | BLS | C6-C5-C4 | 4.24 | 119.53 | 117.51 |
| 31 | A | 4001 | BLS | O3-C6'-C5' | -3.32 | 109.32 | 121.10 |
| 31 | A | 4001 | BLS | C13-N12-C11 | 3.01 | 121.48 | 115.72 |
| 31 | A | 4001 | BLS | O4-C6'-O3 | 2.95 | 130.67 | 124.05 |
| 31 | A | 4001 | BLS | C3'-C4'-N6 | -2.75 | 106.24 | 110.12 |
| 31 | A | 4001 | BLS | C2-N3-C4 | 2.53 | 119.29 | 115.65 |
| 31 | A | 4001 | BLS | C4'-N6-C7 | -2.52 | 120.44 | 123.39 |
| 31 | A | 4001 | BLS | C5'-C4'-N6 | -2.48 | 107.41 | 111.10 |
| 31 | A | 4001 | BLS | C2'-C1'-N1 | -2.44 | 109.04 | 111.85 |
| 31 | A | 4001 | BLS | C9-C8-C7 | 2.40 | 115.53 | 112.69 |
| 31 | A | 4001 | BLS | O5'-C5'-C4' | 2.02 | 113.63 | 109.84 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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